Variational Discrete Action Theory

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ABSTRACT

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This thesis focuses on developing new approaches to solving the ground state properties of quantum many-body Hamiltonians, and the goal is to develop a systematic approach which properly balances efficiency and accuracy. Two new formalisms are proposed in this thesis: the Variational Discrete Action Theory (VDAT) and the Off-Shell Effective Energy Theory (OET).

The VDAT exploits the advantages of both variational wavefunctions and many-body Green's functions for solving quantum Hamiltonians. VDAT consists of two central components: the Sequential Product Density matrix (SPD) and the Discrete Action associated with the SPD. The SPD is a *variational* ansatz inspired by the Trotter decomposition and characterized by an integer $\mathcal{N}$, and $\mathcal{N}$ controls the balance of accuracy and cost; monotonically converging to the exact solution for $\mathcal{N} \to \infty$. The Discrete Action emerges by treating the each projector in the SPD as an effective discrete time evolution. We generalize the path integral to our discrete formalism, which converts a dynamic correlation function to a static correlation function in a compound space. We also generalize the usual many-body Green's function formalism, which results in analogous but distinct mathematical structures due to the non-abelian nature of the SPD, yielding discrete versions of the generating functional, Dyson equation, and Bethe-Salpeter equation.

We apply VDAT to two canonical models of interacting electrons: the Anderson impurity model (AIM) and the Hubbard model. We prove that the SPD can be *exactly* evaluated in the AIM, and demonstrate that $\mathcal{N} = 3$ provides a robust description of the exact results with a relatively negligible cost. For the Hubbard model, we introduce the local self-consistent approximation (LSA), which is the analogue of the dynamical mean-field theory, and prove that LSA *exactly* evaluates VDAT for d=∞. Furthermore, VDAT within the LSA at $\mathcal{N} = 2$ exactly recovers the Gutzwiller approximation (GA), and therefore $\mathcal{N} > 2$ provides a new

class of theories which balance efficiency and accuracy. For the d=∞ Hubbard model, we evaluate $\mathcal{N} = 2-4$ and show that $\mathcal{N} = 3$ provides a truly minimal yet precise description of Mott physics with a cost similar to the GA. VDAT provides a flexible scheme for studying quantum Hamiltonians, competing both with state-of-the-art methods and simple, efficient approaches all within a single framework. VDAT will have broad applications in condensed matter and materials physics.

In the second part of the thesis, we propose a different formalism, off-shell effective energy theory (OET), which combines the variational principle and effective energy theory, providing a ground state description of a quantum many-body Hamiltonian. The OET is based on a partitioning of the Hamiltonian and a corresponding density matrix ansatz constructed from an off-shell extension of the equilibrium density matrix; and there are dual realizations based on a given partitioning. To approximate OET, we introduce the central point expansion (CPE), which is an expansion of the density matrix ansatz, and we renormalize the CPE using a standard expansion of the ground state energy. We showcase the OET for the one band Hubbard model in d=1, 2, and ∞, using a partitioning between kinetic and potential energy, yielding two realizations denoted as $\mathcal{K}$ and $\mathcal{X}$. OET shows favorable agreement with exact or state-of-the-art results over all parameter space, and has a negligible computational cost. Physically, $\mathcal{K}$ describes the Fermi liquid, while $\mathcal{X}$ gives an analogous description of both the Luttinger liquid and the Mott insulator. Our approach should find broad applicability in lattice model Hamiltonians, in addition to real materials systems.

The VDAT can immediately be applied to generic quantum models, and in some cases will rival the best existing theories, allowing the discovery of new physics in strongly correlated electron scenarios. Alternatively, the OET provides a practical formalism for encapsulating the complex physics of some model and allowing extrapolation over all phase space. Both of the formalisms should find broad applications in both model Hamiltonians and real materials.

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Chapter 1

Introduction

Here we consider two major approaches to the quantum many body problem. One is based on the Green's function and diagrammatic techniques and the other is based on variational wave functions. In this chapter, we review some necessary formulas for both topics, which is useful for the following discussion. We start with the finite temperature Green's function formalism. For the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{1.1}$$

where $\hat{H}_0$ is non-interacting and $\hat{V}$ is interacting, the Matsubara Green's Function is defined in Heisenberg representation as[5]

$$\mathcal{G}_{p\sigma}\left(\tau - \tau'\right) = -\left\langle \mathrm{T}_\tau \hat{a}_{p\sigma}\left(\tau\right) \hat{a}^\dagger_{p\sigma}\left(\tau'\right)\right\rangle, \tag{1.2}$$

where $\hat{A}\left(\tau\right) = \exp\left(\tau\hat{H}\right)\hat{A}\exp\left(-\tau\hat{H}\right)$, and T_τ is the time ordering operator. The Fourier transformation of Green's Function is

$$\mathcal{G}\left(i\omega_n\right) = \int_0^\beta \exp\left(i\omega_n\tau\right)\mathcal{G}\left(\tau\right)d\tau. \tag{1.3}$$

Now, we show how to use the finite temperature Green function to compute the thermodynamics of the interacting system. In the following, we use the interaction representation,

where $\hat{A}(\tau) = \exp\left(\tau\hat{H}_0\right)\hat{A}\exp\left(-\tau\hat{H}_0\right)$. We denote

$$\hat{U}(\tau) = \exp\left(\tau\hat{H}_0\right)\exp\left(-\tau\hat{H}\right) \tag{1.4}$$

$$= 1 - \int_0^\tau d\tau_1 \hat{V}(\tau)\hat{U}(\tau_1) \tag{1.5}$$

$$= \sum_{n=0}^{\infty}(-1)^n \int_0^\tau d\tau_1 ... \int_0^{\tau_{n-1}} d\tau_n \hat{V}(\tau_1)...\hat{V}(\tau_n) \tag{1.6}$$

$$= \mathrm{T}_\tau \exp\left(-\int_0^\tau d\tau_1 \hat{V}(\tau_1)\right). \tag{1.7}$$

Then we have

$$\mathcal{G}_{p\sigma}(\tau) = -\frac{\mathrm{Tr}\left(\exp\left(-\beta\hat{H}_0\right)\hat{S}(\beta,\tau)\,\hat{a}^\dagger_{p\sigma}(\tau)\,\hat{S}(\tau,0)\,\hat{a}_{p\sigma}(0)\right)}{\mathrm{Tr}\left(\exp\left(-\beta\hat{H}_0\right)\hat{S}(\beta,0)\right)} \tag{1.8}$$

$$= -\frac{\mathrm{Tr}\left(\exp\left(-\beta\hat{H}_0\right)\mathrm{T}_\tau\,\hat{S}(\beta,0)\,\hat{a}^\dagger_{p\sigma}(\tau)\,\hat{a}_{p\sigma}(0)\right)}{\mathrm{Tr}\left(\exp\left(-\beta\hat{H}_0\right)\hat{S}(\beta,0)\right)}, \tag{1.9}$$

where $\hat{S}(\tau_1,\tau_2) = \hat{U}(\tau_1)\hat{U}^{-1}(\tau_2)$. We can perturbatively evaluate the Green's function and this yields the self-energy via the Dyson equation

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma, \tag{1.10}$$

where $\mathcal{G}_0$ is the non-interacting Green's function. Alternatively, one could perturbatively evaluate the self-energy and obtain the Green's function via Dyson's Equation. The self-energy represents an irreducible part of the diagram, and it is a key quantity when making approximations. Additionally, one can compute higher order Green's functions in a similar manner.

The variational principle is another key foundation of many-body physics. For a given

variational wave function $|\varphi(\{\gamma_i\})\rangle$, we can determine the ground state energy as

$$E_0 = \min_{\{\gamma_i\}} \frac{\left\langle \varphi(\{\gamma_i\}) \left| \hat{H} \right| \varphi(\{\gamma_i\}) \right\rangle}{\langle \varphi(\{\gamma_i\}) | \varphi(\{\gamma_i\}) \rangle}, \tag{1.11}$$

where $\{\gamma_i\}$ are variational parameters. The variational wave function is useful in that it provides a rigorous upper bound for the energy, though it can be challenging to systemically improve and evaluate the trial wave function. One particular way to construct the variational wave function is[6–8]

$$|\varphi(g)\rangle = \exp\left(-g\hat{V}\right)|\varphi_0\rangle, \tag{1.12}$$

where $|\varphi_0\rangle$ is the ground state of $\hat{H}_0$ and g is a variational parameter. For the one band Hubbard model, this becomes the well known Gutzwiller wave function.

We will show that the Variational Discrete Action Theory (VDAT), presented in this thesis, is a new formalism which combines the best aspects of both Green's functions and variational wave functions. The VDAT method has an unprecedented combination of efficiency and accuracy. In this thesis, we will use the VDAT to explore two different canonical Hamiltonians for interacting electrons: the Anderson Impurity Model (AIM) and the Hubbard Model. The AIM pertains to a single site with local interactions embedded in a non-interacting bath of electrons:

$$\hat{H} = \hat{H}_0 + \hat{V}, \qquad \hat{H}_0 = \sum_{\sigma,\mathbf{k}} v_{\mathbf{k},\sigma}\left(\hat{f}^\dagger_\sigma \hat{c}_{\mathbf{k},\sigma} + h.c.\right) - \epsilon_{\mathbf{k}\sigma}\sum_{\sigma,\mathbf{k}}\left(\hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} + h.c\right) \tag{1.13}$$

$$\hat{V} = U\left(\hat{f}^\dagger_\uparrow \hat{f}_\uparrow - \frac{1}{2}\right)\left(\hat{f}^\dagger_\downarrow \hat{f}_\downarrow - \frac{1}{2}\right), \tag{1.14}$$

where $\hat{f}_\sigma$ destroys an electron of spin σ from the impurity orbital, $\hat{c}_{\mathbf{k},\sigma}$ destroys an electron of spin σ from the bath orbital $\mathbf{k}$, $v_{\mathbf{k},\sigma}$ is the hybridization between the bath and the impurity, $\epsilon_{\mathbf{k}\sigma}$ is the dispersion within the bath, and U is the Hubbard repulsion among electron within the impurity. While the AIM is a non-trivial many-electron problem, it can be solved

numerically exactly using density matrix renormalization group[1, 9] or quantum Monte-Carlo techniques[10].

The Hubbard model is more complex, having an interaction at each site in the lattice

$$\hat{H} = \hat{H}_0 + \hat{V}, \qquad \hat{H}_0 = \sum_{ij\sigma} t_{ij} \hat{a}^\dagger_{i\sigma} \hat{a}_{j\sigma}, \qquad \hat{V} = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = U \sum_i \hat{d}_i. \tag{1.15}$$

In one dimension, the Hubbard model can be solved via the Bethe Ansatz[11–13]. In infinite dimensions, the dynamical mean-field theory maps the Hubbard model onto an effective AIM subject to a self-consistency condition[3], which can then be solved using various numerical approaches.

Chapter 2

Sequential Product Density Matrix

2.1 Motivation

A quantum many-body Hamiltonian will consist of a non-interacting part $\hat{H}_0$ and an interacting part $\hat{V}$, and the complete solution to this problem scales exponentially; making it insoluble. The key idea of the variational discrete action theory (VDAT) is based on a particular class of variational density matrices, referred to as Sequential Product Density Matrices (SPD), which can be efficiently evaluated. The full generality of the SPD will be presented in Sec. 2.3, but here we first consider the simpler case of the Sequential Product Wave Function (SPW), which can be formulated as

$$|\varphi\big(g_i,\gamma_i\big)\rangle = \exp\big(\gamma_1\hat{H}_0\big)\exp\big(g_1\hat{V}\big)...\exp\big(\gamma_N\hat{H}_0\big)\exp\big(g_N\hat{V}\big)|\varphi_0\rangle, \tag{2.1}$$

where N is a positive integer, γ_i and g_i are variational parameters, and $|\varphi_0\rangle$ is the ground state of $\hat{H}_0$. When $N\to\infty$, this SPW recovers the exact solution

$$|\varphi\rangle = \lim_{\beta\to\infty}\frac{\exp\big(-\beta\hat{H}\big)|\varphi_0\rangle}{\sqrt{\langle\varphi_0|\exp\big(-2\beta\hat{H}\big)|\varphi_0\rangle}} \tag{2.2}$$

when $g_i=\gamma_i=\beta/N$, which follows from the well known Trotter-Suzuki decomposition[14]. Therefore, it seems possible that for finite but small N, this variational wave function might be reasonable, which is our first motivation.

A second motivation is based on the success of the Gutzwiller wave-function[6–8, 15], in

addition to its well known limitations. To focus the discussion, we consider the one band Hubbard model. The idea of the Gutzwiller wave function is to use the interaction as a projector to modify a non-interacting wave-function and describe the competition between kinetic energy and local interaction.

$$|\varphi(g)\rangle = \exp\left(g\sum_n \hat{d}_n\right)|\varphi_0\rangle, \tag{2.3}$$

where $|\varphi_0\rangle$ is usually choose as the ground state of H_0 with same density. When working in the grand canonical ensemble, we extend to

$$|\varphi(g)\rangle = \exp\left(g\sum_n \hat{d}_n + \sum_\sigma \lambda_\sigma \hat{N}_\sigma\right)|\varphi_0\rangle \tag{2.4}$$

to control the density of given spin band, where $\hat{N}_\sigma$ is the total particle number operator for spin σ. For the Hubbard model, the Gutzwiller wave function can be efficiently evaluated using the Gutzwiller approximation, which is an exact evaluation of the Gutzwiller wave function for the case of infinite dimensions[15]. Therefore, in infinite dimensions, any shortcoming of the Gutzwiller approximation is due to the Gutzwiller wave function itself. This motivates us to go beyond the Gutzwiller wave function in a systematic manner.

Let us begin by reviewing how the standard GA works. To make the analysis convenient, we use the physical double occupancy instead to g to parameterize the energy, where

$$d(g) = \frac{\langle\varphi(g)|\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}|\varphi(g)\rangle}{\langle\varphi(g)|\varphi(g)\rangle}. \tag{2.5}$$

We could solve for g as a function of d and thus

$$n_{ij;\sigma}(g) = \frac{\left\langle\varphi(g)|\hat{a}^\dagger_{i\sigma}\hat{a}_{j\sigma}|\varphi(g)\right\rangle}{\langle\varphi(g)|\varphi(g)\rangle} \equiv Z_{ij;\sigma}(d)\, n_{ij;\sigma}(0). \tag{2.6}$$

For half-filling, the on-site renormalization $Z_{ii;\sigma}(d) = 1$, and one can construct the

renormalization between two different sites i and j as $Z_{ij;\sigma}(d) = 1 - (4\Delta d)^2$, where $\Delta d = d - 1/4$. For the Hubbard model, we only need to know the nearest site renormalization, and we denote it as $Z_\sigma(d)$ for short. Then, the minimization of the total energy over g can be effectively expressed as

$$\min_g \frac{\left\langle \varphi(g) | \hat{H} | \varphi(g) \right\rangle}{\langle \varphi(g) | \varphi(g) \rangle} = \min_g \left(\frac{\left\langle \varphi(g) | \hat{H}_0 | \varphi(g) \right\rangle}{\langle \varphi(g) | \varphi(g) \rangle} + \frac{\left\langle \varphi(g) | \hat{V} | \varphi(g) \right\rangle}{\langle \varphi(g) | \varphi(g) \rangle} \right) \tag{2.7}$$

$$= \min_g \left(\sum_{ij\sigma} t_{ij} n_{ij;\sigma}(g) + \sum_i U d(g) \right) \tag{2.8}$$

$$= \min_d \left(\sum_{ij\sigma} t_{ij} n_{ij;\sigma}(0) Z_{ij;\sigma}(d) + \sum_i U d \right), \tag{2.9}$$

where we have assumed translational symmetry, and thus we can minimize over the energy per site as

$$E_{gs} = \min_d \left(\sum_\sigma E_\sigma Z_\sigma(d) + U d \right), \tag{2.10}$$

where E_σ is the non-interacting kinetic energy per site for spin σ. As we will see the Chapter 8.5, we could make this form in principle exact using the concept of constrained search, and the Gutzwiller approximation could be viewed as an insightful non-perturbative approximation for it. The advantage of the Gutzwiller approximation in infinite dimensions could be summarized as the following:

1. It is a non-perturbative approximation from the non-interacting limit which treats the renormalization of the single particle density matrix locally. The renormalization between site i and j only depends on the local reduced density matrix of i and j and it ignore the correlation between them.
2. It has a good description of the metal phase as it is based on a wave-function projected from a non-interacting system.
3. It describes a metal-insulator transition for Hubbard model at half-filling in a straight-

forward way[16], yielding a renormalized fermi liquid for the metal phase and a collection of isolated atoms for the insulating phase.

4. It has a generic expression for Z in the multiband Hubbard model[17–20], and has relatively small computational cost compared with DMFT.

On the other hand, the Gutzwiller wave function (and approximation) has some severe problems. The most prominent is that within the Gutzwiller approximation, the super-exchange is ignored and there is no kinetic energy for the system in the insulating phase, which is not correct. When we study the magnetization and orbital polarization, the super-exchange, manifested in the kinetic energy, has a delicate balance with local interactions, and thus GA completely fails to describes the magnetic susceptibility and orbital susceptibility for Mott-insulators. Another problem is that even though in infinite dimensions the self-energy is local, there is still a complex momentum density distribution, but within the GA the momentum distribution resembles the non-interacting case with a constant renormalization. This problem can be traced to the fact that $Z_{ij;\sigma} = Z_\sigma$ for the off-site renormalization. Furthermore, GA has a wrong second order expansion coefficient compared with weak coupling perturbation theory.

One obvious solution is to perform DMFT calculations, but the cost increase from Gutzwiller to DMFT is tremendous. For example, for the one band Hubbard model, the Gutzwiller approximation has an analytic expression for Z, and the total energy as a function of U can be written analytically in closed form; while the DMFT calculation is much more demanding. Therefore, it is curious whether we can find an approach that has relatively small computational cost similar to GA but with accuracy comparable with DMFT. Or even better, is it possible that one could find a hierarchical class of approximations that connects the Gutzwiller approximation to the DMFT approximation smoothly, with a fine-tuned balance between computational cost and accuracy? We show that this is not only possible, but very practical.

A first step towards the SPD could be considered in terms of the so-called Gutzwiller-

Baeriswyl wave function introduced by Otsuka [21–23], though we write a slightly more general form having a distinct variational parameter for each single particle operator

$$|\varphi\left(g,\gamma_k\right)\rangle = \exp\left(\sum_{k\sigma}\gamma_{k\sigma}\hat{n}_{k\sigma}\right)\exp\left(g\sum_{n}\hat{d}_n\right)|\varphi_0\rangle. \tag{2.11}$$

Intuitively, the extra projection should introduce a non-trivial momentum distribution and will describe superexchange when $g \to -\infty$. Extending this line of reasoning, one could sequentially apply the kinetic and interacting projector N times, bringing us full circle to the motivation based on the Trotter-Suzuki decomposition.

2.2 Introducing the SPD in the Hubbard model

We begin by continuing our simplified discussion of the SPW before proceeding to the SPD. When defining the SPW for the Hubbard model, we have two types of wave-functions, denoted B and G (reminiscent of Baeriswyl and Gutzwiller), where the B type is

$$|\varphi_B\big(g_i,\gamma_{k\sigma;i}\big)\rangle = \exp\big(\sum_{k\sigma}\gamma_{k\sigma;1}\hat{n}_{k\sigma}\big)\exp\big(g_1\sum_{n}\hat{d}_n\big)...\exp\big(\sum_{k\sigma}\gamma_{k\sigma;M}\hat{n}_{k\sigma}\big)\exp\big(g_M\sum_{n}\hat{d}_n\big)|\varphi_0\rangle, \tag{2.12}$$

where M is a positive integer. Type G is

$$|\varphi_G\left(g_i,\gamma_{k\sigma;i}\right)\rangle = \exp\left(g_1\sum_{n}\hat{d}_n\right)...\exp\left(\sum_{k\sigma}\gamma_{k\sigma;M}\hat{n}_{k\sigma}\right)\exp\left(g_M\sum_{n}\hat{d}_n\right)|\varphi_0\rangle. \tag{2.13}$$

Of course, type G could be viewed as a special case of B, and vice versa. A wave function similar to Eq. 2.13 was first suggested by Dzierzawa et al[24], and they realized the importance of iteratively applying these projectors and the connection to the Trotter de-

composition; but we are not aware of any systematic pursuit of this idea. It should be emphasized that Eq. 2.13 has complete variational freedom in the single-particle projectors, while the proposition of Dzierzawa et al did not. More recently, a Wick rotated version of this wave function was proposed in the context of quantum computing by Farhi et. al[25], and further extended by Wecker et. al [26]. It should be noted that Eq. 2.13 is a special case of our more general SPD. In general, the SPD allows for completely general single-particle projectors and many-particle projectors at each time step, which will offer greater flexibility for studying disparate phenomena and increase the rate of convergence (see Section 2.3).

Finally, we elevate the SPW to a density matrix, which will simplify our formal developments and anticipate a generalization to finite temperatures. The type B SPW can be recast in a density matrix form as

$$\begin{aligned}
&\hat{\rho}_B\left(g_i, \gamma_{k\sigma;i}\right) = \\
&\exp\left(\sum_{k\sigma} \gamma_{k\sigma;1}\hat{n}_{k\sigma}\right) \exp\left(g_1 \sum_n \hat{d}_n\right) \ldots \exp\left(\sum_{k\sigma} \gamma_{k\sigma;M}\hat{n}_{k\sigma}\right) \exp\left(g_M \sum_n \hat{d}_n\right) \\
&\times |\varphi_0\rangle\langle\varphi_0| \exp\left(g_M \sum_n \hat{d}_n\right) \exp\left(\sum_{k\sigma} \gamma_{k\sigma;M}\hat{n}_{k\sigma}\right) \ldots \exp\left(g_1 \sum_n \hat{d}_n\right) \exp\left(\sum_{k\sigma} \gamma_{k\sigma;1}\hat{n}_{k\sigma}\right) \qquad (2.14) \\
&= \exp\left(\sum_{k\sigma} \gamma_{k\sigma;1}\hat{n}_{k\sigma}\right) \exp\left(g_1 \sum_n \hat{d}_n\right) \ldots \exp\left(\sum_{k\sigma} \gamma_{k\sigma;N}\hat{n}_{k\sigma}\right) \exp\left(g_N \sum_n \hat{d}_n\right), \qquad (2.15)
\end{aligned}$$

where we used $|\varphi_0\rangle\langle\varphi_0| = C \exp\left(\sum_{k\sigma} \gamma_{k\sigma}\hat{n}_{k\sigma}\right)$ with $N = 2M + 1$ and

$$\gamma_{k\sigma;l} = \gamma_{k\sigma}^{(N+1-l)}, \qquad g_l = g^{(N-l)}, \qquad g_N = 0. \qquad (2.16)$$

Similarly, the type G scenario gives

$$\hat{\rho}_G\left(g_i,\gamma_{k;i}\right)=\exp\left(g_1\sum_n\hat{d}_n\right)...\exp\left(\sum_{k\sigma}\gamma_{k\sigma;N}\hat{n}_{k\sigma}\right)\exp\left(g_N\sum_n\hat{d}_n\right)$$
$$\times\left|\varphi_0\right\rangle\left\langle\varphi_0\right|\exp\left(g_N\sum_n\hat{d}_n\right)\exp\left(\sum_{k\sigma}\gamma_{k\sigma;N}\hat{n}_{k\sigma}\right)...\exp\left(g_1\sum_n\hat{d}_n\right) \tag{2.17}$$
$$=\exp\left(\sum_{k\sigma}\gamma_{k\sigma;1}\hat{n}_{k\sigma}\right)\exp\left(g_1\sum_n\hat{d}_n\right)...\exp\left(\sum_{k\sigma}\gamma_{k\sigma;N}\hat{n}_{k\sigma}\right)\exp\left(g_N\sum_n\hat{d}_n\right) \tag{2.18}$$

with $N=2M$ and

$$g_l=g^{(N+1-l)},\qquad\qquad\gamma_{k\sigma;l}=\gamma_{k\sigma}^{(N-l)},\qquad\qquad\gamma_{k\sigma;1}=0. \tag{2.19}$$

One can also study the B type of $N=2M$ and G type of $N=2M+1$, but they are just special cases corresponding to $N+1$. Furthermore, one could use the more general form to include both $\hat{\rho}_B$ and $\hat{\rho}_G$, which we refer to as the sequential product density matrix (SPD) for the Hubbard model

$$\hat{\rho}\left(g_i,\gamma_{k\sigma;i}\right)=\exp\left(\sum_{k\sigma}\gamma_{k\sigma;1}\hat{n}_{k\sigma}\right)\exp\left(g_1\sum_n\hat{d}_n\right)...\exp\left(\sum_{k\sigma}\gamma_{k\sigma;\mathcal{N}}\hat{n}_{k\sigma}\right)\exp\left(g_{\mathcal{N}}\sum_n\hat{d}_n\right) \tag{2.20}$$

where the integer variable $\mathcal{N}$ characterizes the number of discrete time steps. Notice that the SPD is not explicitly required to be symmetric, and this is very convenient for developing the Lie group structure of the non-interacting density matrix (see Chapter 3.3). However, when applying the variational principle one must constrain $\gamma_{k\sigma;i}$ and g_i so that $\hat{\rho}\left(g_i,\gamma_{k;i}\right)$ is a symmetric matrix. In this thesis, we always choose G-type for $\mathcal{N}=2M$ and B-type for $\mathcal{N}=2M+1$.

Finally, we can also see the connection with the Trotter-Suzuki decomposition, which

recovers the finite temperature density matrix of Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ as

$$\exp\left(\beta\hat{H}\right) = \lim_{\mathcal{N}\to\infty}\left(\exp\left(\beta\hat{H}_0/\mathcal{N}\right)\exp\left(\beta\hat{V}/\mathcal{N}\right)\right)^{\mathcal{N}}. \tag{2.21}$$

For a given $\mathcal{N}$, if we choose the variational parameter for the SPD as

$$\gamma_{k\sigma;i} = \beta\epsilon_{k\sigma}/\mathcal{N}, \qquad\qquad g_i = \beta U/\mathcal{N}, \tag{2.22}$$

we recover the Trotter-Suzuki decomposition. However, the SPD combined with the variational principle will be superior to the Trotter-Suzuki decomposition by construction for finite $\mathcal{N}$. When $\mathcal{N}\to\infty$, the SPD recovers the exact finite temperature density matrix.

2.3 General form of SPD

Here we discuss the general form for the SPD, given as

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1\cdot\hat{\boldsymbol{n}}\right)\hat{P}_1...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}}\cdot\hat{\boldsymbol{n}}\right)\hat{P}_{\mathcal{N}} = \hat{\mathcal{P}}_1...\hat{\mathcal{P}}_{\mathcal{N}}, \quad \hat{P}_\tau = \exp\left(\hat{V}_\tau\right), \quad \hat{\mathcal{P}}_\tau = \exp\left(\boldsymbol{\gamma}_\tau\cdot\hat{\boldsymbol{n}}\right)\hat{P}_\tau, \tag{2.23}$$

where $\tau = 1,..,\mathcal{N}$ is the discrete time label, $\hat{\boldsymbol{n}}$ denotes the matrix collection of all single particle operators as

$$\hat{\boldsymbol{n}} = \begin{pmatrix} \hat{c}_1^\dagger\hat{c}_1 & \hat{c}_1^\dagger\hat{c}_2 & .. & \hat{c}_1^\dagger\hat{c}_L \\ \hat{c}_2^\dagger\hat{c}_1 & \hat{c}_2^\dagger\hat{c}_2 & .. & .. \\ .. & .. & .. & .. \\ \hat{c}_L^\dagger\hat{c}_1 & .. & .. & \hat{c}_L^\dagger\hat{c}_L \end{pmatrix}, \tag{2.24}$$

where L is the number of spin-orbitals of the system, and $\boldsymbol{\gamma}_\tau$ is a real matrix with same dimension as $\hat{\boldsymbol{n}}$; and the dot product of these matrices is defined as

$$\boldsymbol{\gamma} \cdot \hat{\boldsymbol{n}} \equiv \sum_{i=1}^{L} \sum_{j=1}^{L} \gamma_{ij} \hat{n}_{ij}. \tag{2.25}$$

Here, $\hat{V}_\tau$ is a general many-body operator, which may not be explicitly coupled within the Hamiltonian being studied. Eq. 2.23 is the key ansatz of the VDAT formalism, and we will demonstrate that the Discrete Action Theory is a powerful tool for efficiently evaluating this SPD. Notice that the discrete time label τ is opposite to the standard definition, as we label the projections in ascending order from left to right, while the usual definition is the reverse. There is no profound reason for this change in convention, though it does seem slightly more convenient in the context of the discrete form of the SPD. Once again, we remind the reader that we use G-type for even $\mathcal{N}$ and B-type for odd $\mathcal{N}$.

Additionally, each SPD will have an associated non-interacting SPD given as

$$\hat{\rho}_0 = \exp\left(\boldsymbol{\gamma}_1 \hat{\boldsymbol{n}}\right) ... \exp\left(\boldsymbol{\gamma}_\mathcal{N} \hat{\boldsymbol{n}}\right), \tag{2.26}$$

which plays a similar role to the non-interacting Hamiltonian in perturbation theory. While the above exponential can be combined into a single exponential, shown in Section 3.3, this would result in a loss of information, and therefore the above form should be maintained. This is critical to formulating the Discrete Action Theory and its corresponding evaluation within perturbation theory.

2.4 Evaluating the SPD for the Hubbard Plaquette

In this section, we explore the SPD for the Hubbard model on a ring at zero temperature. For small systems, we can directly evaluate the SPD and minimize over the variational parameters. Consider the Hubbard model on the plaquette, i.e, a ring with 4 sites. The

model reads

$$\hat{H} = \sum_{i=1}^{4} t \left(\hat{a}^{\dagger}_{i;\sigma} \hat{a}_{i+1;\sigma} + h.c. \right) + U \sum_{i=1}^{4} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \tag{2.27}$$

For the convenience of comparison with the Trotter-Suzuki formula, we use the SPD with the restriction that it is symmetric. The SPD is characterized by the discretization number $\mathcal{N}$, giving $\hat{\rho}^{(\mathcal{N})}$ as

$$\hat{\rho}^{(1)} = \hat{P}_B(\gamma_1) \tag{2.28}$$

$$\hat{\rho}^{(2)} = \hat{P}_G(g_1) \hat{P}_B(\gamma_1) \hat{P}_G(g_1) \tag{2.29}$$

$$\hat{\rho}^{(3)} = \hat{P}_B(\gamma_2) \hat{P}_G(g_1) \hat{P}_B(\gamma_1) \hat{P}_G(g_1) \hat{P}_B(\gamma_2) \tag{2.30}$$

$$\hat{\rho}^{(4)} = \hat{P}_G(g_2) \hat{P}_B(\gamma_2) \hat{P}_G(g_1) \hat{P}_B(\gamma_1) \hat{P}_G(g_1) \hat{P}_B(\gamma_2) \hat{P}_G(g_2) \tag{2.31}$$

$$\hat{\rho}^{(5)} = \hat{P}_B(\gamma_3) \hat{P}_G(g_2) \hat{P}_B(\gamma_2) \hat{P}_G(g_1) \hat{P}_B(\gamma_1) \hat{P}_G(g_1) \hat{P}_B(\gamma_2) \hat{P}_G(g_2) \hat{P}_B(\gamma_3) \tag{2.32}$$

$$\dots \tag{2.33}$$

We remind the reader that for each $\mathcal{N}$ there are two forms. For example, for $\mathcal{N} = 2$, the B-type, as opposed to the G-type listed above, is

$$\hat{\rho}^{(2)} = \hat{P}_B(\gamma_1) \hat{P}_G(g_1) \hat{P}_B(\gamma_1). \tag{2.34}$$

Given that the plaquette is sufficiently small, the exact solution can easily be computed, and the SPD can be evaluated without using the more advanced mathematical machinery introduced in Chapter 4. We begin be considering the double occupancy, $d = \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$, shown in Figure 2.1. For $\mathcal{N} = 2$, which is equivalent to exactly evaluating the Gutzwiller wave function, we have relatively large disagreement with the exact solution, completely missing the discontinuity at $U/t = 0$. Moving to $\mathcal{N} = 3$, we recover the discontinuity, and move closer to the exact solution. For $\mathcal{N} = 11$, there is almost no discernible difference with the

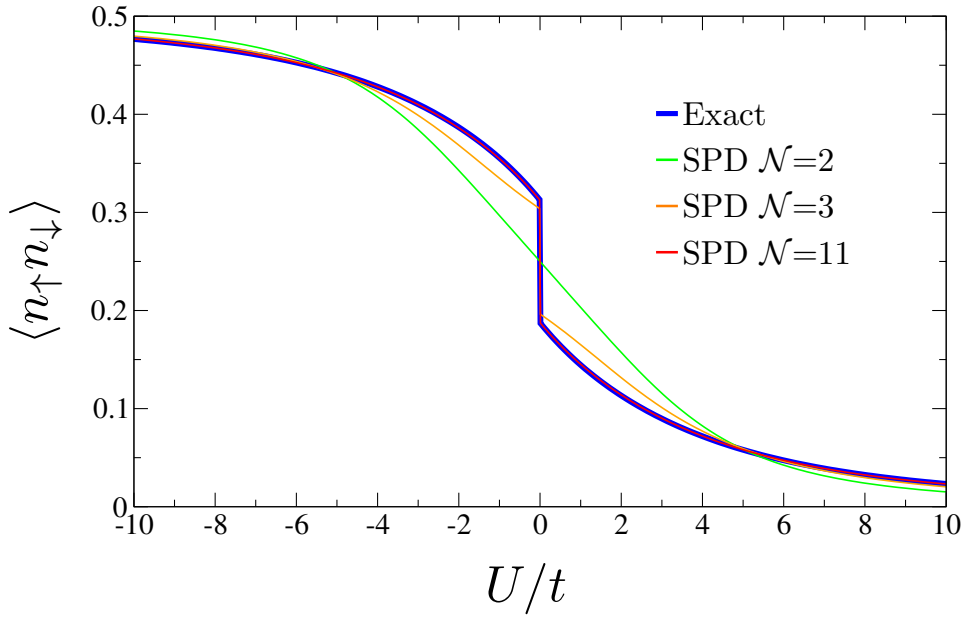

Figure 2.1: Double occupancy vs. U/t for the Hubbard plaquette evaluated using the SPD for $\mathcal{N} = 2$, 3, and 11 compared to the exact solution.

exact solution. Now we move on to the total energy, shown in Figure 2.2. We see that the error monotonically decreases with increasing $\mathcal{N}$. This example showcases the quality of the SPD ansatz, and later in the thesis we will prove that the SPD can be efficiently evaluated even in infinite systems.

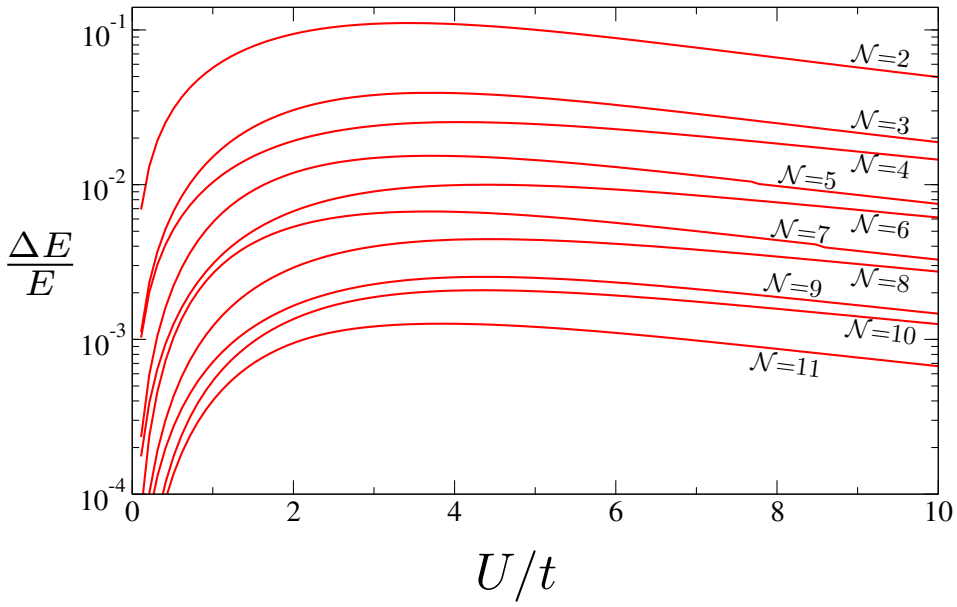

Figure 2.2: Energy error vs. U/t for the Hubbard plaquette evaluated using the SPD for $\mathcal{N}$ = 2-11.

Chapter 3

Discrete Action and Discrete Green's Function Formalism

3.1 Definition of Discrete Action and Discrete Green's function

In Chapter 2, we have seen that SPD provides a generic way to approach the exact ground state of a given Hamiltonian. Recall the general SPD defined in Chapter 2 Section 2.3

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right) \hat{P}_1 ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right) \hat{P}_{\mathcal{N}} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_N, \quad \hat{P}_i = \exp\left(\hat{V}_i\right), \quad \hat{\mathcal{P}}_i = \exp\left(\boldsymbol{\gamma}_i \cdot \hat{\boldsymbol{n}}\right) \hat{P}_i. \tag{3.1}$$

Additionally, recall the definition of the non-interacting SPD

$$\hat{\rho}_0 = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right) ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right). \tag{3.2}$$

Our strategy to evaluate the SPD is completely analogous to the Matsubara Green's function formalism. In fact, we will show that some key concepts from the Green's function based many-body formalism could be generalized to our scenario of discrete imaginary time, including the self-energy, Dyson equation, and diagram rules. Most importantly, the underlying interpretation of the path integral, which maps an N-dimension quantum system to N+1 dimensional classical system is generalized to a mapping from our original N-dimension system to a compound quantum system.

We define the non-interacting and interacting correlation function of the SPD as

$$\left\langle \hat{O}_1;\hat{O}_2;..;\hat{O}_{\mathcal{N}}\right\rangle_{\hat{\rho}_0} \equiv \frac{\mathrm{Tr}\Big(\exp\left(\boldsymbol{\gamma}_1\cdot\hat{\boldsymbol{n}}_1\right)\hat{O}_1\exp\left(\boldsymbol{\gamma}_2\cdot\hat{\boldsymbol{n}}_2\right)\hat{O}_2...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}}\cdot\hat{\boldsymbol{n}}_{\mathcal{N}}\right)\hat{O}_{\mathcal{N}}\Big)}{\mathrm{Tr}(\exp\left(\boldsymbol{\gamma}_1\cdot\hat{\boldsymbol{n}}_1\right)\exp\left(\boldsymbol{\gamma}_2\cdot\hat{\boldsymbol{n}}_2\right)...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}}\cdot\hat{\boldsymbol{n}}_{\mathcal{N}}\right))}, \tag{3.3}$$

and

$$\left\langle \hat{O}_1;\hat{O}_2;..;\hat{O}_{\mathcal{N}}\right\rangle_{\hat{\rho}} \equiv \frac{\mathrm{Tr}\Big(\exp\left(\boldsymbol{\gamma}_1\cdot\hat{\boldsymbol{n}}_1\right)\hat{P}_1\hat{O}_1\exp\left(\boldsymbol{\gamma}_2\cdot\hat{\boldsymbol{n}}_2\right)\hat{P}_2\hat{O}_2...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}}\cdot\hat{\boldsymbol{n}}_{\mathcal{N}}\right)\hat{P}_{\mathcal{N}}\hat{O}_{\mathcal{N}}\Big)}{\mathrm{Tr}\Big(\exp\left(\boldsymbol{\gamma}_1\cdot\hat{\boldsymbol{n}}_1\right)\hat{P}_1\exp\left(\boldsymbol{\gamma}_2\cdot\hat{\boldsymbol{n}}_2\right)\hat{P}_2...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}}\cdot\hat{\boldsymbol{n}}_{\mathcal{N}}\right)\Big)}. \tag{3.4}$$

The concept of discrete action naturally emerges when we introduce a complete basis set of the Fock space $\{|\Gamma_i\rangle\}$

$$\left\langle \hat{O}_1;\hat{O}_2;..;\hat{O}_{\mathcal{N}}\right\rangle_{\hat{\rho}} = \frac{1}{\mathrm{Tr}\left(\hat{\mathcal{P}}_1...\hat{\mathcal{P}}_{\mathcal{N}}\right)}\sum_{\Gamma_1..\Gamma_{\mathcal{N}}}\left\langle\Gamma_1|\hat{\mathcal{P}}_1\hat{O}_1|\Gamma_2\right\rangle\left\langle\Gamma_2|\hat{\mathcal{P}}_2\hat{O}_2|\Gamma_3\right\rangle..\left\langle\Gamma_{\mathcal{N}}|\hat{\mathcal{P}}_{\mathcal{N}}\hat{O}_{\mathcal{N}}|\Gamma_1\right\rangle \tag{3.5}$$

$$\begin{aligned}
&= \frac{1}{\mathrm{Tr}\left(\hat{\mathcal{P}}_1...\hat{\mathcal{P}}_{\mathcal{N}}\right)}\sum_{\Gamma_1..\Gamma_{\mathcal{N}}\eta_1..\eta_{\mathcal{N}}\eta_1'..\eta_{\mathcal{N}}'}\left\langle\Gamma_1|\eta_1\rangle\mathcal{P}_{1;\eta_1\eta_1'}\langle\eta_1'|\hat{O}_1|\Gamma_2\right\rangle\times\\
&\left\langle\Gamma_2|\eta_2\rangle\mathcal{P}_{2;\eta_2\eta_2'}\langle\eta_2'|\hat{O}_2|\Gamma_3\right\rangle..\left\langle\Gamma_{\mathcal{N}}|\eta_{\mathcal{N}}\rangle\mathcal{P}_{\mathcal{N};\eta_{\mathcal{N}}\eta_{\mathcal{N}}'}\langle\eta_{\mathcal{N}}'|\hat{O}_{\mathcal{N}}|\Gamma_1\right\rangle
\end{aligned} \tag{3.6}$$

$$\begin{aligned}
&= \frac{1}{\mathrm{Tr}\left(\hat{\mathcal{P}}_1...\hat{\mathcal{P}}_{\mathcal{N}}\right)}\sum_{\Gamma_1..\Gamma_{\mathcal{N}}\eta_1..\eta_{\mathcal{N}}\eta_1'..\eta_{\mathcal{N}}'}\mathcal{P}_{1;\eta_1\eta_1'}\mathcal{P}_{2;\eta_2\eta_2'}...\mathcal{P}_{\mathcal{N};\eta_{\mathcal{N}}\eta_{\mathcal{N}}'}\times\\
&\left\langle\Gamma_1|\eta_1\rangle\langle\eta_1'|\hat{O}_1|\Gamma_2\right\rangle\left\langle\Gamma_2|\eta_2\rangle\langle\eta_2'|\hat{O}_2|\Gamma_3\right\rangle..\left\langle\Gamma_{\mathcal{N}}|\eta_{\mathcal{N}}\rangle\langle\eta_{\mathcal{N}}'|\hat{O}_{\mathcal{N}}|\Gamma_1\right\rangle,
\end{aligned} \tag{3.7}$$

where $\mathcal{P}_{\tau;\eta\eta'} = \langle\eta|\hat{\mathcal{P}}_\tau|\eta'\rangle$.

We can now recast this expectation value as

$$\left\langle \hat{O}_1; \hat{O}_2; ..; \hat{O}_{\mathcal{N}} \right\rangle_{\mathcal{A}} = \sum_{\Gamma_1..\Gamma_{\mathcal{N}}\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \times \left\langle \Gamma_1|\eta_1\right\rangle\langle\eta'_1|\hat{O}_1|\Gamma_2\right\rangle \left\langle \Gamma_2|\eta_2\right\rangle\langle\eta'_2|\hat{O}_2|\Gamma_3\right\rangle .. \left\langle \Gamma_{\mathcal{N}}|\eta_{\mathcal{N}}\right\rangle\langle\eta'_{\mathcal{N}}|\hat{O}_{\mathcal{N}}|\Gamma_1\right\rangle , \quad (3.8)$$

where

$$\mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} = \frac{1}{\mathrm{Tr}\left(\hat{\mathcal{P}}_1...\hat{\mathcal{P}}_{\mathcal{N}}\right)} \mathcal{P}_{1;\eta_1\eta'_1}\mathcal{P}_{2;\eta_2\eta'_2}...\mathcal{P}_{\mathcal{N};\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}. \quad (3.9)$$

We refer to $\mathcal{A}$ as the discrete action of the SPD, in the sense that it encodes all the discrete dynamical information. The coefficient $\mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}}$ contains the full correlation between all time steps.

For an arbitrary quantum system, which may not be described by the SPD at finite $\mathcal{N}$, the effective action is given as

$$\mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} = \left\langle \hat{X}_{\eta'_1\eta_2}, \hat{X}_{\eta'_2\eta_3}, ..., \hat{X}_{\eta'_{\mathcal{N}}\eta_1} \right\rangle_{\mathcal{A}}, \quad (3.10)$$

where $\hat{X}_{\eta\eta'} = |\eta\rangle\langle\eta'|$, and the correlator of any operators is given as

$$\left\langle \hat{O}_1; \hat{O}_2; ..; \hat{O}_{\mathcal{N}} \right\rangle_{\mathcal{A}} = \sum_{\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \times \langle\eta'_1|\hat{O}_1|\eta_2\rangle\langle\eta'_2|\hat{O}_2|\eta_3\rangle..\langle\eta'_{\mathcal{N}}|\hat{O}_{\mathcal{N}}|\eta_1\rangle. \quad (3.11)$$

This discrete action fully characterizes the discrete time dynamics of an arbitrary quantum system. In Chapter 6, we will use the SPD to study the AIM, and we will need this more general form of the discrete action when characterizing the discrete dynamics of the impurity site.

Analogous to the continuous time case, we will need to introduce the discrete Green's function in order to determine the ground state properties of some Hamiltonian. The non-

interacting and interacting discrete Green's functions are defined as

$$g_{mn;0}(i,j) = \begin{cases} \left\langle \overbrace{\hat{1};..;\hat{1}}^{i-1}; \hat{a}_m^\dagger; \overbrace{\hat{1};..;\hat{1}}^{j-i-1}; \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-j} \right\rangle_{\hat{\rho}_0} & i < j \\ \left\langle \overbrace{\hat{1};..;\hat{1}}^{i-1}; \hat{a}_m^\dagger \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-i} \right\rangle_{\hat{\rho}_0} & i = j \\ -\left\langle \overbrace{\hat{1};..;\hat{1}}^{j-1}; \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{i-j-1}; \hat{a}_m^\dagger; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-i} \right\rangle_{\hat{\rho}_0} & j < i \end{cases} \tag{3.12}$$

and

$$g_{mn}(i,j) = \begin{cases} \left\langle \overbrace{\hat{1};..;\hat{1}}^{i-1}; \hat{a}_m^\dagger; \overbrace{\hat{1};..;\hat{1}}^{j-i-1}; \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-j} \right\rangle_{\hat{\rho}} & i < j \\ \left\langle \overbrace{\hat{1};..;\hat{1}}^{i-1}; \hat{a}_m^\dagger \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-i} \right\rangle_{\hat{\rho}} & i = j \\ -\left\langle \overbrace{\hat{1};..;\hat{1}}^{j-1}; \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{i-j-1}; \hat{a}_m^\dagger; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-i} \right\rangle_{\hat{\rho}} & j < i \end{cases} \tag{3.13}$$

Furthermore, for the most generic discrete action, the discrete Green's function is given as

$$g_{mn}(i,j) = \begin{cases} \left\langle \overbrace{\hat{1};..;\hat{1}}^{i-1}; \hat{a}_m^\dagger; \overbrace{\hat{1};..;\hat{1}}^{j-i-1}; \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-j} \right\rangle_{\mathcal{A}} & i < j \\ \left\langle \overbrace{\hat{1};..;\hat{1}}^{i-1}; \hat{a}_m^\dagger \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-i} \right\rangle_{\mathcal{A}} & i = j \\ -\left\langle \overbrace{\hat{1};..;\hat{1}}^{j-1}; \hat{a}_n; \overbrace{\hat{1};..;\hat{1}}^{i-j-1}; \hat{a}_m^\dagger; \overbrace{\hat{1};..;\hat{1}}^{\mathcal{N}-i} \right\rangle_{\mathcal{A}} & j < i \end{cases} \tag{3.14}$$

Once again, we remind the reader that we have chosen the opposite time ordering convention as compared to the usual many-body Green's function.

3.2 Mapping the Discrete Action to an Effective Density Matrix of a Compound System

To proceed, we prescribe a mathematical trick to recast the dynamical correlation of a discrete action as a static measurement under an effective density matrix in a compound system. In the path integral formalism of the usual action, one can interpret the action as the effective energy of a classical system (though for fermions one needs Grassmann numbers, which have no classical counterpart) with the same spatial structure and one more axis for the time correlation. Thus, we have the well-known fact that d dimensional quantum fields correspond to a (d+1) dimensional classical system. In the following, we generalize this mapping, resulting in two key differences:

1. As the number of time steps is finite, the number of points within extra dimension is also finite. Instead of saying the new system is in a higher dimension, we refer to it as a compound quantum system, with a Hilbert space of $\mathbb{H}_c = \otimes_{\tau=1}^{\mathcal{N}} \mathbb{H}$.
2. For the evolution of each time step, since the $\hat{\mathcal{P}}_i$ can not be treated as an infinitesimally small expansion from identity matrix, we need to keep its exact form. Therefore, the resulting system is still quantum mechanical.

To begin, we must define how we represent operators from the original system in the compound system. Each creation and destruction operator will be attached to a given time index when promoted to the compound space. For example, for a system with L spin orbitals, any operator can be built algebraically from the $2L$ operators $\hat{a}_1^\dagger, \ldots, \hat{a}_L^\dagger$ and $\hat{a}_1, \ldots, \hat{a}_L$. Given $\mathcal{N}$ time steps, any operator for the compound system can be built algebraically from $2L\mathcal{N}$ operators $\hat{a}_1^{\dagger(1)}, \ldots, \hat{a}_L^{\dagger(1)}, \ldots, \hat{a}_1^{\dagger(\tau)}, \ldots, \hat{a}_L^{\dagger(\tau)}, \ldots, \hat{a}_1^{\dagger(\mathcal{N})}, \ldots, \hat{a}_L^{\dagger(\mathcal{N})}$ and $\hat{a}_1^{(1)}, \ldots, \hat{a}_L^{(1)}, \ldots, \hat{a}_1^{(\tau)}, \ldots, \hat{a}_L^{(\tau)}, \ldots, \hat{a}_1^{(\mathcal{N})}, \ldots, \hat{a}_L^{(\mathcal{N})}$. These operators in the compound space must obey the fermionic anti-commutation relations. In order to promote some generic operator $\hat{O} = f(\hat{a}_1^\dagger, \ldots, \hat{a}_L^\dagger, \hat{a}_1, \ldots, \hat{a}_L)$ for a given τ, we obtain the corresponding operator in the compound space as $\hat{O}^{(\tau)} = f(\hat{a}_1^{\dagger(\tau)}, \ldots, \hat{a}_L^{\dagger(\tau)}, \hat{a}_1^{(\tau)}, \ldots, \hat{a}_L^{(\tau)})$.

Recalling the definition of the expectation value in terms of the effective action, we can embed into the compound system as

$$\left\langle \hat{O}_1;\hat{O}_2;..;\hat{O}_{\mathcal{N}} \right\rangle_{\mathcal{A}} = \sum_{\Gamma_1..\Gamma_{\mathcal{N}}\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \times$$

$$\left\langle \Gamma_1|\eta_1\right\rangle\langle\eta'_1|\hat{O}_1|\Gamma_2\rangle \left\langle \Gamma_2|\eta_2\right\rangle\langle\eta'_2|\hat{O}_2|\Gamma_3\rangle .. \left\langle \Gamma_{\mathcal{N}}|\eta_{\mathcal{N}}\right\rangle\langle\eta'_{\mathcal{N}}|\hat{O}_{\mathcal{N}}|\Gamma_1\rangle \tag{3.15}$$

$$= \sum_{\Gamma_1..\Gamma_{\mathcal{N}}\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \times \tag{3.16}$$

$$\left\langle \Gamma_1|\hat{X}_{\eta_1\eta'_1}\hat{O}_1|\Gamma_2\right\rangle \left\langle \Gamma_2|\hat{X}_{\eta_2\eta'_2}\hat{O}_2|\Gamma_3\right\rangle .. \left\langle \Gamma_{\mathcal{N}}|\hat{X}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}|\hat{O}_{\mathcal{N}}|\Gamma_1\right\rangle \tag{3.17}$$

$$= \sum_{\Gamma_1..\Gamma_{\mathcal{N}}\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \times$$

$$\theta_{\Gamma_2\Gamma_3..\Gamma_1}\langle\Gamma_1\otimes\Gamma_2...\otimes\Gamma_{\mathcal{N}}|\hat{X}^{(1)}_{\eta_1\eta'_1}\hat{O}^{(1)}_1\hat{X}^{(2)}_{\eta_2\eta'_2}\hat{O}^{(2)}_2..\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{O}^{(\mathcal{N})}_{\mathcal{N}}|\Gamma_2\otimes\Gamma_3..\otimes\Gamma_1\rangle, \tag{3.18}$$

where

$$\theta_{\Gamma_2\Gamma_3..\Gamma_1} = \langle\Gamma_1\otimes\Gamma_2...\otimes\Gamma_{\mathcal{N}}|\left(\hat{X}_{\Gamma_1\Gamma_2}\right)^{(1)}...\left(\hat{X}_{\Gamma_{\mathcal{N}-1}\Gamma_{\mathcal{N}}}\right)^{(\mathcal{N}-1)}\left(\hat{X}_{\Gamma_{\mathcal{N}}\Gamma_1}\right)^{(\mathcal{N})}|\Gamma_2\otimes\Gamma_3..\otimes\Gamma_1\rangle \tag{3.19}$$

$$= \langle\Gamma_2\otimes\Gamma_3..\otimes\Gamma_1|\left(\hat{X}_{\Gamma_1\Gamma_{\mathcal{N}}}\right)^{(\mathcal{N})}\left(\hat{X}_{\Gamma_{\mathcal{N}}\Gamma_{\mathcal{N}-1}}\right)^{(\mathcal{N}-1)}..\left(\hat{X}_{\Gamma_2\Gamma_1}\right)^{(1)}|\Gamma_1\otimes\Gamma_2...\otimes\Gamma_{\mathcal{N}}\rangle. \tag{3.20}$$

In order to convert Eq. 3.16 into a trace, we must define a permutation matrix as

$$\theta_{\Gamma_2\Gamma_3..\Gamma_1}|\Gamma_2\otimes\Gamma_3..\otimes\Gamma_1\rangle = \hat{Q}|\Gamma_1\otimes\Gamma_2...\otimes\Gamma_{\mathcal{N}}\rangle, \tag{3.21}$$

where

$$\hat{Q} = \sum_{\Gamma_1\Gamma_2..\Gamma_{\mathcal{N}}} \theta_{\Gamma_2\Gamma_3..\Gamma_1} |\Gamma_2 \otimes \Gamma_3 .. \otimes \Gamma_1\rangle\langle\Gamma_1 \otimes \Gamma_2 ... \otimes \Gamma_{\mathcal{N}}| \tag{3.22}$$

$$= \sum_{\Gamma_1\Gamma_2..\Gamma_{\mathcal{N}}} \left(\hat{X}_{\Gamma_1\Gamma_{\mathcal{N}}}\right)^{(\mathcal{N})} \left(\hat{X}_{\Gamma_{\mathcal{N}}\Gamma_{\mathcal{N}-1}}\right)^{(\mathcal{N}-1)} .. \left(\hat{X}_{\Gamma_2\Gamma_1}\right)^{(1)}. \tag{3.23}$$

Using the permutation matrix, we can then achieve the desired result

$$\left\langle \hat{O}_1; \hat{O}_2; ..; \hat{O}_{\mathcal{N}} \right\rangle_{\mathcal{A}} = \sum_{\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \mathrm{Tr}\left(\hat{Q} X^{(1)}_{\eta_1\eta'_1} \hat{O}^{(1)}_1 \hat{X}^{(\mathcal{N})}_{\eta_2\eta'_2} \hat{O}^{(2)}_2 ... \hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}} \hat{O}^{(\mathcal{N})}_{\mathcal{N}}\right) \tag{3.24}$$

$$= \mathrm{Tr}\Bigg(\hat{Q}\Big(\sum_{\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \varphi_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \hat{X}^{(1)}_{\eta_1\eta'_1} ... \hat{X}^{(\mathcal{N})}_{\eta_2\eta'_2}\Big) \times \hat{O}^{(1)}_1 \hat{O}^{(2)}_2 ... \hat{O}^{(\mathcal{N})}_{\mathcal{N}}\Bigg) \tag{3.25}$$

$$= \mathrm{Tr}\left(\hat{Q}\hat{\mathcal{A}} \hat{O}^{(1)}_1 \hat{O}^{(2)}_2 ... \hat{O}^{(\mathcal{N})}_{\mathcal{N}}\right) \tag{3.26}$$

$$= \mathrm{Tr}\left(\hat{\rho}_{eff} \hat{O}^{(1)}_1 \hat{O}^{(2)}_2 ... \hat{O}^{(\mathcal{N})}_{\mathcal{N}}\right), \tag{3.27}$$

where

$$\hat{\mathcal{A}} = \sum_{\eta_1..\eta_{\mathcal{N}}\eta'_1..\eta'_{\mathcal{N}}} \mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \varphi_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}} \hat{X}^{(1)}_{\eta_1\eta'_1} ... \hat{X}^{(\mathcal{N})}_{\eta_2\eta'_2} \tag{3.28}$$

and

$$\varphi_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}}$$
$$= \mathrm{Tr}\left(\left(\hat{X}_{\eta_1\eta_{\mathcal{N}}}\right)^{(\mathcal{N})} \left(\hat{X}_{\eta_{\mathcal{N}}\eta_{\mathcal{N}-1}}\right)^{(\mathcal{N}-1)} .. \left(\hat{X}_{\eta_2\eta_1}\right)^{(1)} \hat{X}^{(1)}_{\eta_1\eta'_1} ... \hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}} \hat{X}^{(1)}_{\eta'_1\eta_2} ... \hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right). \tag{3.29}$$

We determined $\varphi_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}}$ by taking an explicit choice of $\hat{O}_i^{(i)} = \hat{X}^{(i)}_{\eta'_i\eta_{i+1}}$, resulting in

$$\varphi_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}}\mathrm{Tr}\left(\hat{Q}\hat{X}^{(1)}_{\eta_1\eta'_1}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{X}^{(1)}_{\eta'_1\eta_2}\hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right) \equiv \mathrm{Tr}\left(\hat{Q}\hat{X}^{(1)}_{\eta_1\eta'_1}\hat{X}^{(1)}_{\eta'_1\eta_2}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right). \tag{3.30}$$

We can evaluate the right hand side as

$$\mathrm{Tr}\left(\hat{Q}\hat{X}^{(1)}_{\eta_1\eta'_1}\hat{X}^{(1)}_{\eta'_1\eta_2}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right) = \mathrm{Tr}\left(\hat{Q}\hat{X}^{(1)}_{\eta_1\eta_2}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta_1}\right) \tag{3.31}$$

$$= \mathrm{Tr}\left(\left(\hat{X}_{\eta_1\eta_{\mathcal{N}}}\right)^{(\mathcal{N})}\left(\hat{X}_{\eta_{\mathcal{N}}\eta_{\mathcal{N}-1}}\right)^{(\mathcal{N}-1)}..\left(\hat{X}_{\eta_2\eta_1}\right)^{(1)}\hat{X}^{(1)}_{\eta_1\eta_2}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta_1}\right) = 1 \tag{3.32}$$

and the left hand side as

$$\mathrm{Tr}\left(\hat{Q}\hat{X}^{(1)}_{\eta_1\eta'_1}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{X}^{(1)}_{\eta'_1\eta_2}\hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right) \tag{3.33}$$

$$= \mathrm{Tr}\left(\left(\hat{X}_{\eta_1\eta_{\mathcal{N}}}\right)^{(\mathcal{N})}\left(\hat{X}_{\eta_{\mathcal{N}}\eta_{\mathcal{N}-1}}\right)^{(\mathcal{N}-1)}..\left(\hat{X}_{\eta_2\eta_1}\right)^{(1)}\hat{X}^{(1)}_{\eta_1\eta'_1}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{X}^{(1)}_{\eta'_1\eta_2}\hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right) \tag{3.34}$$

$$= \mathrm{Tr}\left(\left(\hat{X}_{\eta_1\eta_{\mathcal{N}}}\right)^{(\mathcal{N})}\left(\hat{X}_{\eta_{\mathcal{N}}\eta_{\mathcal{N}-1}}\right)^{(\mathcal{N}-1)}..\left(\hat{X}_{\eta_2\eta_1}\right)^{(1)}\hat{X}^{(1)}_{\eta_1\eta'_1}...\hat{X}^{(\mathcal{N})}_{\eta_{\mathcal{N}}\eta'_{\mathcal{N}}}\hat{X}^{(1)}_{\eta'_1\eta_2}\hat{X}^{(\mathcal{N})}_{\eta'_{\mathcal{N}}\eta_1}\right). \tag{3.35}$$

Given that φ can only have values of ± 1, we have derived Eq. 3.29. In summary, we have

$$\left\langle \hat{O}_1; \hat{O}_2; ..; \hat{O}_{\mathcal{N}} \right\rangle_{\mathcal{A}} = \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{O}_1^{(1)}\hat{O}_2^{(2)}...\hat{O}_{\mathcal{N}}^{(\mathcal{N})}\right),$$

which proves that we can recast the dynamical correlation of a discrete action as a static measurement under an effective density matrix in a compound system. It should be noted that $\hat{\rho}_{eff}$ is not a Hermitian matrix in general.

Finally, notice that when $\mathcal{A}_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}}$ corresponds to an SPD that conserves particle number at each time step and is nonzero, $\varphi_{\eta_1\eta_2..\eta_{\mathcal{N}},\eta'_1\eta'_2..\eta'_{\mathcal{N}}}$=1 , as $\hat{X}^{(i)}_{\eta_i\eta'_i}$ is bosonic for such an SPD. Consequently, we have

$$\hat{\rho}_{eff} = \hat{Q}\hat{\mathcal{P}}_1^{(1)}...\hat{\mathcal{P}}_{\mathcal{N}}^{(\mathcal{N})}. \tag{3.36}$$

It is useful to appreciate that the mapping to the compound space can be considered to be a generalization of the usual path integral. First consider the standard path integral representation of the partition function

$$\left\langle \exp(-\beta\hat{H}) \right\rangle_{\hat{1}} = \frac{\int D\bar{\varphi}D\varphi \exp\left(-\int_0^\beta d\tau \left(\sum_i \bar{\varphi}_i(\tau)\frac{\partial}{\partial\tau}\varphi_i(\tau) + H\left(\{\bar{\varphi}(\tau)\},\{\varphi(\tau)\}\right)\right)\right.}{\int D\bar{\varphi}D\varphi \exp\left(-\int_0^\beta d\tau \left(\sum_i \bar{\varphi}_i(\tau)\frac{\partial}{\partial\tau}\varphi_i(\tau)\right)\right.}. \tag{3.37}$$

In order to directly compare with our discrete theory, we change variables as $\tau \to \beta - \tau$, yielding

$$\left\langle \exp(-\beta\hat{H}) \right\rangle_{\hat{1}} = \frac{\int D\bar{\varphi}D\varphi \exp\left(\int_0^\beta d\tau \left(\sum_i \bar{\varphi}_i(\tau)\frac{\partial}{\partial\tau}\varphi_i(\tau) - H\left(\{\bar{\varphi}(\tau)\},\{\varphi(\tau)\}\right)\right)\right.}{\int D\bar{\varphi}D\varphi \exp\left(\int_0^\beta d\tau \left(\sum_i \bar{\varphi}_i(\tau)\frac{\partial}{\partial\tau}\varphi_i(\tau)\right)\right.} \tag{3.38}$$

$$\approx \frac{\int \left(\prod_{\tau=1}^{\mathcal{N}}\prod_{i=1}^{L} d\bar{\varphi}_{i,\tau}d\varphi_{i,\tau}\right) \exp\left(\sum_{i\tau\tau'} \bar{\varphi}_{i,\tau}\Delta_{\tau,\tau'}\varphi_{i,\tau'} - \frac{\beta}{\mathcal{N}}\sum_{\tau=1}^{\mathcal{N}} H\left(\{\bar{\varphi}_\tau\},\{\varphi_\tau\}\right)\right)}{\int \left(\prod_{\tau=1}^{\mathcal{N}}\prod_{i=1}^{L} d\bar{\varphi}_{i,\tau}d\varphi_{i,\tau}\right) \exp\left(\sum_{i\tau\tau'} \bar{\varphi}_{i,\tau}\Delta_{\tau,\tau'}\varphi_{i,\tau'}\right)}, \tag{3.39}$$

where $\Delta_{\tau,\tau'}$ is the discretization of $\partial/\partial\tau$. Now we consider the same quantity expressed in the compound system for a given finite $\mathcal{N}$

$$\left\langle \exp(-\beta\hat{H}) \right\rangle_{\hat{1}} = \left\langle \prod_{\tau=1}^{\mathcal{N}} \exp(-\frac{\beta}{\mathcal{N}}\hat{H}) \right\rangle_{\hat{1}} \tag{3.40}$$

$$= \left\langle \exp(-\frac{\beta}{\mathcal{N}}\hat{H}); \exp(-\frac{\beta}{\mathcal{N}}\hat{H}); \ldots; \exp(-\frac{\beta}{\mathcal{N}}\hat{H}) \right\rangle_{\hat{1}} \tag{3.41}$$

$$= \left\langle \exp(-\frac{\beta}{\mathcal{N}}\hat{H}^{(1)}) \exp(-\frac{\beta}{\mathcal{N}}\hat{H}^{(2)}) \ldots \exp(-\frac{\beta}{\mathcal{N}}\hat{H}^{(\mathcal{N})}) \right\rangle_{\hat{Q}} \tag{3.42}$$

$$= \left\langle \exp\left(-\frac{\beta}{\mathcal{N}}\sum_{\tau=1}^{\mathcal{N}} \hat{H}^{(\tau)}\right) \right\rangle_{\hat{Q}}. \tag{3.43}$$

One can see that for any $\mathcal{N}$, the mapping to the compound system is exact, in contrast to the discretized path integral, which is only exact for $\mathcal{N} \to \infty$. In order to see the connection

between these two representations at finite $\mathcal{N}$, we can show that the discretized path integral is an approximation to the exact expression in the compound space. Specifically, one can show

$$\left\langle \exp\left(-\frac{\beta}{\mathcal{N}}\sum_{\tau=1}^{\mathcal{N}}\hat{H}^{(\tau)}\right)\right\rangle_{\hat{Q}} = \tag{3.44}$$

$$\frac{\int(\prod_{\tau=1}^{\mathcal{N}}\prod_{i=1}^{L}d\bar{\varphi}_{i,\tau}d\varphi_{i,\tau})\exp\left(\sum_{ij\tau\tau'}\bar{\varphi}_{i,\tau}[(\boldsymbol{g}_Q^{-1})^T]_{i\tau,j\tau'}\varphi_{j,\tau'}-\frac{\beta}{\mathcal{N}}\sum_{\tau=1}^{\mathcal{N}}H\left(\{\bar{\varphi}_\tau\},\{\varphi_\tau\}\right)\right)}{\int(\prod_{\tau=1}^{\mathcal{N}}\prod_{i=1}^{L}d\bar{\varphi}_{i,\tau}d\varphi_{i,\tau})\exp\left(\sum_{ij\tau\tau'}\bar{\varphi}_{i,\tau}[(\boldsymbol{g}_Q^{-1})^T]_{ij}\varphi_{j,\tau'}\right)} \tag{3.45}$$

$$+\mathcal{O}(\frac{1}{\mathcal{N}}), \tag{3.46}$$

where

$$\left[\left(\boldsymbol{g}_Q^{-1}\right)^T\right]_{i\tau,j\tau'}=\begin{cases}-\delta_{ij} & \tau=\tau'+1\\ \delta_{ij} & \tau=\tau'\\ 0 & \text{otherwise}\end{cases}. \tag{3.47}$$

In order to prove this, we begin by introducing a shorthand notation for the classical average over $2M$ Grassman variables which have a correspondence to the creation and destruction operators

$$\left\langle\left\langle\hat{A}\right\rangle\right\rangle_{\boldsymbol{g}_0}=\frac{\int\prod_{i=1}^{M}d\bar{\varphi}_i d\varphi_i\exp\left(\sum_{ij}\bar{\varphi}_i[(\boldsymbol{g}_0^{-1})^T]_{ij}\varphi_j\right)A\left(\{\bar{\varphi}\},\{\varphi\}\right)}{\int\prod_{i=1}^{M}d\bar{\varphi}_i d\varphi_i\exp\left(\sum_{ij}\bar{\varphi}_i[(\boldsymbol{g}_0^{-1})^T]_{ij}\varphi_j\right)}. \tag{3.48}$$

In order to prove Eq. 3.44, it is sufficient to prove a more general relation

$$\left\langle\exp\left(\hat{O}_M\right)\right\rangle_{\hat{\rho}_0}=\left\langle\left\langle\exp(\hat{O}_M)\right\rangle\right\rangle_{\boldsymbol{g}_0}+\mathcal{O}(\frac{1}{M}), \tag{3.49}$$

where $\hat{O}_M$ is an operator in the compound space built from $M = \mathcal{N} \times L$ spin orbitals

$$\hat{O}_M = \frac{1}{M} \sum_n \epsilon_n a_n^\dagger a_n + \frac{1}{M^2} \sum_{n \neq n'} v_{nn'} a_n^\dagger a_{n'} + \frac{1}{M^4} \sum_{ijkl} u_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \dots \tag{3.50}$$

which has a well defined limit for $M \to \infty$. Given a non-interacting density matrix $\hat{\rho}_0$ with $\boldsymbol{g}_0$ as the corresponding single-particle density matrix, the following equality holds for any operator

$$\left\langle \left\langle \hat{A} \right\rangle \right\rangle_{\boldsymbol{g}_0} = \left\langle : \hat{A} : \right\rangle_{\hat{\rho}_0} . \tag{3.51}$$

For example, we have

$$\left\langle \left\langle \hat{a}_{i_1}^\dagger \hat{a}_{i_2}^\dagger \dots \hat{a}_{i_n}^\dagger \hat{a}_{j_1} \hat{a}_{j_2} \dots \hat{a}_{j_n} \right\rangle \right\rangle_{\boldsymbol{g}_0} = \left\langle \hat{a}_{i_1}^\dagger \hat{a}_{i_2}^\dagger \dots \hat{a}_{i_n}^\dagger \hat{a}_{j_1} \hat{a}_{j_2} \dots \hat{a}_{j_n} \right\rangle_{\hat{\rho}_0} . \tag{3.52}$$

For an alternate example, consider

$$\left\langle \left\langle \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger \hat{a}_i \right\rangle \right\rangle_{\boldsymbol{g}_0} = 0, \qquad \left\langle \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger \hat{a}_i \right\rangle_{\hat{\rho}_0} \neq 0$$

where for former is zero because $\{\bar{\varphi}, \bar{\varphi}\} = 0$ and $\{\varphi, \bar{\varphi}\} = 0$, but the latter is nonzero as $\left\{\hat{a}, \hat{a}^\dagger\right\} = 1$. We can then prove that $\hat{O}_M$ raised to any integer satifies

$$\hat{O}_M^n =: \hat{O}_M^n : + \mathcal{O}(\frac{1}{M}). \tag{3.53}$$

For example, for $n = 2$ we have

$$\left(\frac{1}{M} \sum_n \epsilon_n a_n^\dagger a_n \right)^2 = \frac{1}{M^2} \sum_{nn'} \epsilon_n \epsilon_{n'} a_n^\dagger a_n a_{n'}^\dagger a_{n'} = \frac{1}{M^2} \sum_{nn'} \epsilon_n \epsilon_{n'} a_n^\dagger (\delta_{nn'} - a_{n'}^\dagger a_n)) a_{n'} \tag{3.54}$$

$$=: \left(\frac{1}{M} \sum_n \epsilon_n a_n^\dagger a_n \right)^2 : + \frac{1}{M^2} \sum_n \epsilon_n^2 a_n^\dagger a_n. \tag{3.55}$$

We can see that the latter will contribute $\mathcal{O}\left(\frac{1}{M}\right)$ given that there are M terms in the summation. For a general product, we have

$$\left(\frac{1}{M^{2\ell}} \sum_{n_1 \ldots n_\ell n'_1 \ldots n'_\ell} \epsilon_{n_1 \ldots n_\ell} a^\dagger_{n_1} \ldots a^\dagger_{n_\ell} a_{n'_1} \ldots a_{n'_\ell}\right) \times \tag{3.56}$$

$$\left(\frac{1}{M^{2r}} \sum_{m_1 \ldots m_r m'_1 \ldots m'_r} \epsilon_{m_1 \ldots m_r} a^\dagger_{m_1} \ldots a^\dagger_{m_r} a_{m'_1} \ldots a_{m'_r}\right) = \tag{3.57}$$

$$\frac{1}{M^{2(\ell+r)}} \sum_{\substack{n_1 \ldots n_\ell n'_1 \ldots n'_\ell \\ m_1 \ldots m_r m'_1 \ldots m'_r}} \epsilon_{n_1 \ldots n_\ell} \epsilon_{m_1 \ldots m_r} a^\dagger_{n_1} \ldots a^\dagger_{n_\ell} a_{n'_1} \ldots a_{n'_\ell} a^\dagger_{m_1} \ldots a^\dagger_{m_r} a_{m'_1} \ldots a_{m'_r}. \tag{3.58}$$

Applying Wick's theorem, a nonzero single contraction term contains a Kronecker delta function which will ensure that the corresponding summation will scale like $1/M$. Similarly, for a nonzero double contraction, the resulting summation will scale like $1/M^2$, etc. This proves Eq. 3.53. We then have

$$\left\langle \hat{O}^n_M \right\rangle_{\hat{\rho}_0} = \left\langle : \hat{O}^n_M : \right\rangle_{\hat{\rho}_0} + \mathcal{O}(\frac{1}{M}) = \left\langle \left\langle \hat{O}^n_M \right\rangle \right\rangle_{\boldsymbol{g}_0} + \mathcal{O}(\frac{1}{M}),$$

which proves Eq. 3.49.

3.3 Lie group structure of the non-interacting density matrix in the non-symmetric case

In Section 3.2, we have seen that in general, the discrete action $\mathcal{A}$ can be mapped to an effective density matrix of a compound system as

$$\hat{\rho}_{eff} = \hat{Q}\hat{\mathcal{A}}. \tag{3.59}$$

Unlike the usual density matrix, $\hat{\rho}_{eff}$ is not symmetric due the presence of the shift operator $\hat{Q}$, defined in Eq. 3.23, which is a very complex object as it consists of products of Hubbard operators in the compound space. In this section, we study the group structure of the general non-interacting density matrix, which provides the foundation of our theory and gives many insights into defining the self-energy and shift operator $\hat{Q}$.

We start with a system containing L spin-orbitals, and we define the non-interacting many-body density matrix as

$$\hat{\rho}\left(v\right)=\exp\left(\sum_{ij}v_{ij}\hat{a}_{i}^{\dagger}\hat{a}_{j}\right)=\exp\left(\sum_{\Gamma}v_{\Gamma}\hat{O}_{\Gamma}\right), \tag{3.60}$$

where $\Gamma=(i,j)$ denotes the index, $\hat{O}_{(i,j)}=\hat{a}_{i}^{\dagger}\hat{a}_{j}$, and v_{ij} is a real matrix but not necessarily symmetric. Notice from the anti-commutation relation $\left\{\hat{a}_{i}^{\dagger},\hat{a}_{j}\right\}=\delta_{ij}$,

$$\left[\hat{O}_{(i,j)},\hat{O}_{(k,l)}\right]=\hat{a}_{i}^{\dagger}\hat{a}_{j}\hat{a}_{k}^{\dagger}\hat{a}_{l}-\hat{a}_{k}^{\dagger}\hat{a}_{l}\hat{a}_{i}^{\dagger}\hat{a}_{j} \tag{3.61}$$

$$=\hat{a}_{i}^{\dagger}\hat{a}_{j}\hat{a}_{k}^{\dagger}\hat{a}_{l}-\hat{a}_{k}^{\dagger}\left(\delta_{il}-\hat{a}_{i}^{\dagger}\hat{a}_{l}\right)\hat{a}_{j}=\hat{a}_{i}^{\dagger}\hat{a}_{j}\hat{a}_{k}^{\dagger}\hat{a}_{l}-\delta_{il}\hat{a}_{k}^{\dagger}\hat{a}_{j}+\hat{a}_{i}^{\dagger}\hat{a}_{k}^{\dagger}\hat{a}_{j}\hat{a}_{l} \tag{3.62}$$

$$=-\delta_{il}\hat{a}_{k}^{\dagger}\hat{a}_{j}+\hat{a}_{i}^{\dagger}\left(\delta_{kj}-\hat{a}_{j}\hat{a}_{k}^{\dagger}\right)\hat{a}_{l}+\hat{a}_{i}^{\dagger}\hat{a}_{j}\hat{a}_{k}^{\dagger}\hat{a}_{l}=\hat{a}_{i}^{\dagger}\hat{a}_{l}\delta_{kj}-\hat{a}_{k}^{\dagger}\hat{a}_{j}\delta_{il} \tag{3.63}$$

$$=\hat{O}_{(i,l)}\delta_{kj}-\hat{O}_{(k,j)}\delta_{il}. \tag{3.64}$$

Therefore, $\hat{O}_{\Gamma}$ forms a Lie algebra and $\hat{\rho}\left(v\right)$ forms a Lie group. Notice that it is impractical to directly compute the non-interacting density in the Fock space for a large system, and therefore we need a more efficient approach, which can be achieved by finding an isomorphism of the Lie algebra $\hat{O}_{\Gamma}\rightarrow A_{\Gamma}$. The matrices A_{Γ} are defined as

$$\left[A_{(i,j)}\right]_{ml}=\delta_{im}\delta_{jl}\qquad\leftrightarrow\qquad A_{(i,j)}=\begin{pmatrix}0 & \cdots & \cdots\\ \cdots & 1\,(\text{ith row, jth column}) & \cdots\\ \cdots & \cdots & \cdots\end{pmatrix} \tag{3.65}$$

and the dimension of these matrices is $L \times L$. The commutation relations are given as

$$\left[A_{(i,j)}, A_{(k,l)}\right] = A_{(i,j)}A_{(k,l)} - A_{(k,l)}A_{(i,j)} = A_{(i,l)}\delta_{k,j} - A_{(k,j)}\delta_{il}, \tag{3.66}$$

which has the same algebraic relation as $\hat{O}_{(i,j)}$, proving the isomorphism. So we have the map

$$\hat{\rho}\left(\boldsymbol{v}\right) = \exp\left(\sum_{\Gamma} v_{\Gamma}\hat{O}_{\Gamma}\right) \leftrightarrow \exp\left(\sum_{\Gamma} v_{\Gamma}A_{\Gamma}\right) = \exp\left(\boldsymbol{v}\right). \tag{3.67}$$

The single-particle density matrix is defined as

$$\boldsymbol{g}\left(\boldsymbol{v}\right) = \frac{\mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{\boldsymbol{n}}\right)}{\mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\right)} = \frac{1}{\mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\right)}\begin{pmatrix} \mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{a}_1^{\dagger}\hat{a}_1\right) & \mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{a}_1^{\dagger}\hat{a}_2\right) & .. & \mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{a}_1^{\dagger}\hat{a}_L\right) \\ \mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{a}_2^{\dagger}\hat{a}_1\right) & ... & .. & ... \\ .. & .. & .. & .. \\ \mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{a}_L^{\dagger}\hat{a}_1\right) & ... & .. & \mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\hat{a}_L^{\dagger}\hat{a}_L\right) \end{pmatrix} \tag{3.68}$$

$$= \left(\frac{\mathbf{1}}{\mathbf{1} + \exp\left(-\boldsymbol{v}\right)}\right)^{T}. \tag{3.69}$$

The above equation can be derived as following, using

$$\mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\right) = \det\left(\mathbf{1} + \exp\left(\boldsymbol{v}\right)\right), \tag{3.70}$$

$$\boldsymbol{g}\left(\boldsymbol{v}\right) = \frac{\partial \ln\left(\mathrm{Tr}\left(\hat{\rho}\left(\boldsymbol{v}\right)\right)\right)}{\partial \boldsymbol{v}} = \frac{\partial \ln\left(\det\left(\mathbf{1} + \exp\left(\boldsymbol{v}\right)\right)\right)}{\partial \boldsymbol{v}} = \frac{\partial \mathrm{Tr}\left(\ln\left(\mathbf{1} + \exp\left(\boldsymbol{v}\right)\right)\right)}{\partial \boldsymbol{v}} \tag{3.71}$$

$$= \left(\exp\left(\boldsymbol{v}\right)\frac{\mathbf{1}}{\mathbf{1} + \exp\left(\boldsymbol{v}\right)}\right)^{T} = \left(\frac{\mathbf{1}}{\mathbf{1} + \exp\left(-\boldsymbol{v}\right)}\right)^{T}. \tag{3.72}$$

Notice that we use the name $\boldsymbol{g}$ to refer to the single-particle density matrix. We choose this convention given that the single-particle density matrix of the compound space will be the discrete Green's function in the original space.

Now we consider group multiplication in terms of $\boldsymbol{g}$. We being by parametrizing the group element in terms of $\boldsymbol{g}$ as

$$\exp(\boldsymbol{v}) = \left(\frac{\mathbf{1}}{\boldsymbol{g}(\boldsymbol{v})^{-1} - \mathbf{1}}\right)^{T}. \tag{3.73}$$

Recall the group multiplication

$$\exp(\boldsymbol{v}) = \exp(\boldsymbol{v}_1)\exp(\boldsymbol{v}_2). \tag{3.74}$$

In terms of $\boldsymbol{g}$, this becomes

$$\left(\boldsymbol{g}^{-1} - \mathbf{1}\right) = \left(\boldsymbol{g}_1^{-1} - \mathbf{1}\right)\left(\boldsymbol{g}_2^{-1} - \mathbf{1}\right), \tag{3.75}$$

$$\boldsymbol{g}^{-1} = \boldsymbol{g}_1^{-1}\boldsymbol{g}_2^{-1} - \boldsymbol{g}_2^{-1} - \boldsymbol{g}_1^{-1} + 2, \tag{3.76}$$

$$\boldsymbol{g} = \boldsymbol{g}_2\left(\mathbf{1} - \boldsymbol{g}_1 - \boldsymbol{g}_2 + 2\boldsymbol{g}_1\boldsymbol{g}_2\right)^{-1}\boldsymbol{g}_1 = \boldsymbol{g}_1 \star \boldsymbol{g}_2. \tag{3.77}$$

Note that we have introduced the symbol $\star$ to denote group multiplication for the single particle density matrix, and we see that it is relatively complex.

Now, we discuss how to find $\hat{Q}$ using the group theory. We will need to consider the

single-particle operators in the compound space

$$\hat{\boldsymbol{N}} = \begin{pmatrix} \hat{c}_1^{\dagger(1)}\hat{c}_1^{(1)} & \dots & \hat{c}_1^{\dagger(1)}\hat{c}_L^{(1)} & \dots & \dots & \dots & \dots & \hat{c}_1^{\dagger(1)}\hat{c}_1^{(\mathcal{N})} & \dots & \hat{c}_1^{\dagger(1)}\hat{c}_L^{(\mathcal{N})} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \hat{c}_L^{\dagger(1)}\hat{c}_1^{(1)} & \dots & \hat{c}_L^{\dagger(1)}\hat{c}_L^{(1)} & \dots & \dots & \dots & \dots & \hat{c}_L^{\dagger(1)}\hat{c}_1^{(\mathcal{N})} & \dots & \hat{c}_L^{\dagger(1)}\hat{c}_L^{(\mathcal{N})} \\ \dots & \dots & \dots & \hat{c}_1^{\dagger(2)}\hat{c}_1^{(2)} & \dots & \hat{c}_1^{\dagger(2)}\hat{c}_L^{(2)} & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \hat{c}_L^{\dagger(2)}\hat{c}_1^{(2)} & \dots & \hat{c}_L^{\dagger(2)}\hat{c}_L^{(2)} & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \hat{c}_1^{\dagger(\mathcal{N})}\hat{c}_1^{(1)} & \dots & \hat{c}_1^{\dagger(\mathcal{N})}\hat{c}_L^{(1)} & \dots & \dots & \dots & \dots & \hat{c}_1^{\dagger(\mathcal{N})}\hat{c}_1^{(\mathcal{N})} & \dots & \hat{c}_1^{\dagger(\mathcal{N})}\hat{c}_L^{(\mathcal{N})} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \hat{c}_L^{\dagger(\mathcal{N})}\hat{c}_1^{(1)} & \dots & \hat{c}_L^{\dagger(\mathcal{N})}\hat{c}_L^{(1)} & \dots & \dots & \dots & \dots & \hat{c}_L^{\dagger(\mathcal{N})}\hat{c}_1^{(\mathcal{N})} & \dots & \hat{c}_L^{\dagger(\mathcal{N})}\hat{c}_L^{(\mathcal{N})} \end{pmatrix} \tag{3.78}$$

Notice that the representation of $\hat{Q}$ in the compound space is completely determined from the manner in which we combine the $\mathcal{N}$ copies of the original system into the compound system. Therefore, we can straightforwardly determine $\hat{Q}$ by studying $\hat{\rho}_{eff}$ in the special case of an SPD with $\hat{\mathcal{P}}_i = \hat{1}$, then we have

$$\frac{\mathrm{Tr}\left(\hat{\rho}_{eff}\hat{\boldsymbol{N}}\right)}{\mathrm{Tr}(\hat{\rho}_{eff})} = \frac{\mathrm{Tr}\left(\hat{Q}\hat{\boldsymbol{N}}\right)}{\mathrm{Tr}(\hat{Q})} = \boldsymbol{g}_Q, \tag{3.79}$$

where $\boldsymbol{g}_Q$ is the single-particle density matrix of the compound system when $\hat{\rho}_{eff} = \hat{Q}$. Recall the relation for a correlator in the original space in terms of the compound space

$$\left\langle \hat{O}_1; \hat{O}_2; ..; \hat{O}_{\mathcal{N}} \right\rangle_{\mathcal{A}} = \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{O}_1^{(1)}\hat{O}_2^{(2)}...\hat{O}_{\mathcal{N}}^{(\mathcal{N})}\right).$$

Given that any correlator within the noninteracting SPD (see Eq. 3.3) can be evaluated using Wick's theorem, this indicates that the corresponding $\hat{\rho}_{eff}$ must also be a noninteracting density matrix in the compound space. Then we have

$$\hat{Q} = \hat{\rho}\left(\boldsymbol{v}_Q\right), \qquad\qquad \boldsymbol{v}_Q = -\log\left(\boldsymbol{g}_Q^{-1} - \mathbf{1}\right)^T. \tag{3.80}$$

Given that $\hat{Q}$ is independent of the SPD, the specific determination of $\hat{Q}$ applies in general.

Before computing $\hat{Q}$ for particular cases, we first define our conventions for the discrete Green's function. Now, consider a system of L spin-orbitals and $\mathcal{N}$ time steps. The discrete Green's function will have dimension $L\mathcal{N} \times L\mathcal{N}$. There are two obvious way to group these entries. First, we can use the time index to build a sub-block, and use the orbital index to specify the entries within a sub-block. We refer to this as the time index major form. In the time index major form, we have

$$\boldsymbol{g} = \begin{pmatrix} \boldsymbol{g}^{(11)} & .. & \\ .. & .. & \\ & & \boldsymbol{g}^{(\mathcal{N}\mathcal{N})} \end{pmatrix} \tag{3.81}$$

where

$$\boldsymbol{g}^{(\tau_1\tau_2)} = \begin{pmatrix} \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{a}_1^{\dagger(\tau_1)}\hat{a}_1^{(\tau_2)}\right) & \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{a}_1^{\dagger(\tau_1)}\hat{a}_2^{(\tau_2)}\right) & \\ ... & ... & \\ & & \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{a}_L^{\dagger(\tau_1)}\hat{a}_L^{(\tau_2)}\right) \end{pmatrix} \tag{3.82}$$

For $\hat{\rho}_{eff} = \hat{Q}$, we have

$$\boldsymbol{g}^{(\tau_1\tau_2)} = \frac{1}{2}\mathrm{sign}(\tau_2 - \tau_1)\mathbf{1}, \qquad \mathrm{sign}(x) = \begin{cases} 1 & x \geq 0 \\ -1 & x < 0 \end{cases} \tag{3.83}$$

Alternatively, we can use the orbital index to build the sub-block, and use the time index to specify the entries within a sub-block. We refer to this as the orbital index major form. In the orbital index major form, we have

$$\boldsymbol{g} = \begin{pmatrix} \boldsymbol{g}_{11} & .. & \\ .. & .. & \\ & & \boldsymbol{g}_{LL} \end{pmatrix} \tag{3.84}$$

where

$$\boldsymbol{g}_{i_1 i_2} = \begin{pmatrix} \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{a}_{i_1}^{\dagger(1)}\hat{a}_{i_2}^{(1)}\right) & \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{a}_{i_1}^{\dagger(1)}\hat{a}_{i_2}^{(2)}\right) & \\ ... & ... & \\ & & \mathrm{Tr}\left(\hat{\rho}_{eff}\hat{a}_{i_1}^{\dagger(\mathcal{N})}\hat{a}_{i_2}^{(\mathcal{N})}\right) \end{pmatrix} \tag{3.85}$$

For $\hat{\rho}_{eff} = \hat{Q}$, we have

$$\boldsymbol{g}_{i_1 i_2} = \delta_{i_1 i_2} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \\ -\frac{1}{2} & \frac{1}{2} & \\ -\frac{1}{2} & -\frac{1}{2} & ... \end{pmatrix} \tag{3.86}$$

For this special case of $\hat{\mathcal{P}}_i = \hat{1}$, the different orbitals have no coupling between each other, and as a result we have

$$\hat{Q} = \otimes_{i=1}^{L} \hat{Q}_i, \tag{3.87}$$

where $\hat{Q}_i$ is the shift matrix for orbital i. Thus, we only need to study a single degree of freedom for $\mathcal{N}$ times steps and then we can construct the $\hat{Q}$ for any system. In the following, we will give some examples to show the procedure. Recall the basic formulas,

$$\hat{Q} = \hat{\rho}\left(\boldsymbol{v}_Q\right), \qquad\qquad \boldsymbol{v}_Q = -\log\left(\boldsymbol{g}_Q^{-1} - \mathbf{1}\right)^T. \tag{3.88}$$

For a single degree of freedom and $\mathcal{N} = 2$, we have

$$\boldsymbol{g}_Q = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}, \qquad\qquad \boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{\pi}{2} \\ \frac{\pi}{2} & 0 \end{pmatrix}. \tag{3.89}$$

Using the occupation number representation of $|n_L ... n_1\rangle = \left(\hat{a}_L^\dagger\right)^{n_1} ... \left(\hat{a}_1^\dagger\right)^{n_1} |00..0\rangle$, we can

choose a basis ordered as

$$|00\rangle, \qquad |01\rangle, \qquad |10\rangle, \qquad |11\rangle, \tag{3.90}$$

where this ordering follows the convention of increasing binary values. Finally, $\hat{Q}$ can be represented in this basis as

$$\hat{Q} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.91}$$

For a single degree of freedom and $\mathcal{N} = 3$, we have

$$\boldsymbol{g}_Q = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \qquad \boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{2\pi}{3\sqrt{3}} & -\frac{2\pi}{3\sqrt{3}} \\ \frac{2\pi}{3\sqrt{3}} & 0 & -\frac{2\pi}{3\sqrt{3}} \\ \frac{2\pi}{3\sqrt{3}} & \frac{2\pi}{3\sqrt{3}} & 0 \end{pmatrix} \tag{3.92}$$

and $\hat{Q}$ is given as

$$\hat{Q} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.93}$$

For a single degree of freedom and $\mathcal{N} = 4$, we have

$$\boldsymbol{g}_Q = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \qquad \boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{\pi}{2\sqrt{2}} & -\frac{\pi}{4} & -\frac{\pi}{2\sqrt{2}} \\ \frac{\pi}{2\sqrt{2}} & 0 & -\frac{\pi}{2\sqrt{2}} & -\frac{\pi}{4} \\ \frac{\pi}{4} & \frac{\pi}{2\sqrt{2}} & 0 & -\frac{\pi}{2\sqrt{2}} \\ \frac{\pi}{2\sqrt{2}} & \frac{\pi}{4} & \frac{\pi}{2\sqrt{2}} & 0 \end{pmatrix} \tag{3.94}$$

and

$$\hat{Q} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.95}$$

For a single degree of freedom and $\mathcal{N} = 5$, we have

$$\boldsymbol{g}_Q = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{3.96}$$

$$\boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & -\frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & -\frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & -\frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi \\ \frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & 0 & -\frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & -\frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & -\frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi \\ \frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & \frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & 0 & -\frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & -\frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi \\ \frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & \frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & \frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & 0 & -\frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi \\ \frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & \frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & \frac{1}{5}\sqrt{2-\frac{2}{\sqrt{5}}}\pi & \frac{1}{5}\sqrt{2+\frac{2}{\sqrt{5}}}\pi & 0 \end{pmatrix} \tag{3.97}$$

and we do not show $\hat{Q}$ due to the large dimension. The above examples should serve to illustrate the intrinsic correlations of the compound space due to the time structure of the original system.

3.4 Computing the Green's function for a non-interacting SPD

In this section, we will illustrate the general way to compute the Green's function for a non-interacting SPD (Eq. 2.26). We first consider how to compute the Green's function for a single fermionic degree of freedom for various $\mathcal{N}$ using two different approaches: using the discrete action of the original space and the effective density matrix of the compound space. Consider the non-interacting SPD for a single fermionic degree of freedom with $\mathcal{N} = 2$, where $\hat{\rho} = \exp(\gamma_1 \hat{n}) \exp(\gamma_2 \hat{n})$. We first consider the discrete action in the original space, where the time correlator is given as

$$\left\langle \hat{O}_1; \hat{O}_2 \right\rangle = \frac{\mathrm{Tr}\left(\exp(\gamma_1 \hat{n})\, \hat{O}_1 \exp(\gamma_2 \hat{n})\, \hat{O}_2\right)}{\mathrm{Tr}\left(\exp(\gamma_1 \hat{n}) \exp(\gamma_2 \hat{n})\right)} \tag{3.98}$$

and the Green's function can be evaluated as

$$\boldsymbol{g}(\gamma_i) = \begin{pmatrix} \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2)} & \frac{\exp(\gamma_1)}{1+\exp(\gamma_1+\gamma_2)} \\ -\frac{\exp(\gamma_2)}{1+\exp(\gamma_1+\gamma_2)} & \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2)} \end{pmatrix}. \tag{3.99}$$

We can see that the parameter γ will influence $\boldsymbol{g}$ in a non-linear manner.

Now, we consider how to evaluate the discrete Green's function in the compound space. The shift matrix for $\mathcal{N} = 2$ is

$$\boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{\pi}{2} \\ \frac{\pi}{2} & 0 \end{pmatrix}, \qquad \hat{Q} = \hat{\rho}(\boldsymbol{v}_Q), \tag{3.100}$$

and

$$\hat{\rho}_{eff} = \hat{Q}\hat{\mathcal{P}}_1^{(1)}\hat{\mathcal{P}}_2^{(2)} = \hat{Q} \exp\left(\sum_{i=1}^{2} \gamma_i a^{\dagger(i)} a^{(i)}\right) = \hat{\rho}(\boldsymbol{v}_Q)\, \hat{\rho}(\boldsymbol{\gamma}) = \hat{\rho}(\boldsymbol{v}), \tag{3.101}$$

where

$$\boldsymbol{\gamma} = \begin{pmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{pmatrix}, \qquad \boldsymbol{v} = \log\left(\exp\left(\boldsymbol{v}_Q\right)\exp\left(\boldsymbol{\gamma}\right)\right) = \begin{pmatrix} \frac{\gamma_1+\gamma_2}{2} & -\frac{1}{2}\pi e^{\frac{\gamma_2-\gamma_1}{2}} \\ \frac{1}{2}\pi e^{\frac{\gamma_1-\gamma_2}{2}} & \frac{\gamma_1+\gamma_2}{2} \end{pmatrix}. \tag{3.102}$$

The Green function can then be computed in the compound space as

$$\boldsymbol{g}\left(\gamma_i\right) = \left(\frac{\mathbf{1}}{\mathbf{1}+\exp\left(-\boldsymbol{v}\right)}\right)^T = \begin{pmatrix} 1-\frac{1}{e^{\gamma_1+\gamma_2}+1} & \frac{1}{e^{-\gamma_1}+e^{\gamma_2}} \\ -\frac{e^{\gamma_2}}{e^{\gamma_1+\gamma_2}+1} & 1-\frac{1}{e^{\gamma_1+\gamma_2}+1} \end{pmatrix} \tag{3.103}$$

$$= \begin{pmatrix} \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2)} & \frac{\exp(\gamma_1)}{1+\exp(\gamma_1+\gamma_2)} \\ -\frac{\exp(\gamma_2)}{1+\exp(\gamma_1+\gamma_2)} & \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2)} \end{pmatrix}. \tag{3.104}$$

We see the two approaches yield the same result, as they must.

Now, we repeat the same analysis for $\mathcal{N}=3$. In the original system, we have

$$\left\langle \hat{O}_1; \hat{O}_2; \hat{O}_3 \right\rangle = \frac{\mathrm{Tr}\left(\exp\left(\gamma_1\hat{n}\right)\hat{O}_1\exp\left(\gamma_2\hat{n}\right)\hat{O}_2\exp\left(\gamma_3\hat{n}\right)\hat{O}_3\right)}{\mathrm{Tr}\left(\exp\left(\gamma_1\hat{n}\right)\exp\left(\gamma_2\hat{n}\right)\exp\left(\gamma_3\hat{n}\right)\right)}. \tag{3.105}$$

Thus, we can evaluate the Green's function as

$$\boldsymbol{g}\left(\{\gamma_i\}\right) = \begin{pmatrix} \frac{\exp(\gamma_1+\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} \\ -\frac{\exp(\gamma_2)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} \\ -\frac{\exp(\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & -\frac{\exp(\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} \end{pmatrix}. \tag{3.106}$$

Similarly, in the compound space, we have

$$\boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{2\pi}{3\sqrt{3}} & -\frac{2\pi}{3\sqrt{3}} \\ \frac{2\pi}{3\sqrt{3}} & 0 & -\frac{2\pi}{3\sqrt{3}} \\ \frac{2\pi}{3\sqrt{3}} & \frac{2\pi}{3\sqrt{3}} & 0 \end{pmatrix}, \qquad \boldsymbol{\gamma} = \begin{pmatrix} \gamma_1 & 0 & 0 \\ 0 & \gamma_2 & 0 \\ 0 & 0 & \gamma_3 \end{pmatrix}, \tag{3.107}$$

and

$$\boldsymbol{v} = \log\left(\exp\left(\boldsymbol{v}_Q\right)\exp\left(\boldsymbol{\gamma}\right)\right) = \begin{pmatrix} \frac{1}{3}(\gamma_1+\gamma_2+\gamma_3) & -\frac{2\pi e^{\frac{1}{3}(-\gamma_1+2\gamma_2-\gamma_3)}}{3\sqrt{3}} & -\frac{2\pi e^{\frac{1}{3}(-2\gamma_1+\gamma_2+\gamma_3)}}{3\sqrt{3}} \\ \frac{2\pi e^{\frac{1}{3}(\gamma_1-2\gamma_2+\gamma_3)}}{3\sqrt{3}} & \frac{1}{3}(\gamma_1+\gamma_2+\gamma_3) & -\frac{2\pi e^{\frac{1}{3}(-\gamma_1-\gamma_2+2\gamma_3)}}{3\sqrt{3}} \\ \frac{2\pi e^{\frac{1}{3}(2\gamma_1-\gamma_2-\gamma_3)}}{3\sqrt{3}} & \frac{2\pi e^{\frac{1}{3}(\gamma_1+\gamma_2-2\gamma_3)}}{3\sqrt{3}} & \frac{1}{3}(\gamma_1+\gamma_2+\gamma_3) \end{pmatrix} \tag{3.108}$$

and

$$\boldsymbol{g}\left(\{\gamma_i\}\right) = \left(\frac{\mathbf{1}}{\mathbf{1}+\exp\left(-\boldsymbol{v}\right)}\right)^T \tag{3.109}$$

$$= \begin{pmatrix} 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3}+1} & \frac{e^{\gamma_1+\gamma_3}}{e^{\gamma_1+\gamma_2+\gamma_3}+1} & \frac{e^{\gamma_1}}{e^{\gamma_1+\gamma_2+\gamma_3}+1} \\ -\frac{e^{\gamma_2}}{e^{\gamma_1+\gamma_2+\gamma_3}+1} & 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3}+1} & \frac{e^{\gamma_1+\gamma_2}}{e^{\gamma_1+\gamma_2+\gamma_3}+1} \\ -\frac{e^{\gamma_2+\gamma_3}}{e^{\gamma_1+\gamma_2+\gamma_3}+1} & -\frac{e^{\gamma_3}}{e^{\gamma_1+\gamma_2+\gamma_3}+1} & 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3}+1} \end{pmatrix} \tag{3.110}$$

$$= \begin{pmatrix} \frac{\exp(\gamma_1+\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} \\ -\frac{\exp(\gamma_2)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} \\ -\frac{\exp(\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & -\frac{\exp(\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3)} \end{pmatrix}. \tag{3.111}$$

Now, we repeat the same analysis for $\mathcal{N}=4$. In the original system, we have

$$\left\langle \hat{O}_1;\hat{O}_2;\hat{O}_3;\hat{O}_4 \right\rangle = \frac{\mathrm{Tr}\left(\exp\left(\gamma_1\hat{n}\right)\hat{O}_1\exp\left(\gamma_2\hat{n}\right)\hat{O}_2\exp\left(\gamma_3\hat{n}\right)\hat{O}_3\exp\left(\gamma_4\hat{n}\right)\hat{O}_4\right)}{\mathrm{Tr}\left(\exp\left(\gamma_1\hat{n}\right)\exp\left(\gamma_2\hat{n}\right)\exp\left(\gamma_3\hat{n}\right)\exp\left(\gamma_4\hat{n}\right)\right)} \tag{3.112}$$

and the Green function is

$$\boldsymbol{g}\left(\gamma_i\right) = \begin{pmatrix} \frac{\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} \\ -\frac{\exp(\gamma_2)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_2)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} \\ -\frac{\exp(\gamma_2+\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & -\frac{\exp(\gamma_3)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} \\ -\frac{\exp(\gamma_2+\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & -\frac{\exp(\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & -\frac{\exp(\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} & \frac{\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)}{1+\exp(\gamma_1+\gamma_2+\gamma_3+\gamma_4)} \end{pmatrix} \tag{3.113}$$

In the compound system, we have

$$\boldsymbol{v}_Q = \begin{pmatrix} 0 & -\frac{\pi}{2\sqrt{2}} & -\frac{\pi}{4} & -\frac{\pi}{2\sqrt{2}} \\ \frac{\pi}{2\sqrt{2}} & 0 & -\frac{\pi}{2\sqrt{2}} & -\frac{\pi}{4} \\ \frac{\pi}{4} & \frac{\pi}{2\sqrt{2}} & 0 & -\frac{\pi}{2\sqrt{2}} \\ \frac{\pi}{2\sqrt{2}} & \frac{\pi}{4} & \frac{\pi}{2\sqrt{2}} & 0 \end{pmatrix}, \qquad \boldsymbol{\gamma} = \begin{pmatrix} \gamma_1 & 0 & 0 & 0 \\ 0 & \gamma_2 & 0 & 0 \\ 0 & 0 & \gamma_3 & 0 \\ 0 & 0 & 0 & \gamma_4 \end{pmatrix}, \tag{3.114}$$

and

$$\boldsymbol{v} = \begin{pmatrix} \frac{1}{4}(\gamma_1+\gamma_2+\gamma_3+\gamma_4) & -\frac{\pi e^{\frac{1}{4}(-\gamma_1+3\gamma_2-\gamma_3-\gamma_4)}}{2\sqrt{2}} & -\frac{1}{4}\pi e^{\frac{1}{2}(-\gamma_1+\gamma_2+\gamma_3-\gamma_4)} & -\frac{\pi e^{\frac{1}{4}(-3\gamma_1+\gamma_2+\gamma_3+\gamma_4)}}{2\sqrt{2}} \\ \frac{\pi e^{\frac{1}{4}(\gamma_1-3\gamma_2+\gamma_3+\gamma_4)}}{2\sqrt{2}} & \frac{1}{4}(\gamma_1+\gamma_2+\gamma_3+\gamma_4) & -\frac{\pi e^{\frac{1}{4}(-\gamma_1-\gamma_2+3\gamma_3-\gamma_4)}}{2\sqrt{2}} & -\frac{1}{4}\pi e^{\frac{1}{2}(-\gamma_1-\gamma_2+\gamma_3+\gamma_4)} \\ \frac{1}{4}\pi e^{\frac{1}{2}(\gamma_1-\gamma_2-\gamma_3+\gamma_4)} & \frac{\pi e^{\frac{1}{4}(\gamma_1+\gamma_2-3\gamma_3+\gamma_4)}}{2\sqrt{2}} & \frac{1}{4}(\gamma_1+\gamma_2+\gamma_3+\gamma_4) & -\frac{\pi e^{\frac{1}{4}(-\gamma_1-\gamma_2-\gamma_3+3\gamma_4)}}{2\sqrt{2}} \\ \frac{\pi e^{\frac{1}{4}(3\gamma_1-\gamma_2-\gamma_3-\gamma_4)}}{2\sqrt{2}} & \frac{1}{4}\pi e^{\frac{1}{2}(\gamma_1+\gamma_2-\gamma_3-\gamma_4)} & \frac{\pi e^{\frac{1}{4}(\gamma_1+\gamma_2+\gamma_3-3\gamma_4)}}{2\sqrt{2}} & \frac{1}{4}(\gamma_1+\gamma_2+\gamma_3+\gamma_4) \end{pmatrix} \tag{3.115}$$

and

$$\boldsymbol{g}(\gamma_i) = \left(\frac{1}{1+\exp(-v)}\right)^T \tag{3.116}$$

$$= \begin{pmatrix} 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & \frac{e^{\gamma_1+\gamma_3+\gamma_4}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & \frac{e^{\gamma_1+\gamma_4}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & \frac{e^{\gamma_1}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} \\ -\frac{e^{\gamma_2}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & \frac{e^{\gamma_1+\gamma_2+\gamma_4}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & \frac{e^{\gamma_1+\gamma_2}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} \\ -\frac{e^{\gamma_2+\gamma_3}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & -\frac{e^{\gamma_3}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & \frac{e^{\gamma_1+\gamma_2+\gamma_3}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} \\ -\frac{e^{\gamma_2+\gamma_3+\gamma_4}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & -\frac{e^{\gamma_3+\gamma_4}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & -\frac{e^{\gamma_4}}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} & 1-\frac{1}{e^{\gamma_1+\gamma_2+\gamma_3+\gamma_4}+1} \end{pmatrix} \tag{3.117}$$

The preceding exercises should give good insight into how the compound system is used.

There is one drawback for parameterizing the SPD with γ_i: when we consider the ground-state, $\gamma_i \to \pm\infty$, and we can see that the Green's function is well defined though there are some intermediate values which may diverge; and this could pose difficulties for numerical evaluation. One solution is to bound the γ_i with some cutoff Λ, i.e, $|\gamma_i| < \Lambda$. We propose

an alternative solution where we use the single-particle density matrix of $\exp(\boldsymbol{\gamma}_i \cdot \hat{\boldsymbol{n}})$ to parameterize $\boldsymbol{\gamma}_i$, which should be superior, and we first illustrate this for a non-interacting SPD in a system with L spin-orbitals and $\mathcal{N} = 2$ with

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1 \hat{\boldsymbol{n}}\right) \exp\left(\boldsymbol{\gamma}_2 \hat{\boldsymbol{n}}\right), \tag{3.118}$$

where $\boldsymbol{\gamma}_1$ and $\boldsymbol{\gamma}_2$ are arbitrary real $L \times L$ matrices. We then parameterize $\boldsymbol{\gamma}_1$ and $\boldsymbol{\gamma}_2$ using the corresponding density matrices

$$\boldsymbol{n}_1 = \left(\frac{\mathbf{1}}{\mathbf{1} + \exp\left(-\boldsymbol{\gamma}_1\right)}\right)^T, \qquad \boldsymbol{n}_2 = \left(\frac{\mathbf{1}}{\mathbf{1} + \exp\left(-\boldsymbol{\gamma}_2\right)}\right)^T. \tag{3.119}$$

We can then evaluate the Green's function in the compound space, where we use the time index major convention, yielding

$$\boldsymbol{g}_Q = \frac{1}{2}\begin{pmatrix} \mathbf{1} & \mathbf{1} \\ -\mathbf{1} & \mathbf{1} \end{pmatrix}, \tag{3.120}$$

where $\mathbf{1}$ is the $L \times L$ identity matrix. We can then follow the usual procedure to compute $\boldsymbol{g}$

$$\exp\left(\boldsymbol{v}_Q\right) = \left(\frac{\mathbf{1}}{\boldsymbol{g}_Q^{-1} - \mathbf{1}}\right)^T = \begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \tag{3.121}$$

$$\exp\left(\boldsymbol{\gamma}\right) = \begin{pmatrix} \exp\left(\boldsymbol{\gamma}_1\right) & \\ & \exp\left(\boldsymbol{\gamma}_2\right) \end{pmatrix} = \begin{pmatrix} \left(\frac{\mathbf{1}}{\boldsymbol{n}_1^{-1} - \mathbf{1}}\right)^T & \\ & \left(\frac{\mathbf{1}}{\boldsymbol{n}_2^{-1} - \mathbf{1}}\right)^T \end{pmatrix}, \tag{3.122}$$

$$\exp\left(\boldsymbol{v}\right) = \exp\left(\boldsymbol{v}_Q\right) \exp\left(\boldsymbol{\gamma}\right) = \begin{pmatrix} & -\left(\frac{\mathbf{1}}{\boldsymbol{n}_2^{-1} - \mathbf{1}}\right)^T \\ \left(\frac{\mathbf{1}}{\boldsymbol{n}_1^{-1} - \mathbf{1}}\right)^T & \end{pmatrix}, \tag{3.123}$$

$$\exp(-\boldsymbol{v}) = \begin{pmatrix} & \left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right)^T \\ -\left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right)^T & \end{pmatrix}, \tag{3.124}$$

$$\boldsymbol{g}^{-1} = (\mathbf{1} + \exp(-\boldsymbol{v}))^T = \begin{pmatrix} \mathbf{1} & -\left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right) \\ \left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right) & \mathbf{1} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \boldsymbol{A}_{12} \\ \boldsymbol{A}_{21} & \mathbf{1} \end{pmatrix}. \tag{3.125}$$

We can then solve for $\boldsymbol{g}$ using the matrix inverse as

$$\begin{pmatrix} \mathbf{1} & \boldsymbol{A}_{12} \\ \boldsymbol{A}_{21} & \mathbf{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{g}_{11} & \boldsymbol{g}_{12} \\ \boldsymbol{g}_{21} & \boldsymbol{g}_{22} \end{pmatrix} = \mathbf{1}. \tag{3.126}$$

So we have

$$\boldsymbol{g}_{11} + \boldsymbol{A}_{12}\boldsymbol{g}_{21} = \mathbf{1}, \tag{3.127}$$

$$\boldsymbol{g}_{12} + \boldsymbol{A}_{12}\boldsymbol{g}_{22} = \mathbf{0}, \tag{3.128}$$

$$\boldsymbol{A}_{21}\boldsymbol{g}_{11} + \boldsymbol{g}_{21} = \mathbf{0}, \tag{3.129}$$

$$\boldsymbol{A}_{21}\boldsymbol{g}_{12} + \boldsymbol{g}_{22} = \mathbf{1}, \tag{3.130}$$

which yields the first two shift relations

$$\boldsymbol{g}_{21} = -\boldsymbol{A}_{21}\boldsymbol{g}_{11}, \tag{3.131}$$

$$\boldsymbol{g}_{12} = -\boldsymbol{A}_{12}\boldsymbol{g}_{22}, \tag{3.132}$$

and we can solve

$$\boldsymbol{g}_{11} = \left(\mathbf{1} - \boldsymbol{A}_{12}\boldsymbol{A}_{21}\right)^{-1}, \tag{3.133}$$

$$\boldsymbol{g}_{22} = \left(\mathbf{1} - \boldsymbol{A}_{21}\boldsymbol{A}_{21}\right)^{-1}. \tag{3.134}$$

Plugging in the expression for $\boldsymbol{A}_{ij}$, we have

$$\boldsymbol{g}_{11} = \left(\mathbf{1} + \left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right)\left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right)\right)^{-1}. \tag{3.135}$$

Notice that

$$\mathbf{1} + \left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right)\left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right) = \boldsymbol{n}_2^{-1}\boldsymbol{n}_1^{-1} - \boldsymbol{n}_1^{-1} - \boldsymbol{n}_2^{-1} + 2\mathbf{1} \tag{3.136}$$

$$= \boldsymbol{n}_2^{-1}\left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)\boldsymbol{n}_1^{-1}, \tag{3.137}$$

which results in

$$\boldsymbol{g}_{11} = \boldsymbol{n}_1\left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1}\boldsymbol{n}_2. \tag{3.138}$$

Recalling the group multiplication rules for $\boldsymbol{g}$ (see Eq. 3.77), we can rewrite $\boldsymbol{g}_{11}$ as

$$\boldsymbol{g}_{11} = \boldsymbol{n}_2 \star \boldsymbol{n}_1. \tag{3.139}$$

Similarly, we find

$$\boldsymbol{g}_{22} = \boldsymbol{n}_2\left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1}\boldsymbol{n}_1 = \boldsymbol{n}_1 \star \boldsymbol{n}_2. \tag{3.140}$$

Considering the off-diagonal terms, we have

$$\boldsymbol{g}_{12} = \left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right) \boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \tag{3.141}$$

$$= \left(\mathbf{1} - \boldsymbol{n}_2\right) \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \tag{3.142}$$

$$\left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right) \boldsymbol{n}_1 \star \boldsymbol{n}_2 \tag{3.143}$$

and

$$\boldsymbol{g}_{21} = -\left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right) \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 \tag{3.144}$$

$$= -\left(\mathbf{1} - \boldsymbol{n}_1\right) \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 \tag{3.145}$$

$$= -\left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right) \boldsymbol{n}_2 \star \boldsymbol{n}_1. \tag{3.146}$$

In summary, we have the following expression for $\boldsymbol{g}$ using the group multiplication operations

$$\boldsymbol{g} = \begin{pmatrix} \boldsymbol{n}_2 \star \boldsymbol{n}_1 & \left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right) \boldsymbol{n}_1 \star \boldsymbol{n}_2 \\ -\left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right) \boldsymbol{n}_2 \star \boldsymbol{n}_1 & \boldsymbol{n}_1 \star \boldsymbol{n}_2 \end{pmatrix}. \tag{3.147}$$

However, the above expression will be numerically difficult to work with given that it contains the inversion of individual $\boldsymbol{n}_i$. A numerically stable expression to compute $\boldsymbol{g}$ can be obtained as

$$\boldsymbol{g} = \begin{pmatrix} \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 & \left(\mathbf{1} - \boldsymbol{n}_2\right) \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \\ -\left(\mathbf{1} - \boldsymbol{n}_1\right) \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 & \boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \end{pmatrix}. \tag{3.148}$$

We can also derive an alternative form which is numerically stable, which is obtained using the alternative definition for the matrix inverse as

$$\begin{pmatrix} \boldsymbol{g}_{11} & \boldsymbol{g}_{12} \\ \boldsymbol{g}_{21} & \boldsymbol{g}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{1} & \boldsymbol{A}_{12} \\ \boldsymbol{A}_{21} & \mathbf{1} \end{pmatrix} = \mathbf{1}. \tag{3.149}$$

Following the same logic, we have

$$\boldsymbol{g}_{11} + \boldsymbol{g}_{12}\boldsymbol{A}_{21} = \mathbf{1}, \tag{3.150}$$

$$\boldsymbol{g}_{11}\boldsymbol{A}_{12} + \boldsymbol{g}_{12} = \mathbf{0}, \tag{3.151}$$

$$\boldsymbol{g}_{21} + \boldsymbol{g}_{22}\boldsymbol{A}_{21} = \mathbf{0}, \tag{3.152}$$

$$\boldsymbol{g}_{21}\boldsymbol{A}_{12} + \boldsymbol{g}_{22} = \mathbf{1}, \tag{3.153}$$

and

$$\boldsymbol{g}_{12} = -\boldsymbol{g}_{11}\boldsymbol{A}_{12}, \tag{3.154}$$

$$\boldsymbol{g}_{21} = -\boldsymbol{g}_{22}\boldsymbol{A}_{21}, \tag{3.155}$$

and

$$\boldsymbol{g}_{11} = \left(\mathbf{1} - \boldsymbol{A}_{12}\boldsymbol{A}_{21}\right)^{-1}, \tag{3.156}$$

$$\boldsymbol{g}_{22} = \left(\mathbf{1} - \boldsymbol{A}_{21}\boldsymbol{A}_{12}\right)^{-1}. \tag{3.157}$$

We then have four relations for the off-diagonal components

$$\boldsymbol{g}_{21} = -\boldsymbol{A}_{21}\boldsymbol{g}_{11}, \tag{3.158}$$

$$\boldsymbol{g}_{12} = -\boldsymbol{A}_{12}\boldsymbol{g}_{22}, \tag{3.159}$$

$$\boldsymbol{g}_{12} = -\boldsymbol{g}_{11}\boldsymbol{A}_{12}, \tag{3.160}$$

$$\boldsymbol{g}_{21} = -\boldsymbol{g}_{22}\boldsymbol{A}_{21}, \tag{3.161}$$

resulting in

$$\boldsymbol{g}_{12} = -\boldsymbol{g}_{11}\boldsymbol{A}_{12} = \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 \left(\boldsymbol{n}_2^{-1} - \mathbf{1}\right) \tag{3.162}$$

$$= \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \left(\mathbf{1} - \boldsymbol{n}_2\right), \tag{3.163}$$

$$\boldsymbol{g}_{21} = -\boldsymbol{g}_{22}\boldsymbol{A}_{21} = -\boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \left(\boldsymbol{n}_1^{-1} - \mathbf{1}\right) \tag{3.164}$$

$$= -\boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \left(\mathbf{1} - \boldsymbol{n}_1\right). \tag{3.165}$$

In conclusion, we have two equivalent approaches to compute $\boldsymbol{g}$ which will be numerically stable

$$\boldsymbol{g} = \begin{pmatrix} \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 & \left(\mathbf{1} - \boldsymbol{n}_2\right) \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \\ -\left(\mathbf{1} - \boldsymbol{n}_1\right) \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 & \boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \end{pmatrix} \tag{3.166}$$

$$= \begin{pmatrix} \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \boldsymbol{n}_2 & \boldsymbol{n}_1 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_2\boldsymbol{n}_1\right)^{-1} \left(\mathbf{1} - \boldsymbol{n}_2\right) \\ -\boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \left(\mathbf{1} - \boldsymbol{n}_1\right) & \boldsymbol{n}_2 \left(\mathbf{1} - \boldsymbol{n}_1 - \boldsymbol{n}_2 + 2\boldsymbol{n}_1\boldsymbol{n}_2\right)^{-1} \boldsymbol{n}_1 \end{pmatrix}. \tag{3.167}$$

Now, we can use a similar method to study the general case. For a non-interacting SPD $\hat{\rho} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_{\mathcal{N}}$, with $\hat{\mathcal{P}}_i = \exp\left(\boldsymbol{\gamma}_i \cdot \hat{\boldsymbol{n}}\right)$, we can parameterize it using

$$\boldsymbol{n}_i = \left(\frac{\mathbf{1}}{\mathbf{1} + \exp\left(-\boldsymbol{\gamma}_i\right)}\right)^T. \tag{3.168}$$

Using the group notation, we can abstractly write

$$\boldsymbol{g} = \boldsymbol{g}_Q \star \boldsymbol{g}_\gamma = \boldsymbol{g}_Q \star \begin{pmatrix} \boldsymbol{n}_1 & & & & \\ & \boldsymbol{n}_2 & & & \\ & & \boldsymbol{n}_3 & & \\ & & & .. & \\ & & & & \boldsymbol{n}_N \end{pmatrix} \tag{3.169}$$

Following the previous procedure, we reach the expression for Green's function as

$$\boldsymbol{g}^{-1} = \begin{pmatrix} \mathbf{1} & \boldsymbol{A}_{12} & & \\ & \mathbf{1} & \boldsymbol{A}_{23} & \\ & & & \\ \boldsymbol{A}_{\mathcal{N}1} & & & \mathbf{1} \end{pmatrix} \tag{3.170}$$

with

$$\boldsymbol{A}_{i,i+1} = \theta_i \left(\boldsymbol{n}_{i+1}^{-1} - \mathbf{1} \right), \qquad \theta_i = \begin{cases} -1 & i = 1, .., \mathcal{N} - 1 \\ & \\ 1 & i = \mathcal{N} \end{cases}, \tag{3.171}$$

and $\mathcal{N} + 1 \to 1$ when evaluating $\boldsymbol{A}_{\mathcal{N},\mathcal{N}+1}$.

We continue by considering the first approach for inverting $\boldsymbol{g}$, where

$$\begin{pmatrix} \mathbf{1} & \boldsymbol{A}_{12} & & \\ & \mathbf{1} & \boldsymbol{A}_{23} & \\ & & & \\ \boldsymbol{A}_{\mathcal{N}1} & & & \mathbf{1} \end{pmatrix} \boldsymbol{g} = \mathbf{1}. \tag{3.172}$$

For diagonal part, we have

$$\boldsymbol{g}_{ii} + \boldsymbol{A}_{i,i+1} \boldsymbol{g}_{i+1,i} = \mathbf{1}, \tag{3.173}$$

and for the non-diagonal part ($i \neq j$), we have

$$\boldsymbol{g}_{ij} + \boldsymbol{A}_{i,i+1} \boldsymbol{g}_{i+1,j} = \mathbf{0}, \tag{3.174}$$

resulting in

$$\boldsymbol{g}_{i+1,i} = -\boldsymbol{A}_{i+1,i+2} \boldsymbol{g}_{i+2,i}. \tag{3.175}$$

Thus

$$\boldsymbol{g}_{ii} + (-\mathbf{1})^{N-1} \boldsymbol{A}_{i,i+1}\boldsymbol{A}_{i+1,i+2}..\boldsymbol{A}_{i-1,i}\boldsymbol{g}_{ii} = \mathbf{1}, \tag{3.176}$$

so we have

$$\boldsymbol{g}_{ii} = \left(\mathbf{1} + (-\mathbf{1})^{N-1} \boldsymbol{A}_{i,i+1}\boldsymbol{A}_{i+1,i+2}..\boldsymbol{A}_{i-1,i}\right). \tag{3.177}$$

Similarly, we can invert using the second approach, where

$$\boldsymbol{g}\begin{pmatrix} \mathbf{1} & \boldsymbol{A}_{12} & & \\ & \mathbf{1} & \boldsymbol{A}_{23} & \\ & & & \\ \boldsymbol{A}_{N1} & & & \mathbf{1} \end{pmatrix} = \mathbf{1}. \tag{3.178}$$

So for diagonal part, we have

$$\boldsymbol{g}_{ii} + \boldsymbol{g}_{i,i-1}\boldsymbol{A}_{i-1,i} = \mathbf{1}, \tag{3.179}$$

and for the non-diagonal part, we have

$$\boldsymbol{g}_{ij} + \boldsymbol{g}_{i,j-1}\boldsymbol{A}_{j-1,j} = \mathbf{0}. \tag{3.180}$$

Combining these two approaches, we have two relations for the off-diagonal components $(i \neq j)$

$$\boldsymbol{g}_{ij} + \boldsymbol{A}_{i,i+1}\boldsymbol{g}_{i+1,j} = \mathbf{0}, \qquad \boldsymbol{g}_{ij} + \boldsymbol{g}_{i,j-1}\boldsymbol{A}_{j-1,j} = \mathbf{0}. \tag{3.181}$$

Using the group multiplication, we have

$$\boldsymbol{g}_{ii} = \boldsymbol{n}_{i+1} \star \boldsymbol{n}_{i+2} \star .. \star \boldsymbol{n}_N \star \boldsymbol{n}_1 ... \star \boldsymbol{n}_i. \tag{3.182}$$

Therefore, we have a numerically stable formulation for the diagonal terms in general. While the off-diagonal terms can be determined from Eq. 3.181, there will be numerically instabilities if $\boldsymbol{n}_{ij}$ has 0 or 1 as eigenvalues. The general reliable way is iteratively apply the $\mathcal{N} = 2$ formulas. The trick is to realize that to compute the i and j block, we could reinterpret the SPD $\hat{\rho} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_N$ as

$$\hat{\rho}' = \left(\hat{\mathcal{P}}_{j+1} ... \hat{\mathcal{P}}_{i-1} \hat{\mathcal{P}}_i\right) \left(\hat{\mathcal{P}}_{i+1} .. \hat{\mathcal{P}}_j\right) = \hat{\mathcal{P}}'_1 \hat{\mathcal{P}}'_2. \tag{3.183}$$

So effectively, if we use

$$\boldsymbol{n}'_1 = \boldsymbol{n}_{j+1} .. \star \boldsymbol{n}_{i-1} \star \boldsymbol{n}_i, \tag{3.184}$$

$$\boldsymbol{n}'_2 = \boldsymbol{n}_{i+1} .. \star \boldsymbol{n}_j, \tag{3.185}$$

in the $\mathcal{N} = 2$ formulas, then we could obtain the sub-block of the $\boldsymbol{g}$ for i and j. This method is less efficient than the previous methods using Eq. 3.181, but it is guaranteed to produce reliable result in general.

One can see that in general the expression for $\boldsymbol{g}$ is quite involved as we are assuming $\boldsymbol{\gamma}_i$ to be arbitrary matrices. The situation can be greatly simplified if we assume the $\boldsymbol{\gamma}_i$ are commutative with each other, which will often result in sufficient variational freedom to accurately solve many practical applications. If all $\boldsymbol{\gamma}_i$ commute with each other, then $\boldsymbol{n}_i$ are also commutative with each other, and for $\mathcal{N} = 2$ we have

$$\boldsymbol{g} = \frac{1}{2\boldsymbol{n}_2\boldsymbol{n}_1 - \boldsymbol{n}_1 - \boldsymbol{n}_2 + \mathbf{1}} \begin{pmatrix} \boldsymbol{n}_1\boldsymbol{n}_2 & -\boldsymbol{n}_1(\boldsymbol{n}_2 - \mathbf{1}) \\ (\boldsymbol{n}_1 - \mathbf{1})\boldsymbol{n}_2 & \boldsymbol{n}_1\boldsymbol{n}_2 \end{pmatrix}, \tag{3.186}$$

and for $\mathcal{N}=3$, we have

$$\boldsymbol{g}=\frac{\mathbf{1}}{\boldsymbol{n}_2\boldsymbol{n}_1+\boldsymbol{n}_3\boldsymbol{n}_1-\boldsymbol{n}_1-\boldsymbol{n}_2+\boldsymbol{n}_2\boldsymbol{n}_3-\boldsymbol{n}_3+\mathbf{1}}\times \tag{3.187}$$

$$\begin{pmatrix} \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3 & -\boldsymbol{n}_1\left(\boldsymbol{n}_2-\mathbf{1}\right)\boldsymbol{n}_3 & \boldsymbol{n}_1\left(\boldsymbol{n}_2-\mathbf{1}\right)\left(\boldsymbol{n}_3-\mathbf{1}\right) \\ -\left(\boldsymbol{n}_1-\mathbf{1}\right)\boldsymbol{n}_2\left(\boldsymbol{n}_3-\mathbf{1}\right) & \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3 & -\boldsymbol{n}_1\boldsymbol{n}_2\left(\boldsymbol{n}_3-\mathbf{1}\right) \\ \left(\boldsymbol{n}_1-\mathbf{1}\right)\boldsymbol{n}_2\boldsymbol{n}_3 & -\left(\boldsymbol{n}_1-\mathbf{1}\right)\left(\boldsymbol{n}_2-\mathbf{1}\right)\boldsymbol{n}_3 & \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3 \end{pmatrix}, \tag{3.188}$$

and for $\mathcal{N}=4$, we have

$$\boldsymbol{g}=\frac{\mathbf{1}}{C}\times$$

$$\begin{pmatrix} \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4 & -\boldsymbol{n}_1\left(\boldsymbol{n}_2-\mathbf{1}\right)\boldsymbol{n}_3\boldsymbol{n}_4 & \boldsymbol{n}_1\left(\boldsymbol{n}_2-\mathbf{1}\right)\left(\boldsymbol{n}_3-\mathbf{1}\right)\boldsymbol{n}_4 & \begin{pmatrix}-\boldsymbol{n}_1\left(\boldsymbol{n}_2-\mathbf{1}\right)\times\\ \left(\boldsymbol{n}_3-\mathbf{1}\right)\left(\boldsymbol{n}_4-\mathbf{1}\right)\end{pmatrix} \\ \begin{pmatrix}\left(\boldsymbol{n}_1-\mathbf{1}\right)\boldsymbol{n}_2\times\\ \left(\boldsymbol{n}_3-\mathbf{1}\right)\left(\boldsymbol{n}_4-\mathbf{1}\right)\end{pmatrix} & \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4 & -\boldsymbol{n}_1\boldsymbol{n}_2\left(\boldsymbol{n}_3-\mathbf{1}\right)\boldsymbol{n}_4 & \boldsymbol{n}_1\boldsymbol{n}_2\left(\boldsymbol{n}_3-\mathbf{1}\right)\left(\boldsymbol{n}_4-\mathbf{1}\right) \\ -\left(\boldsymbol{n}_1-\mathbf{1}\right)\boldsymbol{n}_2\boldsymbol{n}_3\left(\boldsymbol{n}_4-\mathbf{1}\right) & \begin{pmatrix}\left(\boldsymbol{n}_1-\mathbf{1}\right)\left(\boldsymbol{n}_2-\mathbf{1}\right)\times\\ \boldsymbol{n}_3\left(\boldsymbol{n}_4-\mathbf{1}\right)\end{pmatrix} & \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4 & -\boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3\left(\boldsymbol{n}_4-\mathbf{1}\right) \\ \left(\boldsymbol{n}_1-\mathbf{1}\right)\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4 & -\left(\boldsymbol{n}_1-\mathbf{1}\right)\left(\boldsymbol{n}_2-\mathbf{1}\right)\boldsymbol{n}_3\boldsymbol{n}_4 & \begin{pmatrix}\left(\boldsymbol{n}_1-\mathbf{1}\right)\left(\boldsymbol{n}_2-\mathbf{1}\right)\times\\ \left(\boldsymbol{n}_3-\mathbf{1}\right)\boldsymbol{n}_4\end{pmatrix} & \boldsymbol{n}_1\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4 \end{pmatrix} \tag{3.189}$$

where $C=\boldsymbol{n}_2\boldsymbol{n}_1-\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_1+\boldsymbol{n}_3\boldsymbol{n}_1-\boldsymbol{n}_2\boldsymbol{n}_4\boldsymbol{n}_1+2\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_1-\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_1+\boldsymbol{n}_4\boldsymbol{n}_1-\boldsymbol{n}_1-\boldsymbol{n}_2+\boldsymbol{n}_2\boldsymbol{n}_3-\boldsymbol{n}_3+\boldsymbol{n}_2\boldsymbol{n}_4-\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4+\boldsymbol{n}_3\boldsymbol{n}_4-\boldsymbol{n}_4+1$.We can check that for $\mathcal{N}=5$, the common factor is

$$\boldsymbol{n}_2\boldsymbol{n}_1-\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_1+\boldsymbol{n}_3\boldsymbol{n}_1-\boldsymbol{n}_2\boldsymbol{n}_4\boldsymbol{n}_1+\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_1-\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_1+\boldsymbol{n}_4\boldsymbol{n}_1-\boldsymbol{n}_2\boldsymbol{n}_5\boldsymbol{n}_1+\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_5\boldsymbol{n}_1-\boldsymbol{n}_3\boldsymbol{n}_5\boldsymbol{n}_1+\boldsymbol{n}_2\boldsymbol{n}_4\boldsymbol{n}_5\boldsymbol{n}_1+\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_5\boldsymbol{n}_1-\boldsymbol{n}_4\boldsymbol{n}_5\boldsymbol{n}_1+\boldsymbol{n}_5\boldsymbol{n}_1-\boldsymbol{n}_1-\boldsymbol{n}_2+\boldsymbol{n}_2\boldsymbol{n}_3-\boldsymbol{n}_3+\boldsymbol{n}_2\boldsymbol{n}_4-\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4+\boldsymbol{n}_3\boldsymbol{n}_4-\boldsymbol{n}_4+\boldsymbol{n}_2\boldsymbol{n}_5-\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_5+\boldsymbol{n}_3\boldsymbol{n}_5-\boldsymbol{n}_2\boldsymbol{n}_4\boldsymbol{n}_5+\boldsymbol{n}_2\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_5-\boldsymbol{n}_3\boldsymbol{n}_4\boldsymbol{n}_5+\boldsymbol{n}_4\boldsymbol{n}_5-\boldsymbol{n}_5+\mathbf{1}$. For arbitrary $\mathcal{N}$, we have

$$\boldsymbol{C}=\frac{\boldsymbol{n}_1\star\boldsymbol{n}_2\star\boldsymbol{n}_3..\star\boldsymbol{n}_{\mathcal{N}}}{\boldsymbol{n}_1\boldsymbol{n}_2...\boldsymbol{n}_{\mathcal{N}}},\qquad\qquad \boldsymbol{g}_{ij}=\mathrm{sign}(j-i)\boldsymbol{C}\prod_{\ell=1}^{N}f\left(\ell,i,j\right), \tag{3.190}$$

where

$$f(\ell, i, j) = \begin{cases} \boldsymbol{n}_\ell & \text{if } \ell \in [i+1, j] \\ \mathbf{1} - \boldsymbol{n}_\ell & \text{otherwise} \end{cases} . \tag{3.191}$$

Chapter 4

Generating Functional and n-particle Discrete Green's Functions

In this chapter, we generalize the standard techniques of the generating functional to our discrete action formalism. This provides a unified approach for computing n-particle Green's functions, and the construction of effective potential which relate the discrete non-interacting Green's function to the discrete interacting Green's function, generalizing the Dyson equation and the self-energy to our discrete action formalism. We also provide explicit expressions for the two-particle discrete Green's function.

4.1 Generating Functional via a Source

In Chapter 3 Section 3.4, we have extensively studied how to compute the discrete Green's function for a non-interacting SPD. Now, we move to compute the interacting case. Our goal here is to obtain a complete description of the SPD using the generating functional. The key theoretical foundation is Wick's Theorem, which provides the generic way to compute the expectation values of any operator under a non-interacting density matrix. We will specifically consider the single-particle and two-particle discrete Green's functions, and derive the discrete analogues of the Dyson equation and Bethe-Salpeter equation.

Recall that the general interacting SPD

$$\hat{\rho} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_{\mathcal{N}} = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right) \hat{P}_1 ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right) \hat{P}_{\mathcal{N}} \tag{4.1}$$

can be mapped to a compound system with an effective density matrix

$$\hat{\rho}_{eff} = \hat{\rho}_{eff;0}\hat{P}_1^{(1)}..\hat{P}_{\mathcal{N}}^{(\mathcal{N})} = \hat{\rho}_{eff;0}\hat{P}, \qquad \hat{\rho}_{eff;0} = \hat{Q}\exp\left(\sum_i \boldsymbol{\gamma}_i \cdot \hat{\boldsymbol{n}}^{(i)}\right), \tag{4.2}$$

where we used the fact that the single particle operators are Bosonic. Recall that $\hat{\boldsymbol{N}}$ is the matrix collection for the single particle operators of the compound system (see Eq. 3.78). Furthermore, recall that a discrete time n-particle correlation function of the physical space corresponds to a n-particle density matrix in the compound space. Therefore, it will be necessary to construct the generating functional for static observables. The static generating functional of the compound space will then generate the discrete time information of the physical system.

The static generating functional for up to an M-particle density matrix for $\hat{\rho} = \hat{\rho}_0\hat{P}$ is given by

$$\tilde{Z}\left(\boldsymbol{v}^{(1)},\ldots,\boldsymbol{v}^{(M)}\right) = \frac{\left\langle \hat{P}\exp\left(v_{ij}^{(1)}\hat{n}_{ij}\right)\ldots\exp\left(v_{lk}^{(M)}\hat{n}_{lk}\right)\right\rangle_{\hat{\rho}_0}}{\left\langle \exp\left(v_{ij}^{(1)}\hat{n}_{ij}\right)\ldots\exp\left(v_{lk}^{(M)}\hat{n}_{lk}\right)\right\rangle_{\hat{\rho}_0}},$$

where $\boldsymbol{v}^{(i)}$ is the source, $\hat{\rho}_0$ is the non-interacting density matrix, $\hat{P}$ is a general projector, and Einstein notation for summations has been employed (and will be used only throughout this section). While we have written the generating functional in general, we can specifically apply this to the compound space as

$$\tilde{Z}\left(\boldsymbol{v}^{(1)},\ldots,\boldsymbol{v}^{(M)}\right) = \frac{\left\langle \hat{P}\exp\left(v_{ij}^{(1)}\hat{N}_{ij}\right)\ldots\exp\left(v_{lk}^{(M)}\hat{N}_{lk}\right)\right\rangle_{\hat{\rho}_0}}{\left\langle \exp\left(v_{ij}^{(1)}\hat{N}_{ij}\right)\ldots\exp\left(v_{lk}^{(M)}\hat{N}_{lk}\right)\right\rangle_{\hat{\rho}_0}},$$

where $\hat{\rho}_0 = \hat{\rho}_{eff;0}$, $\hat{P} = \hat{P}_1^{(1)}..\hat{P}_{\mathcal{N}}^{(\mathcal{N})}$, and $\hat{N}_{ij}$ is defined in the compound space (see Eq. 3.78). However, we will work with the general version in this section, which can then be applied to any system, including the compound system. It should be noted that the Lie

group properties of the non-interacting density matrix demand that

$$\tilde{Z}\left(\boldsymbol{v}^{(1)},\ldots,\boldsymbol{v}^{(M)}\right)=\tilde{Z}\left(\boldsymbol{v}\right),\qquad\qquad \boldsymbol{v}=\ln(\exp(\boldsymbol{v}^{(1)})\ldots\exp(\boldsymbol{v}^{(M)})).$$

The first step is to derive the static observables in terms of derivatives of $\tilde{Z}\left(\boldsymbol{v}^{(1)},\ldots,\boldsymbol{v}^{(M)}\right)$. Given that we are only concerned with the single-particle and two-particle density matrix, we restrict ourselves to $M=2$. Recalling the expansion for the exponential of an operator

$$\exp\left(v_{ij}^{(1)}\hat{n}_{ij}\right)\exp\left(v_{lk}^{(2)}\hat{n}_{lk}\right)=1+v_{ij}^{(1)}\hat{n}_{ij}+v_{lk}^{(2)}\hat{n}_{lk}+v_{ij}^{(1)}v_{lk}^{(2)}\hat{n}_{ij}\hat{n}_{lk}+\ldots \tag{4.3}$$

Taking the expectation value, we have

$$\left\langle\exp\left(v_{ij}^{(1)}\hat{n}_{ij}\right)\exp\left(v_{lk}^{(2)}\hat{n}_{lk}\right)\right\rangle_{\hat{\rho}_0}=1+v_{ij}^{(1)}\left\langle\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}+v_{lk}^{(2)}\left\langle\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}+v_{ij}^{(1)}v_{lk}^{(2)}\left\langle\hat{n}_{ij}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}+\ldots$$

and

$$\begin{aligned}\left\langle\hat{P}\exp\left(v_{ij}^{(1)}\hat{n}_{ij}\right)\exp\left(v_{lk}^{(2)}\hat{n}_{lk}\right)\right\rangle_{\hat{\rho}_0}=&\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}+v_{ij}^{(1)}\left\langle\hat{P}\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}+v_{lk}^{(2)}\left\langle\hat{P}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}+\\&v_{ij}^{(1)}v_{lk}^{(2)}\left\langle\hat{P}\hat{n}_{ij}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}+\ldots\end{aligned} \tag{4.4}$$

Recalling the following Taylor series

$$\frac{1}{1+x}=1-x+x^2+\ldots \tag{4.5}$$

we have

$$\begin{aligned}\left\langle\exp\left(v_{ij}^{(1)}\hat{n}_{ij}\right)\exp\left(v_{lk}^{(2)}\hat{n}_{lk}\right)\right\rangle_{\hat{\rho}_0}^{-1}=&1-v_{ij}^{(1)}\left\langle\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}-v_{lk}^{(2)}\left\langle\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}-\\&v_{ij}^{(1)}v_{lk}^{(2)}\left(\left\langle\hat{n}_{ij}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}-2\left\langle\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}\left\langle\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}\right)+\ldots\end{aligned} \tag{4.6}$$

Plugging into the expression for $\tilde{Z}$

$$\tilde{Z}\left(\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)}\right)=\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}+v_{ij}^{(1)}\left(\left\langle\hat{P}\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}-\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\right)+v_{lk}^{(2)}\left(\left\langle\hat{P}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}-\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0}\right)$$
$$v_{ij}^{(1)}v_{lk}^{(2)}\Bigg(\left\langle\hat{P}\hat{n}_{ij}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}-\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}\langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}_0}+$$
$$2\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0}-\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\left\langle\hat{P}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}-\left\langle\hat{P}\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0}\Bigg)+\ldots \tag{4.7}$$

We can now evaluate the first and second derivatives of $\tilde{Z}\left(\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)}\right)$ divided by $\tilde{Z}(\mathbf{0},\mathbf{0})$

$$\frac{1}{\tilde{Z}(\mathbf{0},\mathbf{0})}\frac{\partial\tilde{Z}\left(\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)}\right)}{\partial v_{ij}^{(1)}}\bigg|_{\boldsymbol{v}=\mathbf{0}}=\frac{\left\langle\hat{P}\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}}{\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}}-\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}=\langle\hat{n}_{ij}\rangle_{\hat{\rho}}-\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\,, \tag{4.8}$$

and

$$\frac{1}{\tilde{Z}(\mathbf{0},\mathbf{0})}\frac{\partial^2\tilde{Z}\left(\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)}\right)}{\partial v_{ij}^{(1)}\partial v_{lk}^{(2)}}\bigg|_{\boldsymbol{v}=\mathbf{0}}=\frac{\left\langle\hat{P}\hat{n}_{ij}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}}{\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}}-\langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}_0}+$$
$$2\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0}-\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\frac{\left\langle\hat{P}\hat{n}_{lk}\right\rangle_{\hat{\rho}_0}}{\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}}-\frac{\left\langle\hat{P}\hat{n}_{ij}\right\rangle_{\hat{\rho}_0}}{\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0} \tag{4.9}$$
$$=\langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}}-\langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}_0}+2\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0}-$$
$$\langle\hat{n}_{ij}\rangle_{\hat{\rho}_0}\langle\hat{n}_{lk}\rangle_{\hat{\rho}}-\langle\hat{n}_{ij}\rangle_{\hat{\rho}}\langle\hat{n}_{lk}\rangle_{\hat{\rho}_0}\,, \tag{4.10}$$

where $\boldsymbol{v}=\mathbf{0}$ implies that all $\boldsymbol{v}^{(i)}=0$, and we used

$$\frac{\left\langle\hat{P}\hat{O}\right\rangle_{\hat{\rho}_0}}{\left\langle\hat{P}\right\rangle_{\hat{\rho}_0}}=\langle\hat{O}\rangle_{\hat{\rho}}. \tag{4.11}$$

We now have all of the information we need to construct an arbitrary one and two particle density matrix. However, this formulation is somewhat inconvenient given that it

results in an infinite series for $\tilde{Z}\left(\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}\right)$, and requires the use of Wick's theorem order by order. Therefore, it is convenient to perform a change of variables, expressing $\tilde{Z}$ as a function of the non-interacting single-particle density matrix $\boldsymbol{g}_0$, which would correspond to the non-interacting discrete Green's function when working in the compound space.

4.2 Generating Functional in Terms of the Non-interacting Discrete Green's Function

We continue by performing a change of variables for $\tilde{Z}$, writing it in terms of the non-interacting single-particle density matrix $\boldsymbol{g}_0$ as

$$Z(\boldsymbol{g}_0) \equiv \left\langle \hat{P} \right\rangle_{\hat{\varrho}(\boldsymbol{g}_0)} = \tilde{Z}\left(\boldsymbol{v}(\boldsymbol{g}_0)\right), \qquad \hat{\varrho}(\boldsymbol{g}_0) = \exp\left(\ln\left(\frac{\mathbf{1}}{\boldsymbol{g}_0^{-1} - \mathbf{1}}\right)^T \cdot \hat{\boldsymbol{n}}\right), \tag{4.12}$$

where

$$\boldsymbol{v}(\boldsymbol{g}_0) = \ln\left(\left(\frac{\mathbf{1}}{\boldsymbol{g}_0^{-1} - \mathbf{1}}\right)^T \left(\boldsymbol{g}_0^{\star -1} - \mathbf{1}\right)^T\right), \tag{4.13}$$

where $\boldsymbol{g}_0^\star$ is the single-particle density matrix corresponding to $\hat{\rho}_0$, and this was obtained by inverting either of the following equivalent relations

$$\boldsymbol{g}_0(\boldsymbol{v}) = \langle \hat{\boldsymbol{n}} \rangle_{\exp(v_{ij}\hat{n}_{ij})\hat{\rho}_0} = \frac{\mathrm{Tr}(\exp\left(v_{lk}\hat{n}_{lk}\right)\hat{\rho}_0 \hat{\boldsymbol{n}})}{\mathrm{Tr}(\exp\left(v_{lk}\hat{n}_{lk}\right)\hat{\rho}_0)}, \tag{4.14}$$

$$\left(\frac{\mathbf{1}}{\boldsymbol{g}_0(\boldsymbol{v})^{-1} - \mathbf{1}}\right)^T = \exp(\boldsymbol{v})\left(\frac{\mathbf{1}}{\boldsymbol{g}_0^{\star -1} - \mathbf{1}}\right)^T. \tag{4.15}$$

We now consider a general function $\tilde{f}\left(\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}\right) = f(\boldsymbol{g}_0(\boldsymbol{v}))$, and we translate the deriva-

tives using the chain rule. First, we need the cross derivatives between $\boldsymbol{g}_0$ and $\boldsymbol{v}^{(i)}$

$$\left.\frac{\partial[\boldsymbol{g}_0]_{ij}}{\partial v_{lk}^{(n)}}\right|_{\boldsymbol{v}^{(\ell)}=\boldsymbol{0}} = \langle \hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}_0} - \langle \hat{n}_{ij}\rangle_{\hat{\rho}_0}\langle \hat{n}_{lk}\rangle_{\hat{\rho}_0} = [\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{lj}, \quad \left.\frac{\partial[\boldsymbol{p}_0]_{ij}}{\partial v_{lk}^{(n)}}\right|_{\boldsymbol{v}^{(\ell)}=\boldsymbol{0}} = -[\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{lj}, \tag{4.16}$$

where $\boldsymbol{p}_0 = \boldsymbol{1} - \boldsymbol{g}_0$. We can now construct the first derivative of $\tilde{f}$ as

$$\left.\frac{\partial \tilde{f}}{\partial v_{ij}^{(1)}}\right|_{\boldsymbol{v}^{(\ell)}=\boldsymbol{0}} = \frac{\partial f}{\partial[\boldsymbol{g}_0]_{mn}}\frac{\partial[\boldsymbol{g}_0]_{mn}}{\partial v_{ij}^{(1)}} = \frac{\partial f}{\partial[\boldsymbol{g}_0]_{mn}}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in}. \tag{4.17}$$

Similarly for the second derivative

$$\begin{aligned}\left.\frac{\partial \tilde{f}}{\partial v_{ij}^{(1)}\partial v_{lk}^{(2)}}\right|_{\boldsymbol{v}^{(\ell)}=\boldsymbol{0}} &= \frac{\partial f}{\partial[\boldsymbol{g}_0]_{mn}\partial[\boldsymbol{g}_0]_{st}}\frac{\partial[\boldsymbol{g}_0]_{st}}{\partial v_{lk}^{(2)}}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in} + \\ &\frac{\partial f}{\partial[\boldsymbol{g}_0]_{mn}}\left(\frac{\partial[\boldsymbol{g}_0]_{mj}}{\partial v_{lk}^{(2)}}[\boldsymbol{p}_0]_{in} + [\boldsymbol{g}_0]_{mj}\frac{\partial[\boldsymbol{p}_0]_{in}}{\partial v_{lk}^{(2)}}\right) \\ &= \frac{\partial f}{\partial[\boldsymbol{g}_0]_{mn}\partial[\boldsymbol{g}_0]_{st}}[\boldsymbol{g}_0]_{sk}[\boldsymbol{p}_0]_{lt}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in} + \\ &\frac{\partial f}{\partial[\boldsymbol{g}_0]_{mn}}\left([\boldsymbol{g}_0]_{mk}[\boldsymbol{p}_0]_{lj}[\boldsymbol{p}_0]_{in} - [\boldsymbol{g}_0]_{mj}[\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{ln}\right).\end{aligned} \tag{4.18}$$

We now have all derivatives of $\tilde{f}$ up to second order in terms of derivatives of f.

Let us proceed to rewrite the derivatives of $\tilde{Z}$ in terms of the derivatives of Z as

$$\frac{1}{\tilde{Z}(\boldsymbol{0},\boldsymbol{0})}\left.\frac{\partial \tilde{Z}\left(\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)}\right)}{\partial v_{ij}^{(1)}}\right|_{\boldsymbol{v}^{(\ell)}=\boldsymbol{0}} = [\boldsymbol{g}^{\star}]_{ij} - [\boldsymbol{g}_0^{\star}]_{ij} = \frac{1}{Z(\boldsymbol{g}_0^{\star})}\left.\frac{\partial Z(\boldsymbol{g}_0)}{\partial[\boldsymbol{g}_0]_{mn}}\right|_{\boldsymbol{g}_0=\boldsymbol{g}_0^{\star}}[\boldsymbol{g}_0^{\star}]_{mj}[\boldsymbol{p}_0^{\star}]_{in}. \tag{4.19}$$

Given that we will always be evaluating the derivative for $\boldsymbol{g}_0 = \boldsymbol{g}_0^{\star}$, we will suppress the star superscript hereafter. We can then write an equation for $\boldsymbol{g}$ as

$$[\boldsymbol{g}]_{ij} = [\boldsymbol{g}_0]_{ij} + \frac{1}{Z}\frac{\partial Z}{\partial[\boldsymbol{g}_0]_{mn}}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in}. \tag{4.20}$$

We now proceed to the two-particle quantities, where the second derivative of $\tilde{Z}$ is written

as

$$\frac{1}{\tilde{Z}(\mathbf{0},\mathbf{0})}\left.\frac{\partial^2\tilde{Z}\left(\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)}\right)}{\partial v_{ij}^{(1)}\partial v_{lk}^{(2)}}\right|_{\boldsymbol{v}^{(\ell)}=\mathbf{0}} = \langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}} - \langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}_0} + 2[\boldsymbol{g}_0]_{ij}[\boldsymbol{g}_0]_{lk} -$$

$$[\boldsymbol{g}_0]_{ij}[\boldsymbol{g}]_{lk} - [\boldsymbol{g}]_{ij}[\boldsymbol{g}_0]_{lk} \tag{4.21}$$

$$= \frac{1}{Z}\frac{\partial Z}{\partial[\boldsymbol{g}_0]_{mn}\partial[\boldsymbol{g}_0]_{st}}[\boldsymbol{g}_0]_{sk}[\boldsymbol{p}_0]_{lt}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in} +$$

$$\frac{1}{Z}\frac{\partial Z}{\partial[\boldsymbol{g}_0]_{mn}}\left([\boldsymbol{g}_0]_{mk}[\boldsymbol{p}_0]_{lj}[\boldsymbol{p}_0]_{in} - [\boldsymbol{g}_0]_{mj}[\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{ln}\right). \tag{4.22}$$

In summary, we can write the unknown interacting single-particle and two-particle density matrices in terms of the non-interacting density matrices and derivatives of the generating functional as

$$[\boldsymbol{g}]_{ij} = [\boldsymbol{g}_0]_{ij} + \frac{1}{Z}\frac{\partial Z}{\partial[\boldsymbol{g}_0]_{mn}}[\boldsymbol{g}_0]_{mj}[\mathbf{1}-\boldsymbol{g}_0]_{in} \qquad \leftrightarrow \qquad \boldsymbol{g} = \boldsymbol{g}_0 + (\mathbf{1}-\boldsymbol{g}_0)\frac{1}{Z}\frac{\partial Z}{\partial\boldsymbol{g}_0^T}\boldsymbol{g}_0 \tag{4.23}$$

and

$$\begin{aligned}\langle\hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}} =& [\boldsymbol{g}_0]_{ij}[\boldsymbol{g}_0]_{lk} + [\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{lj} + \\ & \frac{1}{Z}\frac{\partial Z}{\partial[\boldsymbol{g}_0]_{mn}}\Big([\boldsymbol{g}_0]_{mk}[\boldsymbol{g}_0]_{ij}[\boldsymbol{p}_0]_{ln} + [\boldsymbol{g}_0]_{mj}[\boldsymbol{g}_0]_{lk}[\boldsymbol{p}_0]_{in} + \\ & [\boldsymbol{g}_0]_{mk}[\boldsymbol{p}_0]_{lj}[\boldsymbol{p}_0]_{in} - [\boldsymbol{g}_0]_{mj}[\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{ln}\Big) + \\ & \frac{1}{Z}\frac{\partial Z}{\partial[\boldsymbol{g}_0]_{mn}\partial[\boldsymbol{g}_0]_{st}}[\boldsymbol{g}_0]_{sk}[\boldsymbol{p}_0]_{lt}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in}.\end{aligned} \tag{4.24}$$

When applying the above two equations in the compound space, they are realizations of the discrete Dyson equation and the discrete Bethe-Salpeter Equation, respectively, in the sense that they relate the non-interacting discrete Green's function and the derivatives of the generating functional to the interacting discrete Green's function. However, it is useful to recast these equations in a form more amenable to approximations. Equation 4.23 can be

rewritten, motivated by the Lie group structure of the non-interacting density matrix (see Section 3.3), as

$$\left(\frac{\mathbf{1}}{\boldsymbol{g}^{-1}-\mathbf{1}}\right)^{T}=\left(\frac{\mathbf{1}}{\boldsymbol{g}_{0}^{-1}-\mathbf{1}}\right)^{T}\exp\left(\boldsymbol{\Sigma}_{P}\right)\quad\leftrightarrow\quad\left(\boldsymbol{g}^{-1}-\mathbf{1}\right)=\left(\boldsymbol{g}_{0}^{-1}-\mathbf{1}\right)\exp\left(-\boldsymbol{\Sigma}_{P}^{T}\right),\quad(4.25)$$

where we have introduced the discrete self-energy $\boldsymbol{\Sigma_P}$, which is an effective non-interacting potential that connects the non-interacting discrete Green's function with the interacting discrete Green's function. Eq. 4.25 is our preferred form of the discrete Dyson equation. In order to connect $\boldsymbol{\Sigma_P}$ in terms of Z and $\boldsymbol{g}_0$, we define the self-energy operator $\boldsymbol{S}=\exp\left(-\boldsymbol{\Sigma}_{P}^{T}\right)$ in addition to $\boldsymbol{\Gamma}=\exp\left(\boldsymbol{\Sigma}_{P}^{T}\right)-\mathbf{1}$, then substituting $\boldsymbol{\Gamma}$ into the discrete Dyson equation

$$\boldsymbol{g}^{-1}-\mathbf{1}=\left(\boldsymbol{g}_{0}^{-1}-\mathbf{1}\right)\frac{\mathbf{1}}{\mathbf{1}+\boldsymbol{\Gamma}},\quad(4.26)$$

and adding the identity to each side

$$\boldsymbol{g}^{-1}=\left(\boldsymbol{g}_{0}^{-1}+\boldsymbol{\Gamma}\right)\frac{\mathbf{1}}{\mathbf{1}+\boldsymbol{\Gamma}},\quad(4.27)$$

and inverting

$$\boldsymbol{g}=\left(\mathbf{1}+\boldsymbol{\Gamma}\right)\frac{\mathbf{1}}{\boldsymbol{\Gamma}+\boldsymbol{g}_{0}^{-1}}=\left(\mathbf{1}+\boldsymbol{\Gamma}\right)\boldsymbol{g}_{0}\frac{\mathbf{1}}{\mathbf{1}+\boldsymbol{\Gamma}\boldsymbol{g}_{0}},\quad(4.28)$$

and subtracting $\boldsymbol{g}_0$ from each side

$$\boldsymbol{g}-\boldsymbol{g}_{0}=\left(\mathbf{1}-\boldsymbol{g}_{0}\right)\boldsymbol{\Gamma}\boldsymbol{g}_{0}\frac{\mathbf{1}}{\mathbf{1}+\boldsymbol{\Gamma}\boldsymbol{g}_{0}}=\left(\mathbf{1}-\boldsymbol{g}_{0}\right)\frac{\mathbf{1}}{\mathbf{1}+\boldsymbol{\Gamma}\boldsymbol{g}_{0}}\boldsymbol{\Gamma}\boldsymbol{g}_{0},\quad(4.29)$$

and comparing to Eq. 4.23, we see that

$$\frac{1}{Z}\frac{\partial Z}{\partial\boldsymbol{g}_{0}^{T}}=\frac{\mathbf{1}}{\mathbf{1}+\boldsymbol{\Gamma}\boldsymbol{g}_{0}}\boldsymbol{\Gamma}=\frac{\mathbf{1}}{\boldsymbol{\Gamma}^{-1}+\boldsymbol{g}_{0}},\quad(4.30)$$

and solving for $\mathbf{\Gamma}^{-1}$, we have

$$\mathbf{\Gamma}^{-1} = \left(\frac{\partial \ln Z}{\partial \boldsymbol{g}_0^T}\right)^{-1} - \boldsymbol{g}_0, \tag{4.31}$$

and inverting, we have

$$\mathbf{\Gamma} = \frac{\mathbf{1}}{\mathbf{1} - \frac{\partial \ln Z}{\partial \boldsymbol{g}_0^T}\boldsymbol{g}_0}\frac{\partial \ln Z}{\partial \boldsymbol{g}_0^T} = \frac{\mathbf{1}}{Z - \frac{\partial Z}{\partial \boldsymbol{g}_0^T}\boldsymbol{g}_0}\frac{\partial Z}{\partial \boldsymbol{g}_0^T}, \tag{4.32}$$

and adding the identity to each side

$$\mathbf{1} + \mathbf{\Gamma} = \exp\left(\mathbf{\Sigma}_P\right)^T = \boldsymbol{S}^{-1} = \frac{\mathbf{1}}{Z - \frac{\partial Z}{\partial \boldsymbol{g}_0^T}\boldsymbol{g}_0}\left(Z + \frac{\partial Z}{\partial \boldsymbol{g}_0^T}\boldsymbol{p}_0\right), \tag{4.33}$$

and inverting, we finally have

$$\boldsymbol{S} = \exp\left(-\mathbf{\Sigma}_P^T\right) = \left(Z\mathbf{1} + \left(\frac{\partial Z}{\partial \boldsymbol{g}_0^T}\right)\boldsymbol{p}_0\right)^{-1}\left(Z\mathbf{1} - \left(\frac{\partial Z}{\partial \boldsymbol{g}_0^T}\right)\boldsymbol{g}_0\right). \tag{4.34}$$

This generalized Dyson equation plays an important role in the discrete action theory, analogous to the usual Dyson equation. We do not perform an analogous manipulation of the two-particle Eq. **??**, as it is sufficient for all of our current applications.

While we have only derived the equations for the one and two particle density matrices, it should be clear that the above procedure can be formally executed for arbitrary order density matrices. It should be emphasized that Z can be written as a finite polynomial of $\boldsymbol{g}_0$ if $\hat{P}$ contains a finite number of terms, which is why it is beneficial to perform the above change in variables from $\boldsymbol{v}$ to $\boldsymbol{g}_0$. Recall that we will be applying this formalism to the density matrices in the compound space, which will correspond to one-particle and two-particle discrete Green's functions in the physical space.

We now consider a special case where $\hat{P} = \exp(\boldsymbol{\mu} \cdot \hat{\boldsymbol{n}})$ is a noninteracting projector

$$Z(\boldsymbol{g}_0) = \left\langle \hat{P} \right\rangle_{\hat{\varrho}(\boldsymbol{g}_0)} = \frac{\mathrm{Tr}(\exp(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}) \exp(\boldsymbol{\mu} \cdot \hat{\boldsymbol{n}}))}{\mathrm{Tr}(\exp(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}))} = \frac{|\mathbf{1} + \exp(\boldsymbol{v}_0) \exp(\boldsymbol{\mu})|}{|\mathbf{1} + \exp(\boldsymbol{v}_0)|} \tag{4.35}$$

$$= |(\mathbf{1} + \exp(\boldsymbol{v}_0))^{-1}(\mathbf{1} + \exp(\boldsymbol{v}_0) \exp(\boldsymbol{\mu}))| = |\mathbf{1} + \boldsymbol{g}_0^T(\exp(\boldsymbol{\mu}) - \mathbf{1})| \tag{4.36}$$

$$= |\mathbf{1} + \boldsymbol{\Gamma}' \boldsymbol{g}_0|, \tag{4.37}$$

where $\boldsymbol{\Gamma}' = \exp(\boldsymbol{\mu}^T) - \mathbf{1}$ and

$$\boldsymbol{g}_0 = \left(\frac{\mathbf{1}}{\mathbf{1} + \exp(-\boldsymbol{v}_0)} \right)^T \qquad \leftrightarrow \qquad \boldsymbol{v}_0 = -\ln(\boldsymbol{g}_0^{-1} - 1)^T, \tag{4.38}$$

and

$$\frac{1}{Z} \frac{\partial Z}{\partial \boldsymbol{g}_0^T} = \frac{\partial \ln Z}{\partial \boldsymbol{g}_0^T} = \frac{\partial \mathrm{Tr}(\ln(\mathbf{1} + \boldsymbol{\Gamma}' \boldsymbol{g}_0))}{\partial \boldsymbol{g}_0^T} = \frac{\mathbf{1}}{\mathbf{1} + \boldsymbol{\Gamma}' \boldsymbol{g}_0} \boldsymbol{\Gamma}' = \frac{\mathbf{1}}{\mathbf{1} + \boldsymbol{\Gamma} \boldsymbol{g}_0} \boldsymbol{\Gamma}, \tag{4.39}$$

so we find that $\boldsymbol{\Gamma}' = \boldsymbol{\Gamma}$ and thus $\boldsymbol{\mu} = \boldsymbol{\Sigma}_P$. Therefore, we can see that in a non-interacting system, if we treat an external potential as our interacting projector, the discrete self-energy is simply the external potential, as one would expect.

Chapter 5

The Local SPD and the Local Discrete Action Model

There are prominent models of interacting electrons which have interactions that only act on a subspace, such as the Anderson impurity model (AIM). Such problems motivate us to study a particular class of SPD, where all interacting projectors $\hat{P}_\tau$ are restricted to the same subspace, which we refer to as the impurity subspace, and the remaining subspace is referred to as the bath (similar to the naming conventions of the AIM). We refer to this class of SPD as the local SPD, denoted SPD-l. The non-interacting projector is allowed to be completely general. Evaluating this class of SPD amounts to solving a discrete action only within the impurity subspace, such that the cost is independent of the size of the bath, and we refer to this scenario as a local discrete action model (LDAM). While the LDAM naturally emerges for the SPD-l, it can also can be used to approximately solve a more general SPD (see Chapter 7).

5.1 Deriving the Local Discrete Action Model (LDAM)

Consider an SPD-l:

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right) \hat{P}_1 ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right) \hat{P}_{\mathcal{N}} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_{\mathcal{N}}, \quad \hat{P}_\tau = \exp\left(\hat{V}_\tau\right), \quad \hat{\mathcal{P}}_\tau = \exp\left(\boldsymbol{\gamma}_\tau \cdot \hat{\boldsymbol{n}}\right) \hat{P}_\tau. \tag{5.1}$$

The resulting effective density matrix in the compound space will then be

$$\hat{\rho}_{eff} = \hat{Q}\hat{\mathcal{P}}_1^{(1)}...\hat{\mathcal{P}}_{\mathcal{N}}^{(\mathcal{N})} = \hat{Q}\exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}^{(1)}\right)\hat{P}_1^{(1)}...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}^{(\mathcal{N})}\right)\hat{P}_{\mathcal{N}}^{(\mathcal{N})} \tag{5.2}$$

$$= \hat{Q}\exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}^{(1)}\right)...\exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}^{(\mathcal{N})}\right)\hat{P}_1^{(1)}...\hat{P}_{\mathcal{N}}^{(\mathcal{N})} \tag{5.3}$$

$$= \hat{\rho}_{eff;0}\hat{P}_1^{(1)}...\hat{P}_{\mathcal{N}}^{(\mathcal{N})}, \tag{5.4}$$

where we used the Bosonic nature of the projectors to shift all $\hat{P}_\tau^{(\tau)}$ to the right. Given that the self-energy is local in this class of problems, we only need to compute the local interacting discrete Green's function, which is given by the following local density matrix in the compound space

$$\hat{\rho}_{loc} = \mathrm{Tr}_{/i}\hat{\rho}_{eff} = \mathrm{Tr}_{/i}(\hat{\rho}_{eff;0})\hat{P}_1^{(1)}...\hat{P}_{\mathcal{N}}^{(\mathcal{N})} \tag{5.5}$$

$$= \hat{\rho}_{loc;0}\hat{P}_1^{(1)}...\hat{P}_{\mathcal{N}}^{(\mathcal{N})}, \tag{5.6}$$

where we have traced out all of the bath orbitals. This resulting local density matrix in the compound space defines the local discrete action model which must be solved. Solving this problem at a given $\mathcal{N}$ yields the solution for the SPD with local interaction projectors. This LDAM can also be obtained via the generating functional. Recall

$$Z(\boldsymbol{g}_0) = \left\langle \hat{P} \right\rangle_{\hat{\varrho}(\boldsymbol{g}_0)} = \left\langle \hat{P} \right\rangle_{\hat{\varrho}(\boldsymbol{g}_{loc;0})},$$

where the last equality follows from the fact that $\hat{P} = \hat{P}_1^{(1)}...\hat{P}_{\mathcal{N}}^{(\mathcal{N})}$ is local, and this implies that the generating functional only depends on $\boldsymbol{g}_{loc;0}$. Furthermore, notice that $\hat{\varrho}(\boldsymbol{g}_{loc;0}) = \hat{\rho}_{loc;0}$, and therefore

$$Z(\boldsymbol{g}_0) = \left\langle \hat{P} \right\rangle_{\hat{\rho}_{loc;0}},$$

where the right hand side of the equality is the generating functional of the LDAM. Therefore, we see that the SPD-l and the LDAM have the same generating functional, and solving the

LDAM will provide all information needed to evaluate the SPD-l.

5.2 Evaluating the SPD-l

Now we proceed to evaluate the SPD-l using the generating functional. Since the projection is purely within the impurity subsystem, the self-energy is local to the impurity subspace

$$\boldsymbol{\Sigma}_P\left(\boldsymbol{g}_0\right) = \boldsymbol{\Sigma}_{P;loc}\left(\boldsymbol{g}_{loc;0}\right) \oplus \mathbf{0}, \tag{5.7}$$

which can be deduced from the generating functional, and this can be used to construct $\boldsymbol{S}_{loc}$, which can also be equivalently computed by measuring the interacting discrete Green's function and evaluating

$$\boldsymbol{S}_{loc} = \left(\boldsymbol{g}_{loc}^{-1} - \mathbf{1}\right)\left(\boldsymbol{g}_{loc;0}^{-1} - \mathbf{1}\right)^{-1}, \tag{5.8}$$

and we can extend to the full space as

$$\boldsymbol{S} = \boldsymbol{S}_{loc} \oplus \mathbf{1}, \tag{5.9}$$

and the interacting Green's function is computed as

$$\left(\boldsymbol{g}^{-1} - \mathbf{1}\right) = \left(\boldsymbol{g}_0^{-1} - \mathbf{1}\right)\boldsymbol{S}, \tag{5.10}$$

$$\boldsymbol{g} = \left(\mathbf{1} + \left(\boldsymbol{g}_0^{-1} - \mathbf{1}\right)\boldsymbol{S}\right)^{-1} = \left(\boldsymbol{g}_0 + \left(\mathbf{1} - \boldsymbol{g}_0\right)\boldsymbol{S}\right)^{-1}\boldsymbol{g}_0, \tag{5.11}$$

If we want to compute a generic operator spanning over multiple sites, we need to collect the corresponding sites to compute

$$\hat{\rho}_{rel} = \hat{\rho}_{rel;0}\hat{P}, \qquad \left\langle \hat{O} \right\rangle = \mathrm{Tr}\left(\hat{\rho}_{rel}\hat{O}\right). \tag{5.12}$$

Alternatively, one can simply use the generating functional and its derivatives to construct the corresponding quantities.

5.3 The Local Discrete Action Model for a Single Orbital with $\mathcal{N} = 3$

The local discrete action model for $\mathcal{N} = 3$ is given by

$$\hat{\rho}_{loc} = \hat{\rho}_{loc;0}\hat{P}_1^{(1)}\hat{P}_2^{(2)}\hat{P}_3^{(3)}, \tag{5.13}$$

where the interaction projectors are

$$\hat{P}_1^{(1)} = \left(1 - \mu - \frac{1}{4}u\right)\hat{1}^{(1)} + \mu\left(\hat{n}_\uparrow^{(1)} + \hat{n}_\downarrow^{(1)}\right) + u\hat{n}_\uparrow^{(1)}\hat{n}_\downarrow^{(1)}, \tag{5.14}$$

$$\hat{P}_2^{(2)} = \left(1 - \mu - \frac{1}{4}u\right)\hat{1}^{(2)} + \mu\left(\hat{n}_\uparrow^{(2)} + \hat{n}_\downarrow^{(2}\right) + u\hat{n}_\uparrow^{(2)}\hat{n}_\downarrow^{(2)}, \tag{5.15}$$

$$\hat{P}_3^{(3)} = \hat{1}^{(3)}, \tag{5.16}$$

where the B-type SPD requires to above form in order to ensure that the SPD is symmetric, and $\hat{\rho}_{loc;0}$ is determined by the noninteracting local discrete Green's functions

$$\boldsymbol{g}_{loc;0\uparrow} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix}, \qquad \boldsymbol{g}_{loc;0} = \begin{pmatrix} c_{11} & 0 & c_{12} & 0 & c_{13} & 0 \\ 0 & c_{11} & 0 & c_{12} & 0 & c_{13} \\ c_{21} & 0 & c_{22} & 0 & c_{23} & 0 \\ 0 & c_{21} & 0 & c_{22} & 0 & c_{23} \\ c_{31} & 0 & c_{32} & 0 & c_{33} & 0 \\ 0 & c_{31} & 0 & c_{32} & 0 & c_{33} \end{pmatrix} \tag{5.17}$$

where we use the time index major scheme and assume spin symmetry.

In general, we have two ways to evaluate the expectation values for the local discrete action model: computing the generating functional or directly evaluating a given observable using Wick's theorem. Here we proceed by using the latter approach, and the final expression will be an order 2 polynomial in u and μ, organized in the following fashion

$$\left\{1, u, u^2, \mu, \mu u, \mu^2\right\}. \tag{5.18}$$

We tabulate the prefactors associated with each of the preceding terms, and store them as a vector. All the relevant expectation values are then given as

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \right\rangle_{\hat{\rho}_{loc;0}} = \begin{pmatrix} 1 \\ c_{11}^2 + c_{22}^2 - \frac{1}{2} \\ \left(c_{22}^2 - \frac{1}{4}\right) c_{11}^2 - 2c_{12}c_{21}c_{22}c_{11} + c_{12}^2 c_{21}^2 - \frac{c_{22}^2}{4} + \frac{1}{16} \\ 2\left(c_{11} + c_{22} - 1\right) \\ \frac{1}{2}\left(\left(4c_{22} - 2\right) c_{11}^2 + \left(4c_{22}^2 - 4c_{12}c_{21} - 1\right) c_{11} - c_{22}\left(4c_{12}c_{21} + 2c_{22} + 1\right) + 1\right) \\ -2c_{12}c_{21} - 2c_{22} + c_{11}\left(4c_{22} - 2\right) + 1 \end{pmatrix} \tag{5.19}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(1)} \hat{a}_\sigma^{(1)} \right\rangle_{\hat{\rho}_{loc;0}} = \tag{5.20}$$

$$\begin{pmatrix} c_{11} \\ c_{11}^2 + \left(c_{22}^2 - \frac{1}{2}\right) c_{11} - c_{12} c_{21} c_{22} \\ \frac{1}{16}\left(4 c_{12} c_{21} \left(4 c_{12} c_{21} + c_{22}\right) + c_{11}\left(-4 c_{22}\left(8 c_{12} c_{21} + c_{22}\right) + 4 c_{11}\left(4 c_{22}^2 - 1\right) + 1\right)\right) \\ c_{11}\left(c_{11} + 2 c_{22} - 1\right) - c_{12} c_{21} \\ \frac{1}{4}\left(\left(4 c_{22}\left(c_{22} + 2\right) - 5\right) c_{11}^2 - \left(2 c_{22} + 8 c_{12} c_{21}\left(c_{22} + 1\right) - 1\right) c_{11} + c_{12} c_{21}\left(4 c_{12} c_{21} + 1\right)\right) \\ c_{11}\left(c_{11}\left(2 c_{22} - 1\right) - 2 c_{12} c_{21}\right) \end{pmatrix} \tag{5.21}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(2)} \hat{a}_\sigma^{\dagger(1)} \hat{a}_\sigma^{(2)} \right\rangle_{\hat{\rho}_{loc;0}} = \begin{pmatrix} c_{12} \\ \frac{1}{2}\left(2 c_{11} - 1\right) c_{12} \\ \frac{1}{16}\left(1 - 4 c_{11}\right) c_{12} \\ c_{12}\left(c_{11} + c_{22} - 1\right) \\ -\frac{1}{4} c_{12}\left(4 c_{12} c_{21} + c_{11}\left(5 - 4 c_{22}\right) + c_{22} - 1\right) \\ c_{12}\left(c_{11}\left(c_{22} - 1\right) - c_{12} c_{21}\right) \end{pmatrix} \tag{5.22}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(1)} \hat{a}_\sigma^{(3)} \right\rangle_{\hat{\rho}_{loc;0}} = \begin{pmatrix} c_{13} \\ c_{13}\left(c_{22}^2 + c_{11} - \frac{1}{2}\right) - c_{12} c_{22} c_{23} \\ \left(\frac{1}{16}\left(c_{13}\left(-4 c_{22}\left(4 c_{12} c_{21} + c_{22}\right) + 4 c_{11}\left(4 c_{22}^2 - 1\right) + 1\right) + \right.\right. \\ \left.\left. 4 c_{12}\left(4 c_{12} c_{21} + \left(1 - 4 c_{11}\right) c_{22}\right) c_{23}\right)\right) \\ c_{13}\left(c_{11} + 2 c_{22} - 1\right) - c_{12} c_{23} \\ \left(\frac{1}{4}\left(c_{13}\left(-2 c_{22} - 4 c_{12} c_{21}\left(c_{22} + 1\right) + c_{11}\left(4 c_{22}\left(c_{22} + 2\right) - 5\right) + 1\right) + \right.\right. \\ \left.\left. c_{12}\left(4 c_{12} c_{21} - 4 c_{11}\left(c_{22} + 1\right) + 1\right) c_{23}\right)\right) \\ c_{11}\left(c_{13}\left(2 c_{22} - 1\right) - c_{12} c_{23}\right) - c_{12} c_{13} c_{21} \end{pmatrix} \tag{5.23}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(2)} \hat{a}_\sigma^{(1)} \right\rangle_{\hat{\rho}_{loc;0}} = \begin{pmatrix} c_{21} \\ \frac{1}{2} c_{21} \left(2c_{22} - 1\right) \\ \frac{1}{16} c_{21} \left(1 - 4c_{22}\right) \\ c_{21} \left(c_{11} + c_{22} - 1\right) \\ -\frac{1}{4} c_{21} \left(c_{11} + 4c_{12}c_{21} + \left(5 - 4c_{11}\right) c_{22} - 1\right) \\ c_{21} \left(\left(c_{11} - 1\right) c_{22} - c_{12}c_{21}\right) \end{pmatrix} \tag{5.24}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(2)} \hat{a}_\sigma^{(2)} \right\rangle_{\hat{\rho}_{loc;0}} = \begin{pmatrix} c_{22} \\ c_{22}^2 + \frac{1}{2} \left(2c_{11}^2 - 1\right) c_{22} - c_{11}c_{12}c_{21} \\ \frac{1}{16} \left(4c_{22} \left(4c_{22} - 1\right) c_{11}^2 + 4c_{12}c_{21} \left(1 - 8c_{22}\right) c_{11} + 16c_{12}^2 c_{21}^2 - 4c_{22}^2 + c_{22}\right) \\ c_{22} \left(2c_{11} + c_{22} - 1\right) - c_{12}c_{21} \\ \frac{1}{4} \left(4c_{12}^2 c_{21}^2 + c_{12} \left(1 - 8 \left(c_{11} + 1\right) c_{22}\right) c_{21} + \left(2c_{11} - 1\right) c_{22} \left(\left(2c_{11} + 5\right) c_{22} - 1\right)\right) \\ c_{22} \left(\left(2c_{11} - 1\right) c_{22} - 2c_{12}c_{21}\right) \end{pmatrix} \tag{5.25}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(2)} \hat{a}_\sigma^{(3)} \right\rangle_{\hat{\rho}_{loc;0}} = \begin{pmatrix} c_{23} \\ \frac{1}{2} \left(2c_{11}^2 + 2c_{22} - 1\right) c_{23} - c_{11}c_{13}c_{21} \\ \begin{pmatrix} \frac{1}{16} \Big(4c_{13}c_{21} \left(4c_{12}c_{21} + c_{11} \left(1 - 4c_{22}\right)\right) + \\ \left(-4c_{22} + 4c_{11} \left(c_{11} \left(4c_{22} - 1\right) - 4c_{12}c_{21}\right) + 1\right) c_{23} \Big) \end{pmatrix} \\ \left(2c_{11} + c_{22} - 1\right) c_{23} - c_{13}c_{21} \\ \begin{pmatrix} \frac{1}{4} \Big(c_{13}c_{21} \left(4c_{12}c_{21} - 4 \left(c_{11} + 1\right) c_{22} + 1\right) + \\ \left(-2c_{11} - 4 \left(c_{11} + 1\right) c_{12}c_{21} + \left(4c_{11} \left(c_{11} + 2\right) - 5\right) c_{22}\right) c_{23} + c_{23} \Big) \end{pmatrix} \\ -c_{13}c_{21}c_{22} - \left(c_{12}c_{21} + \left(1 - 2c_{11}\right) c_{22}\right) c_{23} \end{pmatrix} \tag{5.26}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(3)} \hat{a}_\sigma^{(1)} \right\rangle_{\hat{\rho}_{loc;0}} =$$

$$\begin{pmatrix} c_{31} \\ \left(c_{22}^2 - \frac{1}{2}\right) c_{31} - c_{21} c_{22} c_{32} \\ \frac{1}{16}\left(\left(1 - 4c_{22}^2\right) c_{31} + 4 c_{21} c_{22} c_{32}\right) \\ \left(c_{11} + 2c_{22} - 2\right) c_{31} - c_{21} c_{32} \\ \begin{pmatrix} \frac{1}{4}\Big(\left(-2c_{22}\left(2c_{12}c_{21} + 2c_{22} + 1\right) + c_{11}\left(4c_{22}^2 - 1\right) + 2\right) c_{31} + \\ c_{21}\left(4c_{12}c_{21} - 4\left(c_{11} - 1\right) c_{22} + 1\right) c_{32} \Big) \end{pmatrix} \\ \left(-c_{11} - c_{12}c_{21} + 2\left(c_{11} - 1\right) c_{22} + 1\right) c_{31} - \left(c_{11} - 1\right) c_{21} c_{32} \end{pmatrix} \tag{5.27}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(3)} \hat{a}_\sigma^{(2)} \right\rangle_{\hat{\rho}_{loc;0}} =$$

$$\begin{pmatrix} c_{32} \\ \frac{1}{2}\left(2c_{11}^2 - 1\right) c_{32} - c_{11} c_{12} c_{31} \\ \frac{1}{16}\left(-4c_{32}c_{11}^2 + 4c_{12}c_{31}c_{11} + c_{32}\right) \\ \left(2c_{11} + c_{22} - 2\right) c_{32} - c_{12} c_{31} \\ \begin{pmatrix} \frac{1}{4}\Big(c_{12}\left(4c_{12}c_{21} - 4c_{11}\left(c_{22} - 1\right) + 1\right) c_{31} + \\ \left(2c_{11}\left(-2c_{12}c_{21} + 2c_{11}\left(c_{22} - 1\right) - 1\right) - c_{22} + 2\right) c_{32} \Big) \end{pmatrix} \\ \left(2c_{11} - 1\right)\left(c_{22} - 1\right) c_{32} + c_{12}\left(-\left(c_{22} - 1\right) c_{31} - c_{21} c_{32}\right) \end{pmatrix} \tag{5.28}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{a}_\sigma^{\dagger(3)} \hat{a}_\sigma^{(3)} \right\rangle_{\hat{\rho}_{loc;0}} = \tag{5.29}$$

$$\begin{pmatrix} c_{33} \\ -c_{11} c_{13} c_{31} - c_{22} c_{23} c_{32} + \frac{1}{2}\left(2c_{11}^2 + 2c_{22}^2 - 1\right) c_{33} \\ t_3 \\ -c_{13} c_{31} - c_{23} c_{32} + 2\left(c_{11} + c_{22} - 1\right) c_{33} \\ t_5 \\ \begin{pmatrix} c_{13}\left(\left(1 - 2c_{22}\right) c_{31} + c_{21} c_{32}\right) + c_{12}\left(c_{23} c_{31} - 2c_{21} c_{33}\right) - \\ \left(2c_{11} - 1\right)\left(c_{23} c_{32} + \left(1 - 2c_{22}\right) c_{33}\right) \end{pmatrix} \end{pmatrix} \tag{5.30}$$

where

$t_3 = -c_{22}c_{23}c_{32}c_{11}^2 + c_{22}^2c_{33}c_{11}^2 - \frac{1}{4}c_{33}c_{11}^2 - c_{13}c_{22}^2c_{31}c_{11} + \frac{1}{4}c_{13}c_{31}c_{11} + c_{12}c_{22}c_{23}c_{31}c_{11} + c_{13}c_{21}c_{22}c_{32}c_{11} + c_{12}c_{21}c_{23}c_{32}c_{11} - 2c_{12}c_{21}c_{22}c_{33}c_{11} + c_{12}c_{13}c_{21}c_{22}c_{31} - c_{12}^2c_{21}c_{23}c_{31} - c_{12}c_{13}c_{21}^2c_{32} + \frac{1}{4}c_{22}c_{23}c_{32} + c_{12}^2c_{21}^2c_{33} - \frac{1}{4}c_{22}^2c_{33} + \frac{c_{33}}{16}$

and

$t_5 = -c_{23}c_{32}c_{11}^2 + 2c_{22}c_{33}c_{11}^2 - c_{33}c_{11}^2 + c_{13}c_{31}c_{11} - 2c_{13}c_{22}c_{31}c_{11} + c_{12}c_{23}c_{31}c_{11} + c_{13}c_{21}c_{32}c_{11} - 2c_{22}c_{23}c_{32}c_{11} + 2c_{22}^2c_{33}c_{11} - 2c_{12}c_{21}c_{33}c_{11} - \frac{1}{2}c_{33}c_{11} - c_{13}c_{22}^2c_{31} + \frac{1}{4}c_{13}c_{31} + c_{12}c_{13}c_{21}c_{31} + c_{12}c_{22}c_{23}c_{31} + c_{13}c_{21}c_{22}c_{32} + c_{12}c_{21}c_{23}c_{32} + c_{22}c_{23}c_{32} + \frac{1}{4}c_{23}c_{32} - c_{22}^2c_{33} - 2c_{12}c_{21}c_{22}c_{33} - \frac{1}{2}c_{22}c_{33} + \frac{c_{33}}{2}$

and

$$\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\hat{P}_3^{(3)}\hat{a}_\uparrow^{\dagger(3)}\hat{a}_\uparrow^{(3)}\hat{a}_\downarrow^{\dagger(3)}\hat{a}_\downarrow^{(3)}\right\rangle_{\hat{\rho}_{loc;0}} = \tag{5.31}$$

$$\begin{pmatrix} c_{33}^2 \\ c_{13}^2c_{31}^2 + c_{23}^2c_{32}^2 + \frac{1}{2}\left(2c_{11}^2 + 2c_{22}^2 - 1\right)c_{33}^2 - 2\left(c_{11}c_{13}c_{31} + c_{22}c_{23}c_{32}\right)c_{33} \\ t_3 \\ 2c_{33}\left(-c_{13}c_{31} - c_{23}c_{32} + \left(c_{11} + c_{22} - 1\right)c_{33}\right) \\ t_5 \\ t_6 \end{pmatrix} \tag{5.32}$$

where

$t_3 = c_{23}^2c_{32}^2c_{11}^2 + c_{22}^2c_{33}^2c_{11}^2 - \frac{1}{4}c_{33}^2c_{11}^2 - 2c_{22}c_{23}c_{32}c_{33}c_{11}^2 - 2c_{13}c_{21}c_{23}c_{32}^2c_{11} - 2c_{12}c_{21}c_{22}c_{33}^2c_{11} - 2c_{12}c_{23}^2c_{31}c_{32}c_{11} + 2c_{13}c_{22}c_{23}c_{31}c_{32}c_{11} - 2c_{13}c_{22}^2c_{31}c_{33}c_{11} + \frac{1}{2}c_{13}c_{31}c_{33}c_{11} + 2c_{12}c_{22}c_{23}c_{31}c_{33}c_{11} + 2c_{13}c_{21}c_{22}c_{32}c_{33}c_{11} + 2c_{12}c_{21}c_{23}c_{32}c_{33}c_{11} - \frac{1}{4}c_{13}^2c_{31}^2 + c_{13}^2c_{22}^2c_{31}^2 + c_{12}^2c_{23}^2c_{31}^2 - 2c_{12}c_{13}c_{22}c_{23}c_{31}^2 + c_{13}^2c_{21}^2c_{32}^2 - \frac{1}{4}c_{23}^2c_{32}^2 + c_{12}^2c_{21}^2c_{33}^2 - \frac{1}{4}c_{22}^2c_{33}^2 + \frac{c_{33}^2}{16} - 2c_{13}^2c_{21}c_{22}c_{31}c_{32} + 2c_{12}c_{13}c_{21}c_{23}c_{31}c_{32} + 2c_{12}c_{13}c_{21}c_{22}c_{31}c_{33} - 2c_{12}^2c_{21}c_{23}c_{31}c_{33} - 2c_{12}c_{13}c_{21}^2c_{32}c_{33} + \frac{1}{2}c_{22}c_{23}c_{32}c_{33}$

and

$t_5 = 2c_{22}c_{33}^2c_{11}^2 - c_{33}^2c_{11}^2 - 2c_{23}c_{32}c_{33}c_{11}^2 + 2c_{23}^2c_{32}^2c_{11} + 2c_{22}^2c_{33}^2c_{11} - 2c_{12}c_{21}c_{33}^2c_{11} - \frac{1}{2}c_{33}^2c_{11} + 2c_{13}c_{23}c_{31}c_{32}c_{11} + 2c_{13}c_{31}c_{33}c_{11} - 4c_{13}c_{22}c_{31}c_{33}c_{11} + 2c_{12}c_{23}c_{31}c_{33}c_{11} + 2c_{13}c_{21}c_{32}c_{33}c_{11} - 4c_{22}c_{23}c_{32}c_{33}c_{11} - c_{13}^2c_{31}^2 + 2c_{13}^2c_{22}c_{31}^2 - 2c_{12}c_{13}c_{23}c_{31}^2 - c_{23}^2c_{32}^2 - 2c_{13}c_{21}c_{23}c_{32}^2 - c_{22}^2c_{33}^2 - 2c_{12}c_{21}c_{22}c_{33}^2 - \frac{1}{2}c_{22}c_{33}^2 + \frac{c_{33}^2}{2} - 2c_{12}c_{23}^2c_{31}c_{32} - 2c_{13}^2c_{21}c_{31}c_{32} + 2c_{13}c_{22}c_{23}c_{31}c_{32} - 2c_{13}c_{22}^2c_{31}c_{33} + \frac{1}{2}c_{13}c_{31}c_{33} + 2c_{12}c_{13}c_{21}c_{31}c_{33} + 2c_{12}c_{22}c_{23}c_{31}c_{33} + 2c_{13}c_{21}c_{22}c_{32}c_{33} + 2c_{12}c_{21}c_{23}c_{32}c_{33} +$

$2c_{22}c_{23}c_{32}c_{33} + \frac{1}{2}c_{23}c_{32}c_{33}$

and

$t_6 = -2c_{11}c_{33}^2 - 2c_{12}c_{21}c_{33}^2 + 4c_{11}c_{22}c_{33}^2 - 2c_{22}c_{33}^2 + c_{33}^2 + 2c_{13}c_{31}c_{33} - 4c_{13}c_{22}c_{31}c_{33} + 2c_{12}c_{23}c_{31}c_{33} + 2c_{13}c_{21}c_{32}c_{33} - 4c_{11}c_{23}c_{32}c_{33} + 2c_{23}c_{32}c_{33} + 2c_{13}c_{23}c_{31}c_{32}$.

Notice that the local self-energy is not sufficient to compute the density-density correlation between the impurity and the bath. We denote the non-interacting Green's function of the relevant block as

$$\boldsymbol{g}_0 = \begin{pmatrix} a_{11} & 0 & a_{12} & 0 & a_{13} & 0 & c_{11} & 0 & c_{12} & 0 & c_{13} & 0 \\ 0 & a_{11} & 0 & a_{12} & 0 & a_{13} & 0 & c_{11} & 0 & c_{12} & 0 & c_{13} \\ a_{21} & 0 & a_{22} & 0 & a_{23} & 0 & c_{21} & 0 & c_{22} & 0 & c_{23} & 0 \\ 0 & a_{21} & 0 & a_{22} & 0 & a_{23} & 0 & c_{21} & 0 & c_{22} & 0 & c_{23} \\ a_{31} & 0 & a_{32} & 0 & a_{33} & 0 & c_{31} & 0 & c_{32} & 0 & c_{33} & 0 \\ 0 & a_{31} & 0 & a_{32} & 0 & a_{33} & 0 & c_{31} & 0 & c_{32} & 0 & c_{33} \\ d_{11} & 0 & d_{12} & 0 & d_{13} & 0 & b_{11} & 0 & b_{12} & 0 & b_{13} & 0 \\ 0 & d_{11} & 0 & d_{12} & 0 & d_{13} & 0 & b_{11} & 0 & b_{12} & 0 & b_{13} \\ d_{21} & 0 & d_{22} & 0 & d_{23} & 0 & b_{21} & 0 & b_{22} & 0 & b_{23} & 0 \\ 0 & d_{21} & 0 & d_{22} & 0 & d_{23} & 0 & b_{21} & 0 & b_{22} & 0 & b_{23} \\ d_{31} & 0 & d_{32} & 0 & d_{33} & 0 & b_{31} & 0 & b_{32} & 0 & b_{33} & 0 \\ 0 & d_{31} & 0 & d_{32} & 0 & d_{33} & 0 & b_{31} & 0 & b_{32} & 0 & b_{33} \end{pmatrix} \tag{5.33}$$

where $\boldsymbol{a}$ is the Green's function for the impurity, $\boldsymbol{b}$ is the Green's function for the selected bath orbital, and $\boldsymbol{c}$ and $\boldsymbol{d}$ are the Green's function for the off-diagonal part between the impurity and the bath orbital. Using Wick's theorem, we can compute

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \right\rangle_{\hat{\rho}_{rel;0}} = \begin{pmatrix} 1 \\ a_{11}^2 + a_{22}^2 - \frac{1}{2} \\ \left(a_{22}^2 - \frac{1}{4}\right) a_{11}^2 - 2a_{12}a_{21}a_{22}a_{11} + a_{12}^2 a_{21}^2 - \frac{a_{22}^2}{4} + \frac{1}{16} \\ 2\left(a_{11} + a_{22} - 1\right) \\ \frac{1}{2}\left(\left(4a_{22} - 2\right) a_{11}^2 + \left(4a_{22}^2 - 4a_{12}a_{21} - 1\right) a_{11} - a_{22}\left(4a_{12}a_{21} + 2a_{22} + 1\right) + 1\right) \\ -2a_{12}a_{21} - 2a_{22} + a_{11}\left(4a_{22} - 2\right) + 1 \end{pmatrix} \tag{5.34}$$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{n}_{loc;\sigma}^{(3)} \hat{n}_{bath;\sigma}^{(3)} \right\rangle_{\hat{\rho}_{rel;0}} = \begin{pmatrix} a_{33}b_{33} - c_{33}d_{33} \\ t_2 \\ t_3 \\ t_4 \\ t_5 \\ t_6 \end{pmatrix} \tag{5.35}$$

where

$t_2 = a_{33}a_{11}^2 b_{33} - a_{13}a_{31}a_{11}b_{33} - a_{22}a_{23}a_{32}b_{33} + a_{22}^2 a_{33}b_{33} - \frac{1}{2}a_{33}b_{33} - a_{11}^2 c_{33}d_{33} - a_{33}a_{11}c_{13}d_{31} + a_{13}a_{11}c_{33}d_{31} + a_{31}a_{11}c_{13}d_{33} - a_{22}a_{33}c_{23}d_{32} + a_{22}a_{23}c_{33}d_{32} + a_{22}a_{32}c_{23}d_{33} - a_{22}^2 c_{33}d_{33} + \frac{1}{2}c_{33}d_{33}$

and

$t_3 = -a_{22}a_{23}a_{32}b_{33}a_{11}^2 + a_{22}^2 a_{33}b_{33}a_{11}^2 - \frac{1}{4}a_{33}b_{33}a_{11}^2 - a_{22}a_{33}c_{23}d_{32}a_{11}^2 + a_{22}a_{23}c_{33}d_{32}a_{11}^2 + a_{22}a_{32}c_{23}d_{33}a_{11}^2 - a_{22}^2 c_{33}d_{33}a_{11}^2 + \frac{1}{4}c_{33}d_{33}a_{11}^2 - a_{13}a_{22}^2 a_{31}b_{33}a_{11} + \frac{1}{4}a_{13}a_{31}b_{33}a_{11} + a_{12}a_{22}a_{23}a_{31}b_{33}a_{11} + a_{13}a_{21}a_{22}a_{32}b_{33}a_{11} + a_{12}a_{21}a_{23}a_{32}b_{33}a_{11} - 2a_{12}a_{21}a_{22}a_{33}b_{33}a_{11} + a_{22}a_{23}a_{32}c_{13}d_{31}a_{11} - a_{22}^2 a_{33}c_{13}d_{31}a_{11} + \frac{1}{4}a_{33}c_{13}d_{31}a_{11} - a_{13}a_{22}a_{32}c_{23}d_{31}a_{11} + a_{12}a_{22}a_{33}c_{23}d_{31}a_{11} + a_{13}a_{22}^2 c_{33}d_{31}a_{11} - \frac{1}{4}a_{13}c_{33}d_{31}a_{11} - a_{12}a_{22}a_{23}c_{33}d_{31}a_{11} - a_{22}a_{23}a_{31}c_{13}d_{32}a_{11} + a_{21}a_{22}a_{33}c_{13}d_{32}a_{11} + a_{13}a_{22}a_{31}c_{23}d_{32}a_{11} + a_{12}a_{21}a_{33}c_{23}d_{32}a_{11} - a_{13}a_{21}a_{22}c_{33}d_{32}a_{11} - a_{12}a_{21}a_{23}c_{33}d_{32}a_{11} + a_{22}^2 a_{31}c_{13}d_{33}a_{11} - \frac{1}{4}a_{31}c_{13}d_{33}a_{11} - a_{21}a_{22}a_{32}c_{13}d_{33}a_{11} - a_{12}a_{22}a_{31}c_{23}d_{33}a_{11} - a_{12}a_{21}a_{32}c_{23}d_{33}a_{11} + 2a_{12}a_{21}a_{22}c_{33}d_{33}a_{11} + a_{12}a_{13}a_{21}a_{22}a_{31}b_{33} - a_{12}^2 a_{21}a_{23}a_{31}b_{33} - a_{12}a_{13}a_{21}^2 a_{32}b_{33} + \frac{1}{4}a_{22}a_{23}a_{32}b_{33} + a_{12}^2 a_{21}^2 a_{33}b_{33} - \frac{1}{4}a_{22}^2 a_{33}b_{33} + \frac{1}{16}a_{33}b_{33} - a_{12}a_{21}a_{23}a_{32}c_{13}d_{31} + a_{12}a_{21}a_{22}a_{33}c_{13}d_{31} + a_{12}a_{13}a_{21}a_{32}c_{23}d_{31} - a_{12}^2 a_{21}a_{33}c_{23}d_{31} - a_{12}a_{13}a_{21}a_{22}c_{33}d_{31} + a_{12}^2 a_{21}a_{23}c_{33}d_{31} + a_{12}a_{21}a_{23}a_{31}c_{13}d_{32} - a_{12}a_{21}^2 a_{33}c_{13}d_{32} - a_{12}a_{13}a_{21}a_{31}c_{23}d_{32} + \frac{1}{4}a_{22}a_{33}c_{23}d_{32} + a_{12}a_{13}a_{21}^2 c_{33}d_{32} - \frac{1}{4}a_{22}a_{23}c_{33}d_{32} - a_{12}a_{21}a_{22}a_{31}c_{13}d_{33} + a_{12}a_{21}^2 a_{32}c_{13}d_{33} + a_{12}^2 a_{21}a_{31}c_{23}d_{33} - \frac{1}{4}a_{22}a_{32}c_{23}d_{33} - a_{12}^2 a_{21}^2 c_{33}d_{33} + \frac{1}{4}a_{22}^2 c_{33}d_{33} - \frac{1}{16}c_{33}d_{33}$

and

$t_4 = -a_{13}a_{31}b_{33} - a_{23}a_{32}b_{33} + 2a_{11}a_{33}b_{33} + 2a_{22}a_{33}b_{33} - 2a_{33}b_{33} - a_{33}c_{13}d_{31} + a_{13}c_{33}d_{31} - a_{33}c_{23}d_{32} + a_{23}c_{33}d_{32} + a_{31}c_{13}d_{33} + a_{32}c_{23}d_{33} - 2a_{11}c_{33}d_{33} - 2a_{22}c_{33}d_{33} + 2c_{33}d_{33}$

and

$t_5 = -a_{23}a_{32}b_{33}a_{11}^2 + 2a_{22}a_{33}b_{33}a_{11}^2 - a_{33}b_{33}a_{11}^2 - a_{33}c_{23}d_{32}a_{11}^2 + a_{23}c_{33}d_{32}a_{11}^2 +$

$a_{32}c_{23}d_{33}a_{11}^2 - 2a_{22}c_{33}d_{33}a_{11}^2 + c_{33}d_{33}a_{11}^2 + a_{13}a_{31}b_{33}a_{11} - 2a_{13}a_{22}a_{31}b_{33}a_{11} + a_{12}a_{23}a_{31}b_{33}a_{11} + a_{13}a_{21}a_{32}b_{33}a_{11} - 2a_{22}a_{23}a_{32}b_{33}a_{11} + 2a_{22}^2a_{33}b_{33}a_{11} - 2a_{12}a_{21}a_{33}b_{33}a_{11} - \frac{1}{2}a_{33}b_{33}a_{11} + a_{23}a_{32}c_{13}d_{31}a_{11} - 2a_{22}a_{33}c_{13}d_{31}a_{11} + a_{33}c_{13}d_{31}a_{11} - a_{13}a_{32}c_{23}d_{31}a_{11} + a_{12}a_{33}c_{23}d_{31}a_{11} - a_{13}c_{33}d_{31}a_{11} + 2a_{13}a_{22}c_{33}d_{31}a_{11} - a_{12}a_{23}c_{33}d_{31}a_{11} - a_{23}a_{31}c_{13}d_{32}a_{11} + a_{21}a_{33}c_{13}d_{32}a_{11} + a_{13}a_{31}c_{23}d_{32}a_{11} - 2a_{22}a_{33}c_{23}d_{32}a_{11} - a_{13}a_{21}c_{33}d_{32}a_{11} + 2a_{22}a_{23}c_{33}d_{32}a_{11} + 2a_{22}a_{31}c_{13}d_{33}a_{11} - a_{31}c_{13}d_{33}a_{11} - a_{21}a_{32}c_{13}d_{33}a_{11} - a_{12}a_{31}c_{23}d_{33}a_{11} + 2a_{22}a_{32}c_{23}d_{33}a_{11} - 2a_{22}^2c_{33}d_{33}a_{11} + 2a_{12}a_{21}c_{33}d_{33}a_{11} + \frac{1}{2}c_{33}d_{33}a_{11} - a_{13}a_{22}^2a_{31}b_{33} + \frac{1}{4}a_{13}a_{31}b_{33} + a_{12}a_{13}a_{21}a_{31}b_{33} + a_{12}a_{22}a_{23}a_{31}b_{33} + a_{13}a_{21}a_{22}a_{32}b_{33} + a_{12}a_{21}a_{23}a_{32}b_{33} + a_{22}a_{23}a_{32}b_{33} + \frac{1}{4}a_{23}a_{32}b_{33} - a_{22}^2a_{33}b_{33} - 2a_{12}a_{21}a_{22}a_{33}b_{33} - \frac{1}{2}a_{22}a_{33}b_{33} + \frac{1}{2}a_{33}b_{33} + a_{22}a_{23}a_{32}c_{13}d_{31} - a_{22}^2a_{33}c_{13}d_{31} + a_{12}a_{21}a_{33}c_{13}d_{31} + \frac{1}{4}a_{33}c_{13}d_{31} - a_{13}a_{22}a_{32}c_{23}d_{31} + a_{12}a_{22}a_{33}c_{23}d_{31} + a_{13}a_{22}^2c_{33}d_{31} - \frac{1}{4}a_{13}c_{33}d_{31} - a_{12}a_{13}a_{21}c_{33}d_{31} - a_{12}a_{22}a_{23}c_{33}d_{31} - a_{22}a_{23}a_{31}c_{13}d_{32} + a_{21}a_{22}a_{33}c_{13}d_{32} + a_{13}a_{22}a_{31}c_{23}d_{32} + a_{12}a_{21}a_{33}c_{23}d_{32} + a_{22}a_{33}c_{23}d_{32} + \frac{1}{4}a_{33}c_{23}d_{32} - a_{13}a_{21}a_{22}c_{33}d_{32} - a_{12}a_{21}a_{23}c_{33}d_{32} - a_{22}a_{23}c_{33}d_{32} - \frac{1}{4}a_{23}c_{33}d_{32} + a_{22}^2a_{31}c_{13}d_{33} - a_{12}a_{21}a_{31}c_{13}d_{33} - \frac{1}{4}a_{31}c_{13}d_{33} - a_{21}a_{22}a_{32}c_{13}d_{33} - a_{12}a_{22}a_{31}c_{23}d_{33} - a_{12}a_{21}a_{32}c_{23}d_{33} - a_{22}a_{32}c_{23}d_{33} - \frac{1}{4}a_{32}c_{23}d_{33} + a_{22}^2c_{33}d_{33} + 2a_{12}a_{21}a_{22}c_{33}d_{33} + \frac{1}{2}a_{22}c_{33}d_{33} - \frac{1}{2}c_{33}d_{33}$

and

$t_6 = a_{13}a_{31}b_{33} - 2a_{13}a_{22}a_{31}b_{33} + a_{12}a_{23}a_{31}b_{33} + a_{13}a_{21}a_{32}b_{33} - 2a_{11}a_{23}a_{32}b_{33} + a_{23}a_{32}b_{33} - 2a_{11}a_{33}b_{33} - 2a_{12}a_{21}a_{33}b_{33} + 4a_{11}a_{22}a_{33}b_{33} - 2a_{22}a_{33}b_{33} + a_{33}b_{33} + a_{23}a_{32}c_{13}d_{31} - 2a_{22}a_{33}c_{13}d_{31} + a_{33}c_{13}d_{31} - a_{13}a_{32}c_{23}d_{31} + a_{12}a_{33}c_{23}d_{31} - a_{13}c_{33}d_{31} + 2a_{13}a_{22}c_{33}d_{31} - a_{12}a_{23}c_{33}d_{31} - a_{23}a_{31}c_{13}d_{32} + a_{21}a_{33}c_{13}d_{32} + a_{13}a_{31}c_{23}d_{32} - 2a_{11}a_{33}c_{23}d_{32} + a_{33}c_{23}d_{32} - a_{13}a_{21}c_{33}d_{32} + 2a_{11}a_{23}c_{33}d_{32} - a_{23}c_{33}d_{32} + 2a_{22}a_{31}c_{13}d_{33} - a_{31}c_{13}d_{33} - a_{21}a_{32}c_{13}d_{33} - a_{12}a_{31}c_{23}d_{33} + 2a_{11}a_{32}c_{23}d_{33} - a_{32}c_{23}d_{33} + 2a_{11}c_{33}d_{33} + 2a_{12}a_{21}c_{33}d_{33} - 4a_{11}a_{22}c_{33}d_{33} + 2a_{22}c_{33}d_{33} - c_{33}d_{33}$

and

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{P}_3^{(3)} \hat{n}_{loc;\sigma}^{(3)} \hat{n}_{bath;\bar{\sigma}}^{(3)} \right\rangle_{\hat{\rho}_{rel;0}} = \begin{pmatrix} a_{33}b_{33} \\ t_2 \\ t_3 \\ t_4 \\ t_5 \\ t_6 \end{pmatrix} \tag{5.36}$$

where

$t_2 = a_{33}a_{11}^2b_{33} - a_{13}a_{31}a_{11}b_{33} - a_{22}a_{23}a_{32}b_{33} + a_{22}^2a_{33}b_{33} - \frac{1}{2}a_{33}b_{33} - a_{33}a_{11}c_{13}d_{31} + a_{13}a_{31}c_{13}d_{31} + a_{23}a_{32}c_{23}d_{32} - a_{22}a_{33}c_{23}d_{32}$

and

$t_3 = -a_{22}a_{23}a_{32}b_{33}a_{11}^2 + a_{22}^2a_{33}b_{33}a_{11}^2 - \frac{1}{4}a_{33}b_{33}a_{11}^2 + a_{23}a_{32}c_{23}d_{32}a_{11}^2 - a_{22}a_{33}c_{23}d_{32}a_{11}^2 - a_{13}a_{22}^2a_{31}b_{33}a_{11} + \frac{1}{4}a_{13}a_{31}b_{33}a_{11} + a_{12}a_{22}a_{23}a_{31}b_{33}a_{11} + a_{13}a_{21}a_{22}a_{32}b_{33}a_{11} + a_{12}a_{21}a_{23}a_{32}b_{33}a_{11} - 2a_{12}a_{21}a_{22}a_{33}b_{33}a_{11} + a_{22}a_{23}a_{32}c_{13}d_{31}a_{11} - a_{22}^2a_{33}c_{13}d_{31}a_{11} + \frac{1}{4}a_{33}c_{13}d_{31}a_{11} - a_{12}a_{23}a_{32}c_{23}d_{31}a_{11} + a_{12}a_{22}a_{33}c_{23}d_{31}a_{11} - a_{21}a_{23}a_{32}c_{13}d_{32}a_{11} + a_{21}a_{22}a_{33}c_{13}d_{32}a_{11} + a_{13}a_{22}a_{31}c_{23}d_{32}a_{11} - a_{12}a_{23}a_{31}c_{23}d_{32}a_{11} - a_{13}a_{21}a_{32}c_{23}d_{32}a_{11} + a_{12}a_{21}a_{33}c_{23}d_{32}a_{11} + a_{12}a_{13}a_{21}a_{22}a_{31}b_{33} - a_{12}^2a_{21}a_{23}a_{31}b_{33} - a_{12}a_{13}a_{21}^2a_{32}b_{33} + \frac{1}{4}a_{22}a_{23}a_{32}b_{33} + a_{12}^2a_{21}^2a_{33}b_{33} - \frac{1}{4}a_{22}^2a_{33}b_{33} + \frac{1}{16}a_{33}b_{33} + a_{13}a_{22}^2a_{31}c_{13}d_{31} - \frac{1}{4}a_{13}a_{31}c_{13}d_{31} - a_{12}a_{22}a_{23}a_{31}c_{13}d_{31} - a_{13}a_{21}a_{22}a_{32}c_{13}d_{31} + a_{12}a_{21}a_{22}a_{33}c_{13}d_{31} - a_{12}a_{13}a_{22}a_{31}c_{23}d_{31} + a_{12}^2a_{23}a_{31}c_{23}d_{31} + a_{12}a_{13}a_{21}a_{32}c_{23}d_{31} - a_{12}^2a_{21}a_{33}c_{23}d_{31} - a_{13}a_{21}a_{22}a_{31}c_{13}d_{32} + a_{12}a_{21}a_{23}a_{31}c_{13}d_{32} + a_{13}a_{21}^2a_{32}c_{13}d_{32} - a_{12}a_{21}^2a_{33}c_{13}d_{32} - \frac{1}{4}a_{23}a_{32}c_{23}d_{32} + \frac{1}{4}a_{22}a_{33}c_{23}d_{32}$

and

$t_4 = -a_{13}a_{31}b_{33} - a_{23}a_{32}b_{33} + 2a_{11}a_{33}b_{33} + 2a_{22}a_{33}b_{33} - 2a_{33}b_{33} - a_{33}c_{13}d_{31} - a_{33}c_{23}d_{32}$

and

$t_5 = -a_{23}a_{32}b_{33}a_{11}^2 + 2a_{22}a_{33}b_{33}a_{11}^2 - a_{33}b_{33}a_{11}^2 - a_{33}c_{23}d_{32}a_{11}^2 + a_{13}a_{31}b_{33}a_{11} - 2a_{13}a_{22}a_{31}b_{33}a_{11} + a_{12}a_{23}a_{31}b_{33}a_{11} + a_{13}a_{21}a_{32}b_{33}a_{11} - 2a_{22}a_{23}a_{32}b_{33}a_{11} + 2a_{22}^2a_{33}b_{33}a_{11} - 2a_{12}a_{21}a_{33}b_{33}a_{11} - \frac{1}{2}a_{33}b_{33}a_{11} + a_{23}a_{32}c_{13}d_{31}a_{11} - 2a_{22}a_{33}c_{13}d_{31}a_{11} + a_{33}c_{13}d_{31}a_{11} + a_{12}a_{33}c_{23}d_{31}a_{11} + a_{21}a_{33}c_{13}d_{32}a_{11} + a_{13}a_{31}c_{23}d_{32}a_{11} + 2a_{23}a_{32}c_{23}d_{32}a_{11} - 2a_{22}a_{33}c_{23}d_{32}a_{11} - a_{13}a_{22}^2a_{31}b_{33} + \frac{1}{4}a_{13}a_{31}b_{33} + a_{12}a_{13}a_{21}a_{31}b_{33} + a_{12}a_{22}a_{23}a_{31}b_{33} + a_{13}a_{21}a_{22}a_{32}b_{33} + a_{12}a_{21}a_{23}a_{32}b_{33} + a_{22}a_{23}a_{32}b_{33} + \frac{1}{4}a_{23}a_{32}b_{33} - a_{22}^2a_{33}b_{33} - 2a_{12}a_{21}a_{22}a_{33}b_{33} - \frac{1}{2}a_{22}a_{33}b_{33} + \frac{1}{2}a_{33}b_{33} - a_{13}a_{31}c_{13}d_{31} + 2a_{13}a_{22}a_{31}c_{13}d_{31} - a_{12}a_{23}a_{31}c_{13}d_{31} - a_{13}a_{21}a_{32}c_{13}d_{31} + a_{22}a_{23}a_{32}c_{13}d_{31} - a_{22}^2a_{33}c_{13}d_{31} + a_{12}a_{21}a_{33}c_{13}d_{31} + \frac{1}{4}a_{33}c_{13}d_{31} - a_{12}a_{13}a_{31}c_{23}d_{31} - a_{12}a_{23}a_{32}c_{23}d_{31} + a_{12}a_{22}a_{33}c_{23}d_{31} - a_{13}a_{21}a_{31}c_{13}d_{32} - a_{21}a_{23}a_{32}c_{13}d_{32} + a_{21}a_{22}a_{33}c_{13}d_{32} + a_{13}a_{22}a_{31}c_{23}d_{32} - a_{12}a_{23}a_{31}c_{23}d_{32} - a_{13}a_{21}a_{32}c_{23}d_{32} - a_{23}a_{32}c_{23}d_{32} + a_{12}a_{21}a_{33}c_{23}d_{32} + a_{22}a_{33}c_{23}d_{32} + \frac{1}{4}a_{33}c_{23}d_{32}$

and

$t_6 = a_{13}a_{31}b_{33} - 2a_{13}a_{22}a_{31}b_{33} + a_{12}a_{23}a_{31}b_{33} + a_{13}a_{21}a_{32}b_{33} - 2a_{11}a_{23}a_{32}b_{33} + a_{23}a_{32}b_{33} -$

$2a_{11}a_{33}b_{33} - 2a_{12}a_{21}a_{33}b_{33} + 4a_{11}a_{22}a_{33}b_{33} - 2a_{22}a_{33}b_{33} + a_{33}b_{33} + a_{23}a_{32}c_{13}d_{31} - 2a_{22}a_{33}c_{13}d_{31} + a_{33}c_{13}d_{31} + a_{12}a_{33}c_{23}d_{31} + a_{21}a_{33}c_{13}d_{32} + a_{13}a_{31}c_{23}d_{32} - 2a_{11}a_{33}c_{23}d_{32} + a_{33}c_{23}d_{32}$

Using the above expressions, we have a complete theory to compute the local interacting discrete Green's function, double occupancy, and density-density correlation between the impurity and bath orbital.

It is also pedagogical to demonstrate that the generating functional can be used to obtain the same results. Consider the spin dependent non-interacting discrete Green's function

$$\boldsymbol{g}_0 = \begin{pmatrix} c_{11\uparrow} & 0 & c_{12\uparrow} & 0 & c_{13\uparrow} & 0 \\ 0 & c_{11\downarrow} & 0 & c_{12\downarrow} & 0 & c_{13\downarrow} \\ c_{21\uparrow} & 0 & c_{22\uparrow} & 0 & c_{23\uparrow} & 0 \\ 0 & c_{21\downarrow} & 0 & c_{22\downarrow} & 0 & c_{23\downarrow} \\ c_{31\uparrow} & 0 & c_{32\uparrow} & 0 & c_{33\uparrow} & 0 \\ 0 & c_{31\downarrow} & 0 & c_{32\downarrow} & 0 & c_{33\downarrow} \end{pmatrix}. \tag{5.37}$$

The generating functional is given as

$$Z\left(\boldsymbol{g}_0\right) = \left\langle \hat{P} \right\rangle_{\varrho(\boldsymbol{g}_0)} \tag{5.38}$$

Recall that we represent the generating functional as a vector in the following monomial basis

$$\left\{1, u, u^2, \mu, \mu u, \mu^2\right\}. \tag{5.39}$$

The six components of the generating functional are then given as

$$[Z(\boldsymbol{g}_0)]_1 = 1, \tag{5.40}$$

$$[Z(\boldsymbol{g}_0)]_2 = c_{11\downarrow}c_{11\uparrow} + c_{22\downarrow}c_{22\uparrow} - \frac{1}{2}, \tag{5.41}$$

$$\begin{aligned}[Z(\boldsymbol{g}_0)]_3 =& \frac{1}{16}\Big(- 4c_{22\downarrow}c_{22\uparrow} + 16c_{12\downarrow}c_{21\downarrow}\left(c_{12\uparrow}c_{21\uparrow} - c_{11\uparrow}c_{22\uparrow}\right) + \\ & 4c_{11\downarrow}\left(c_{11\uparrow}\left(4c_{22\downarrow}c_{22\uparrow} - 1\right) - 4c_{22\downarrow}c_{12\uparrow}c_{21\uparrow}\right) + 1\Big),\end{aligned} \tag{5.42}$$

$$[Z(\boldsymbol{g}_0)]_4 = c_{11\downarrow} + c_{22\downarrow} + c_{11\uparrow} + c_{22\uparrow} - 2, \tag{5.43}$$

$$\begin{aligned}[Z(\boldsymbol{g}_0)]_5 =& \frac{1}{4}\Big(- \left(4c_{12\downarrow}c_{21\downarrow} + 1\right)c_{22\uparrow} - c_{22\downarrow}\left(4c_{12\uparrow}c_{21\uparrow} + 4c_{22\uparrow} + 1\right) + \\ & c_{11\uparrow}\left(4c_{22\downarrow}c_{22\uparrow} - 4c_{12\downarrow}c_{21\downarrow} - 1\right) + \\ & c_{11\downarrow}\left(4c_{22\downarrow}c_{22\uparrow} + 4c_{11\uparrow}\left(c_{22\downarrow} + c_{22\uparrow} - 1\right) - 4c_{12\uparrow}c_{21\uparrow} - 1\right) + 2\Big),\end{aligned} \tag{5.44}$$

$$\begin{aligned}[Z(\boldsymbol{g}_0)]_6 =& c_{11\downarrow}\left(c_{22\downarrow} + c_{22\uparrow} - 1\right) + c_{11\uparrow}\left(c_{22\downarrow} + c_{22\uparrow} - 1\right) - c_{12\downarrow}c_{21\downarrow} - \\ & c_{22\downarrow} - c_{12\uparrow}c_{21\uparrow} - c_{22\uparrow} + 1.\end{aligned} \tag{5.45}$$

Recall the expression for the interacting Green function

$$[\boldsymbol{g}]_{ij} = [\boldsymbol{g}_0]_{ij} + \frac{1}{Z}\frac{\partial Z}{\partial [\boldsymbol{g}_0]_{mn}}[\boldsymbol{g}_0]_{mj}[\mathbf{1} - \boldsymbol{g}_0]_{in}. \tag{5.46}$$

We can rewrite the above equation into matrix form as

$$\left\langle \hat{P}\hat{\boldsymbol{N}} \right\rangle - \left\langle \hat{P} \right\rangle \left\langle \hat{\boldsymbol{N}} \right\rangle = \left(1 - \boldsymbol{g}_0\right)\frac{\partial Z}{\partial \boldsymbol{g}_0^T}\boldsymbol{g}_0. \tag{5.47}$$

Taking the first entry of the monomial basis, we get

$$\left[\left\langle \hat{P}\hat{\boldsymbol{N}}_{\uparrow\uparrow} \right\rangle\right]_1 - \left[\left\langle \hat{P} \right\rangle\right]_1 \left[\left\langle \hat{\boldsymbol{N}}_{\uparrow\uparrow} \right\rangle\right]_1 = \left(\mathbf{1} - \boldsymbol{g}_{0;\uparrow\uparrow}\right)\left(\frac{\partial [Z]_1}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow}\boldsymbol{g}_{0;\uparrow\uparrow}, \tag{5.48}$$

where

$$\left(\frac{\partial[Z]_1}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{5.49}$$

and we can compute

$$\left(1 - \boldsymbol{g}_{0;\uparrow\uparrow}\right)\left(\frac{\partial[Z]_1}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow} \boldsymbol{g}_{0;\uparrow\uparrow} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5.50}$$

and

$$\left[\left\langle \hat{P}\hat{\boldsymbol{N}}_{\uparrow\uparrow}\right\rangle\right]_1 = \begin{pmatrix} c_{11\uparrow} & c_{12\uparrow} & c_{13\uparrow} \\ c_{21\uparrow} & c_{22\uparrow} & c_{23\uparrow} \\ c_{31\uparrow} & c_{32\uparrow} & c_{33\uparrow} \end{pmatrix}. \tag{5.51}$$

Notice that $\left\langle \hat{N}_{\uparrow\uparrow}\right\rangle$ only has nonzero entries for the first component $\left[\left\langle \hat{N}_{\uparrow\uparrow}\right\rangle\right]_1$, so then we can construct the second entry as

$$\left[\left\langle \hat{P}\hat{\boldsymbol{N}}_{\uparrow\uparrow}\right\rangle\right]_2 - \left[\left\langle \hat{P}\right\rangle\right]_2\left[\left\langle \hat{\boldsymbol{N}}_{\uparrow\uparrow}\right\rangle\right]_1 = \left(\mathbf{1} - \boldsymbol{g}_{0;\uparrow\uparrow}\right)\left(\frac{\partial[Z]_2}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow} \boldsymbol{g}_{0;\uparrow\uparrow}, \tag{5.52}$$

where

$$\left(\frac{\partial[Z]_2}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow} = \begin{pmatrix} c_{11\downarrow} & 0 & 0 \\ 0 & c_{22\downarrow} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{5.53}$$

and we can compute

$$\left(1 - \boldsymbol{g}_{0;\uparrow\uparrow}\right)\left(\frac{\partial[Z]_2}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow} \boldsymbol{g}_{0;\uparrow\uparrow} =$$

$$\begin{pmatrix} -c_{11\downarrow}\left(c_{11\uparrow}-1\right)c_{11\uparrow} - c_{22\downarrow}c_{12\uparrow}c_{21\uparrow} & c_{12\uparrow}\left(-c_{11\downarrow}\left(c_{11\uparrow}-1\right) - c_{22\downarrow}c_{22\uparrow}\right) & -c_{11\downarrow}\left(c_{11\uparrow}-1\right)c_{13\uparrow} - c_{22\downarrow}c_{12\uparrow}c_{23\uparrow} \\ c_{21\uparrow}\left(-c_{11\downarrow}c_{11\uparrow} - c_{22\downarrow}\left(c_{22\uparrow}-1\right)\right) & -c_{11\downarrow}c_{12\uparrow}c_{21\uparrow} - c_{22\downarrow}\left(c_{22\uparrow}-1\right)c_{22\uparrow} & -c_{11\downarrow}c_{13\uparrow}c_{21\uparrow} - c_{22\downarrow}\left(c_{22\uparrow}-1\right)c_{23\uparrow} \\ -c_{11\downarrow}c_{11\uparrow}c_{31\uparrow} - c_{22\downarrow}c_{21\uparrow}c_{32\uparrow} & -c_{11\downarrow}c_{12\uparrow}c_{31\uparrow} - c_{22\downarrow}c_{22\uparrow}c_{32\uparrow} & -c_{11\downarrow}c_{13\uparrow}c_{31\uparrow} - c_{22\downarrow}c_{23\uparrow}c_{32\uparrow} \end{pmatrix} \tag{5.54}$$

$$= \begin{pmatrix} -c_{11\uparrow}^3 + c_{11\uparrow}^2 - c_{12\uparrow}c_{21\uparrow}c_{22\uparrow} & -c_{12\uparrow}\left(c_{22\uparrow}^2 + \left(c_{11\uparrow}-1\right)c_{11\uparrow}\right) & -\left(c_{11\uparrow}-1\right)c_{11\uparrow}c_{13\uparrow} - c_{12\uparrow}c_{22\uparrow}c_{23\uparrow} \\ -c_{21\uparrow}\left(c_{11\uparrow}^2 + \left(c_{22\uparrow}-1\right)c_{22\uparrow}\right) & -c_{22\uparrow}^3 + c_{22\uparrow}^2 - c_{11\uparrow}c_{12\uparrow}c_{21\uparrow} & -c_{11\uparrow}c_{13\uparrow}c_{21\uparrow} - \left(c_{22\uparrow}-1\right)c_{22\uparrow}c_{23\uparrow} \\ -c_{31\uparrow}c_{11\uparrow}^2 - c_{21\uparrow}c_{22\uparrow}c_{32\uparrow} & -c_{32\uparrow}c_{22\uparrow}^2 - c_{11\uparrow}c_{12\uparrow}c_{31\uparrow} & -c_{11\uparrow}c_{13\uparrow}c_{31\uparrow} - c_{22\uparrow}c_{23\uparrow}c_{32\uparrow} \end{pmatrix} \tag{5.55}$$

and we finally get

$$\left[\left\langle \hat{P}\hat{\boldsymbol{N}}_{\uparrow\uparrow}\right\rangle\right]_2 =$$
$$\begin{pmatrix} \begin{pmatrix} c_{11\uparrow}^2+\left(c_{22\uparrow}^2-\frac{1}{2}\right)c_{11\uparrow}- \\ c_{12\uparrow}c_{21\uparrow}c_{22\uparrow}\end{pmatrix} & \frac{1}{2}\left(2c_{11\uparrow}-1\right)c_{12\uparrow} & \begin{pmatrix} c_{13\uparrow}\left(c_{22\uparrow}^2+c_{11\uparrow}-\frac{1}{2}\right)- \\ c_{12\uparrow}c_{22\uparrow}c_{23\uparrow}\end{pmatrix} \\ \frac{1}{2}c_{21\uparrow}\left(2c_{22\uparrow}-1\right) & \begin{pmatrix} c_{22\uparrow}^2+ \\ \frac{1}{2}\left(2c_{11\uparrow}^2-1\right)c_{22\uparrow}- \\ c_{11\uparrow}c_{12\uparrow}c_{21\uparrow}\end{pmatrix} & \begin{pmatrix} \frac{1}{2}\left(2c_{11\uparrow}^2+2c_{22\uparrow}-1\right)c_{23\uparrow}- \\ c_{11\uparrow}c_{13\uparrow}c_{21\uparrow}\end{pmatrix} \\ \begin{pmatrix} \left(c_{22\uparrow}^2-\frac{1}{2}\right)c_{31\uparrow}- \\ c_{21\uparrow}c_{22\uparrow}c_{32\uparrow}\end{pmatrix} & \begin{pmatrix} \frac{1}{2}\left(2c_{11\uparrow}^2-1\right)c_{32\uparrow}- \\ c_{11\uparrow}c_{12\uparrow}c_{31\uparrow}\end{pmatrix} & \begin{pmatrix} -c_{11\uparrow}c_{13\uparrow}c_{31\uparrow}- \\ c_{22\uparrow}c_{23\uparrow}c_{32\uparrow}+ \\ \left(c_{11\uparrow}^2+c_{22\uparrow}^2-\frac{1}{2}\right)c_{33\uparrow}\end{pmatrix} \end{pmatrix} \tag{5.56}$$

Similary, we can compute the third entry as

$$\left[\left\langle \hat{P}\hat{\boldsymbol{N}}_{\uparrow\uparrow}\right\rangle\right]_3 - \left[\left\langle \hat{P}\right\rangle\right]_3\left[\left\langle \hat{\boldsymbol{N}}_{\uparrow\uparrow}\right\rangle\right]_1 = \left(\mathbf{1}-\boldsymbol{g}_{0;\uparrow\uparrow}\right)\left(\frac{\partial[Z]_3}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow}\boldsymbol{g}_{0;\uparrow\uparrow}, \tag{5.57}$$

where

$$\left(\frac{\partial[Z]_3}{\partial \boldsymbol{g}_0^T}\right)_{\uparrow\uparrow} = \begin{pmatrix} c_{11\downarrow}\left(c_{22\downarrow}c_{22\uparrow}-\frac{1}{4}\right)-c_{12\downarrow}c_{21\downarrow}c_{22\uparrow} & \left(c_{12\downarrow}c_{21\downarrow}-c_{11\downarrow}c_{22\downarrow}\right)c_{12\uparrow} & 0 \\ \left(c_{12\downarrow}c_{21\downarrow}-c_{11\downarrow}c_{22\downarrow}\right)c_{21\uparrow} & \left(c_{11\downarrow}c_{22\downarrow}-c_{12\downarrow}c_{21\downarrow}\right)c_{11\uparrow}-\frac{1}{4}c_{22\downarrow} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{5.58}$$

and we can evaluate a particular matrix element as

$$\begin{aligned}\left[\left\langle \hat{P}\hat{n}_{1\uparrow 1\uparrow}\right\rangle\right]_3 =& \frac{1}{16}\Big(-4c_{11\uparrow}^2+4\left(4c_{11\uparrow}-1\right)c_{22\uparrow}^2c_{11\uparrow}+c_{11\uparrow}+ \\ & 16c_{12\uparrow}^2c_{21\uparrow}^2+4\left(1-8c_{11\uparrow}\right)c_{12\uparrow}c_{21\uparrow}c_{22\uparrow}\Big),\end{aligned} \tag{5.59}$$

which agrees with the previously computed value in Eq. 5.20. It is straightforward to confirm the other elements as well.

We now illustrate the use of the generating functional for the two-particle discrete Green's function, where

$$\begin{aligned}\langle \hat{n}_{ij}\hat{n}_{lk}\rangle_{\hat{\rho}} =& [\boldsymbol{g}_0]_{ij}[\boldsymbol{g}_0]_{lk} + [\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{lj} + \\ & \frac{1}{Z}\frac{\partial Z}{\partial [\boldsymbol{g}_0]_{mn}}\Big([\boldsymbol{g}_0]_{mk}[\boldsymbol{g}_0]_{ij}[\boldsymbol{p}_0]_{ln} + [\boldsymbol{g}_0]_{mj}[\boldsymbol{g}_0]_{lk}[\boldsymbol{p}_0]_{in} + \\ & [\boldsymbol{g}_0]_{mk}[\boldsymbol{p}_0]_{lj}[\boldsymbol{p}_0]_{in} - [\boldsymbol{g}_0]_{mj}[\boldsymbol{g}_0]_{ik}[\boldsymbol{p}_0]_{ln}\Big) + \\ & \frac{1}{Z}\frac{\partial Z}{\partial [\boldsymbol{g}_0]_{mn}\partial [\boldsymbol{g}_0]_{st}}[\boldsymbol{g}_0]_{sk}[\boldsymbol{p}_0]_{lt}[\boldsymbol{g}_0]_{mj}[\boldsymbol{p}_0]_{in}. \end{aligned} \tag{5.60}$$

To illustrate the procedure, we evaluate the double occupancy, and we focus of the first entry of the monomial basis

$$\left[\left\langle \hat{P}\hat{n}_{3\uparrow 3\uparrow}\hat{n}_{3\downarrow 3\downarrow}\right\rangle\right]_1 = \left[\left\langle \hat{P}\right\rangle\right]_1 ([\boldsymbol{g}_0]_{3\uparrow 3\uparrow}[\boldsymbol{g}_0]_{3\downarrow 3\downarrow} + [\boldsymbol{g}_0]_{3\uparrow 3\downarrow}[\boldsymbol{p}_0]_{3\downarrow 3\uparrow}) = c_{33\downarrow}c_{33\uparrow}, \tag{5.61}$$

which can be identified as the Hartree-Fock contribution. The second entry

$$\left[\left\langle \hat{P}\hat{n}_{3\uparrow 3\uparrow}\hat{n}_{3\downarrow 3\downarrow}\right\rangle\right]_2 \tag{5.62}$$

has six contributions denoted as T_i, where

$$T_1 = \left[\left\langle \hat{P}\right\rangle\right]_2 ([\boldsymbol{g}_0]_{3\uparrow 3\uparrow}[\boldsymbol{g}_0]_{3\downarrow 3\downarrow} + [\boldsymbol{g}_0]_{3\uparrow 3\downarrow}[\boldsymbol{p}_0]_{3\downarrow 3\uparrow}) \tag{5.63}$$

$$= c_{33\downarrow}c_{33\uparrow}\left(c_{11\downarrow}c_{11\uparrow} + c_{22\downarrow}c_{22\uparrow} - \frac{1}{2}\right) \tag{5.64}$$

and

$$T_2 = \frac{\partial\,[Z]_2}{\partial [\boldsymbol{g}_0]_{m\downarrow n\downarrow}}[\boldsymbol{g}_0]_{m\downarrow 3\downarrow}[\boldsymbol{g}_0]_{3\uparrow 3\uparrow}[\boldsymbol{p}_0]_{3\downarrow n\downarrow} \tag{5.65}$$

and

$$\left[\frac{\partial\,[Z]_2}{\partial \boldsymbol{g}_0}\right]_{\downarrow\downarrow} = \begin{pmatrix} c_{11\uparrow} & 0 & 0 \\ 0 & c_{22\uparrow} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5.66}$$

and

$$T_2 = c_{33\uparrow}\left(-\left(c_{13\downarrow}c_{31\downarrow}c_{11\uparrow} + c_{23\downarrow}c_{32\downarrow}c_{22\uparrow}\right)\right) \tag{5.67}$$

and

$$T_3 = \frac{\partial\left[Z\right]_2}{\partial[\boldsymbol{g}_0]_{m\uparrow n\uparrow}}[\boldsymbol{g}_0]_{3\uparrow 3\uparrow}[\boldsymbol{g}_0]_{3\downarrow 3\downarrow}[\boldsymbol{p}_0]_{3\uparrow n\uparrow} \tag{5.68}$$

and

$$\left[\frac{\partial\left[Z\right]_2}{\partial\boldsymbol{g}_0}\right]_{\uparrow\uparrow} = \begin{pmatrix} c_{11\downarrow} & 0 & 0 \\ 0 & c_{22\downarrow} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5.69}$$

and

$$T_3 = c_{33\downarrow}\left(-\left(c_{11\downarrow}c_{13\uparrow}c_{31\uparrow} + c_{22\downarrow}c_{23\uparrow}c_{32\uparrow}\right)\right) \tag{5.70}$$

and

$$T_4 = \frac{\partial\left[Z\right]_2}{\partial[\boldsymbol{g}_0]_{m\downarrow n\uparrow}}[\boldsymbol{g}_0]_{m\downarrow 3\downarrow}[\boldsymbol{p}_0]_{3\downarrow 3\uparrow}[\boldsymbol{p}_0]_{3\uparrow n\uparrow} = 0 \tag{5.71}$$

and

$$T_5 = -\frac{\partial\left[Z\right]_2}{\partial[\boldsymbol{g}_0]_{m\uparrow n\downarrow}}[\boldsymbol{g}_0]_{m\uparrow 3\uparrow}[\boldsymbol{g}_0]_{3\uparrow 3\downarrow}[\boldsymbol{p}_0]_{3\downarrow n\downarrow} = 0 \tag{5.72}$$

and

$$T_6 = \frac{\partial Z^{(2)}}{\partial[\boldsymbol{g}_0]_{m\uparrow n\uparrow}\partial[\boldsymbol{g}_0]_{s\downarrow t\downarrow}}[\boldsymbol{g}_0]_{s\downarrow 3\downarrow}[\boldsymbol{p}_0]_{3\downarrow t\downarrow}[\boldsymbol{g}_0]_{m\uparrow 3\uparrow}[\boldsymbol{p}_0]_{3\uparrow n\uparrow} \tag{5.73}$$

and

$$Z^{(2)} = c_{11\downarrow}c_{11\uparrow} + c_{22\downarrow}c_{22\uparrow} - \frac{1}{2} \tag{5.74}$$

and

$$T_6 = \sum_{m=1,2} [\boldsymbol{g}_0]_{m\downarrow 3\downarrow} [\boldsymbol{p}_0]_{3\downarrow m\downarrow} [\boldsymbol{g}_0]_{m\uparrow 3\uparrow} [\boldsymbol{p}_0]_{3\uparrow m\uparrow} \tag{5.75}$$

$$= c_{13\downarrow} c_{31\downarrow} c_{13\uparrow} c_{31\uparrow} + c_{23\downarrow} c_{32\downarrow} c_{23\uparrow} c_{32\uparrow} \tag{5.76}$$

and finally

$$\left[\left\langle \hat{P} \hat{n}_{3\uparrow 3\uparrow} \hat{n}_{3\downarrow 3\downarrow} \right\rangle\right]_2 = T_1 + T_2 + T_3 + T_6 \tag{5.77}$$

$$\begin{aligned} =& c_{13\downarrow} c_{31\downarrow} \left(c_{13\uparrow} c_{31\uparrow} - c_{11\uparrow} c_{33\uparrow}\right) + c_{23\downarrow} c_{32\downarrow} \left(c_{23\uparrow} c_{32\uparrow} - c_{22\uparrow} c_{33\uparrow}\right) + \\ & \frac{1}{2} c_{33\downarrow} \left(c_{33\uparrow} \left(2 c_{11\downarrow} c_{11\uparrow} + 2 c_{22\downarrow} c_{22\uparrow} - 1\right) - 2 \left(c_{11\downarrow} c_{13\uparrow} c_{31\uparrow} + c_{22\downarrow} c_{23\uparrow} c_{32\uparrow}\right)\right) \end{aligned} \tag{5.78}$$

$$\begin{aligned} =& c_{13\uparrow}^2 c_{31\uparrow}^2 + c_{23\uparrow}^2 c_{32\uparrow}^2 + \frac{1}{2} \left(2 c_{11\uparrow}^2 + 2 c_{22\uparrow}^2 - 1\right) c_{33\uparrow}^2 - \\ & 2 \left(c_{11\uparrow} c_{13\uparrow} c_{31\uparrow} + c_{22\uparrow} c_{23\uparrow} c_{32\uparrow}\right) c_{33\uparrow}, \end{aligned} \tag{5.79}$$

which is identical to what was obtained in Eq. 5.31. This exercise illustrates the practicality of using the generating functional to evaluate relevant observables.

Chapter 6

Application to the Anderson Impurity Model

The AIM is a nontrivial many-body problem, yet the single orbital AIM can be precisely solved used density matrix renormalization group (DMRG). Therefore, it serves as a critical test of our VDAT formalism. The AIM will naturally be studied using the SPD-l, as developed in the previous chapter. It is possible that including non-local interacting projectors may allow for faster convergence, but we will show that the SPD-l produces outstanding results for $\mathcal{N} = 3$.

6.1 A Simple Example: AIM with One Bath Orbital

In order to clearly illustrate our theory, we study the AIM with only one bath orbital and particle-hole symmetry. The Hamiltonian is given as

$$\hat{H} = t \sum_{\sigma} \left(\hat{f}_{\sigma}^{\dagger} \hat{c}_{\sigma} + h.c. \right) + U \left(\hat{f}_{\uparrow}^{\dagger} \hat{f}_{\uparrow} - 1/2 \right) \left(\hat{f}_{\downarrow}^{\dagger} \hat{f}_{\downarrow} - 1/2 \right) = t\hat{K} + U\Delta\hat{d}. \tag{6.1}$$

Considering $\mathcal{N} = 2$, the SPD-l is

$$\hat{\rho} = \exp\left(u\Delta\hat{d} \right) \exp\left(\gamma\hat{K} \right) \exp\left(u\Delta\hat{d} \right), \tag{6.2}$$

where u and γ are variational parameters.

We continue by constructing the non-interacting Green's function. As we have spin

symmetry, we only need to compute this for a given spin, and

$$\boldsymbol{g}_{\sigma;Q} = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & -1/2 & 1/2 \end{pmatrix}, \tag{6.3}$$

where we use the orbital index major format, i.e, $f_\sigma^{\dagger(1)}, f_\sigma^{\dagger(2)}$, $c_\sigma^{\dagger(1)}, c_\sigma^{\dagger(2)}$. Using $\boldsymbol{g} = \left(\frac{1}{1+\exp(-v)}\right)^T$, we have

$$\exp\left(\boldsymbol{v}_{\sigma;Q}\right) = \left(\frac{\mathbf{1}}{\left(\boldsymbol{g}_{\sigma;Q}^{-1} - \mathbf{1}\right)}\right)^T = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{6.4}$$

Applying the kinetic projection

$$\boldsymbol{v}_{\sigma;\gamma} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma \\ 0 & 0 & 0 & 0 \\ 0 & \gamma & 0 & 0 \end{pmatrix}, \qquad \exp\left(\boldsymbol{v}_{\sigma;\gamma}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cosh(\gamma) & 0 & \sinh(\gamma) \\ 0 & 0 & 1 & 0 \\ 0 & \sinh(\gamma) & 0 & \cosh(\gamma) \end{pmatrix} \tag{6.5}$$

and

$$\exp\left(\boldsymbol{v}_{\boldsymbol{\sigma}}\right) = \exp\left(\boldsymbol{v}_{\sigma;Q}\right)\exp\left(\boldsymbol{v}_{\sigma;\gamma}\right) = \begin{pmatrix} 0 & -\cosh(\gamma) & 0 & -\sinh(\gamma) \\ 1 & 0 & 0 & 0 \\ 0 & -\sinh(\gamma) & 0 & -\cosh(\gamma) \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{6.6}$$

the non-interacting Green's function can then be computed as

$$\boldsymbol{g}_{\sigma;0} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) & -\frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) \\ -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) & \frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) \\ \frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) & -\frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) & \frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{6.7}$$

So we can effectively parameterize it with $\nu = \frac{1}{2}\tanh\left(\frac{\gamma}{2}\right) \in [-1/2, 1/2]$ or $\gamma = 2\tanh^{-1}(2\nu)$, giving

$$\boldsymbol{g}_{\sigma;0} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \nu & -\nu \\ -\frac{1}{2} & \frac{1}{2} & -\nu & \nu \\ \nu & -\nu & \frac{1}{2} & \frac{1}{2} \\ -\nu & \nu & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{6.8}$$

To compute the self-energy, we only need the local Green's function for the impurity

$$\boldsymbol{g}_{loc;0} = \begin{pmatrix} \boldsymbol{g}_{loc,\uparrow;0} & \\ & \boldsymbol{g}_{loc,\downarrow;0} \end{pmatrix}, \qquad \boldsymbol{g}_{loc,\sigma;0} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{6.9}$$

Recall the discrete time impurity problem

$$\hat{\rho}_{loc} = \hat{\rho}_{loc;0}\hat{P}_1^{(1)}\hat{P}_2^{(2)}, \tag{6.10}$$

where

$$\hat{P} = \hat{P}_1^{(1)}\hat{P}_2^{(2)} = \left(\hat{1}^{(1)} + u\Delta\hat{d}^{(1)}\right)\left(\hat{1}^{(2)} + u\Delta\hat{d}^{(2)}\right). \tag{6.11}$$

So we have

$$\left\langle \hat{P} \right\rangle_{\hat{\rho}_{loc;0}} = \frac{u^2}{16} + 1, \qquad \left\langle \hat{P}\Delta\hat{d}^{(2)} \right\rangle_{\hat{\rho}_{loc;0}} = \frac{u}{8} \tag{6.12}$$

and

$$\left\langle Pa_\sigma^{\dagger(1)}\hat{a}_\sigma^{(1)} \right\rangle_{\hat{\rho}_{loc;0}} = \frac{1}{32}\left(u^2 + 16\right), \qquad \left\langle Pa_\sigma^{\dagger(1)}\hat{a}_\sigma^{(2)} \right\rangle_{\hat{\rho}_{loc;0}} = -\frac{1}{32}(u-4)(u+4), \tag{6.13}$$

$$\left\langle Pa_\sigma^{\dagger(2)}\hat{a}_\sigma^{(1)} \right\rangle_{\hat{\rho}_{loc;0}} = \frac{1}{32}\left(u^2 - 16\right), \qquad \left\langle Pa_\sigma^{\dagger(2)}\hat{a}_\sigma^{(2)} \right\rangle_{\hat{\rho}_{loc;0}} = \frac{1}{32}\left(u^2 + 16\right). \tag{6.14}$$

We can now compute the interacting local Green's function as

$$\boldsymbol{g}_{loc,\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{16}{u^2+16} - \frac{1}{2} \\ \frac{1}{2} - \frac{16}{u^2+16} & \frac{1}{2} \end{pmatrix}, \qquad \Delta d = \frac{2u}{u^2+16}. \tag{6.15}$$

By solving for $u = \frac{1-\sqrt{1-16\Delta \mathrm{d}^2}}{\Delta \mathrm{d}}$, we can rewrite the Green's function in terms of Δd as

$$\boldsymbol{g}_{loc,\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{1-16\Delta \mathrm{d}^2} \\ -\frac{1}{2}\sqrt{1-16\Delta \mathrm{d}^2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} z\left(d\right) \\ -\frac{1}{2} z\left(d\right) & \frac{1}{2} \end{pmatrix}. \tag{6.16}$$

The local self-energy operator is

$$\left(\boldsymbol{g}_{loc,\sigma}^{-1} - \mathbf{1}\right) = \left(\boldsymbol{g}_{loc,\sigma;0}^{-1} - \mathbf{1}\right) \boldsymbol{S}_{loc,\sigma}, \tag{6.17}$$

$$\boldsymbol{S}_{loc;\sigma} = \begin{pmatrix} \frac{2z}{z^2+1} & \frac{2}{z^2+1} - 1 \\ 1 - \frac{2}{z^2+1} & \frac{2z}{z^2+1} \end{pmatrix}. \tag{6.18}$$

We can extend to the full space for the given σ as $\boldsymbol{S}_\sigma = \boldsymbol{S}_{loc;\sigma} \oplus \mathbf{1}$

$$\boldsymbol{S}_\sigma = \begin{pmatrix} \frac{2z}{z^2+1} & \frac{2}{z^2+1} - 1 & 0 & 0 \\ 1 - \frac{2}{z^2+1} & \frac{2z}{z^2+1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{6.19}$$

Now, we apply the self-energy operator in the full block

$$\left(\boldsymbol{g}_{\sigma}^{-1} - 1\right) = \left(\boldsymbol{g}_{\sigma;0}^{-1} - 1\right) \boldsymbol{S}_\sigma, \tag{6.20}$$

$$\boldsymbol{g}_{\sigma;0} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \nu & -\nu \\ -\frac{1}{2} & \frac{1}{2} & -\nu & \nu \\ \nu & -\nu & \frac{1}{2} & \frac{1}{2} \\ -\nu & \nu & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}, \tag{6.21}$$

$$\boldsymbol{g}_{\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{z}{2} & \nu & -\nu \\ -\frac{z}{2} & \frac{1}{2} & -z\nu & z\nu \\ \nu & -z\nu & \frac{1}{2} & \frac{1}{2} \\ -\nu & z\nu & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{6.22}$$

Recalling that we have used orbital major indexing, we can read the physical density matrix from the second time step as

$$\boldsymbol{n}_{\sigma} = \begin{pmatrix} \frac{1}{2} & z\left(d\right)\nu \\ z\left(d\right)\nu & \frac{1}{2} \end{pmatrix}. \tag{6.23}$$

One can clearly see that the hopping between the impurity and the bath is renormalized by $z(d)$.

6.2 Anderson Impurity Model on a Ring

Here we consider the Anderson Impurity model on a ring, given by

$$\hat{H} = \hat{H}_0 + \hat{V} \qquad \hat{H}_0 = v\sum_{\sigma}\left(\hat{f}_{\sigma}^{\dagger}\hat{c}_{0,\sigma} + h.c.\right) - \frac{W}{4}\sum_{\sigma,n=0}^{L-1}\left(\hat{c}_{n,\sigma}^{\dagger}\hat{c}_{n+1,\sigma} + h.c\right) \tag{6.24}$$

$$\hat{V} = U\left(\hat{f}_{\uparrow}^{\dagger}\hat{f}_{\uparrow} - \frac{1}{2}\right)\left(\hat{f}_{\downarrow}^{\dagger}\hat{f}_{\downarrow} - \frac{1}{2}\right) \tag{6.25}$$

The interacting SPD-l is given as

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right)\hat{P}_1 ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right)\hat{P}_{\mathcal{N}} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_{\mathcal{N}}, \quad \hat{P}_{\tau} = \exp\left(\hat{V}_{\tau}\right), \quad \hat{\mathcal{P}}_{\tau} = \exp\left(\boldsymbol{\gamma}_{\tau} \cdot \hat{\boldsymbol{n}}\right)\hat{P}_{\tau}, \tag{6.26}$$

where

$$\hat{P}_\tau = \left(1 - \mu_\tau - \frac{1}{4}u_\tau\right)\hat{1} + \mu_\tau\left(\hat{f}^\dagger_\uparrow\hat{f}_\uparrow + \hat{f}^\dagger_\downarrow\hat{f}_\downarrow\right) + u_\tau\hat{f}^\dagger_\uparrow\hat{f}_\uparrow\hat{f}^\dagger_\downarrow\hat{f}_\downarrow, \tag{6.27}$$

and

$$\exp\left(\boldsymbol{\gamma}_\tau \cdot \hat{\boldsymbol{n}}\right) = \prod_{j\sigma}(1 + h(\epsilon_{j\sigma}(\eta_{1;\tau}, \eta_{2;\tau}, \eta_{3;\tau}))\Delta\hat{n}_{j\sigma}), \tag{6.28}$$

and

$$\begin{aligned}\sum_{j\sigma}\epsilon_{j\sigma}(\eta_{1;\tau}, \eta_{2;\tau}, \eta_{3;\tau})\hat{n}_{j\sigma} = \gamma_{1;\tau}\sum_\sigma\left(\hat{f}^\dagger_\sigma\hat{c}_{0,\sigma} + h.c.\right) - \gamma_{2;\tau}\sum_{\sigma,n=0}^{L-1}\left(\hat{c}^\dagger_{n,\sigma}\hat{c}_{n+1,\sigma} + h.c\right) \\ - \gamma_{3;\tau}(\sum_\sigma(\hat{f}^\dagger_\sigma\hat{f}_\sigma + \sum_n\hat{c}^\dagger_{n,\sigma}\hat{c}_{n,\sigma})),\end{aligned} \tag{6.29}$$

$$h(x) = \begin{cases} 2 & x > 2 \\ x & -2 < x \leq 2 \\ -2 & x \leq -2 \end{cases} \tag{6.30}$$

$$\Delta\hat{n}_{j\sigma} = \hat{n}_{j\sigma} - \frac{1}{2}. \tag{6.31}$$

One simplification has been made: the noninteracting projector at each time step is only parameterized by two parameters, $\gamma_{1;\tau}$ and $\gamma_{2;\tau}$. Given that we are exactly evaluating the SPD, we are guaranteed to have an upper bound on the ground state energy, and therefore restricting the form of the variational parameters still produces a rigorous result.

The procedure for solving $\mathcal{N} = 2$ is easily generalized from the previous section. For $\mathcal{N} > 2$, the only difficulty is to solve the LDAM, which computes the local self-energy from the local non-interacting Green's function, as described in Section 5.3. The computational cost is determined by two factors. First, one needs to compute the non-interacting Green's function for the entire model, which requires diagonalizing a matrix with the size of the bath.

Second, one needs to solve for the LDAM, which amounts to evaluating all local diagrams, which scales exponentially with $\mathcal{N}$; though typically only small $\mathcal{N}$ are needed.

Several different observables will be computed. First we consider the local spin correlation function, defined by

$$C_{ff}^{S}=\left\langle S_{f}^{z}S_{f}^{z}\right\rangle =\frac{1}{4}\left\langle \left(\hat{n}_{f\uparrow}-\hat{n}_{f\downarrow}\right)^{2}\right\rangle =\frac{1}{2}\left(n-d\right). \tag{6.32}$$

In the $L\rightarrow\infty$ limit, we have

$$C_{ff}^{S}=\frac{1}{4}-\frac{1}{2}d. \tag{6.33}$$

The correlation between the impurity and a given bath site is

$$C_{fc}^{S}\left(r\right)=\left\langle S_{f}^{z}S_{r;c}^{z}\right\rangle =\frac{1}{4}\left\langle \left(\hat{n}_{f\uparrow}-\hat{n}_{f\downarrow}\right)\left(\hat{n}_{r\uparrow;c}-\hat{n}_{r\downarrow;c}\right)\right\rangle , \tag{6.34}$$

where c denotes the bath orbital. Notice the inversion symmetry, where we have

$$C_{fc}^{S}\left(r\right)=C_{fc}^{S}\left(L-r\right), \qquad 1\leq r\leq\frac{L-1}{2}, \tag{6.35}$$

where L is the size of the ring, and assumed to be an odd number.

The unscreened spin $\mathcal{S}\left(r\right)$ is defined as the accumulation of spin correlation up to r, and we have

$$\mathcal{S}\left(0\right)=C_{ff}^{S}+C_{fc}^{S}\left(0\right), \qquad \mathcal{S}\left(r\right)-\mathcal{S}\left(r-1\right)=C_{fc}^{S}\left(r\right)+C_{fc}^{S}\left(L-r\right), \tag{6.36}$$

and

$$\mathcal{S}\left(\frac{L-1}{2}\right)=\left\langle S_{f}^{z}\left(S_{f}^{z}+\sum_{r=0}^{L-1}S_{r;c}^{z}\right)\right\rangle =0. \tag{6.37}$$

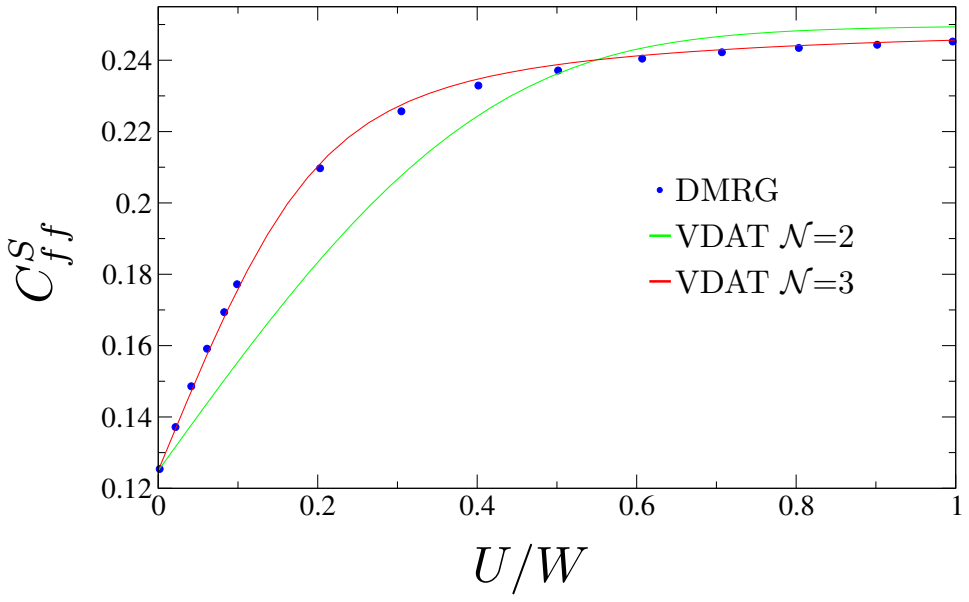

Figure 6.1: A plot of $C^S_{ff} = \langle S^z_f S^z_f \rangle = \frac{1}{4} \langle (\hat{n}_{f\uparrow} - \hat{n}_{f\downarrow})^2 \rangle$ vs. U/W for the Anderson impurity model on a ring with $L = 1397$ evaluated using VDAT and compared to published DMRG results[1].

We now consider the results. We begin by presenting C^S_{ff}, which measures the local spin correlation, as a function of U/W (see Figure 6.1). For $\mathcal{N} = 2$, which is equivalent to the Gutzwiller wave function, one only has a crude approximation to the numerically exact DMRG results. Alternatively, $\mathcal{N} = 3$ is nearly on top of the DMRG results. Clearly the SPD converges extremely rapidly with respect to $\mathcal{N}$. We can also compute the unscreened spin (see Figure 6.2), which is a far more challenging observable given that it involves a long range correlation between the impurity and the bath. Once again, $\mathcal{N} = 2$ has reasonable but relatively inaccurate results, while $\mathcal{N} = 3$ is quantitatively accurate.

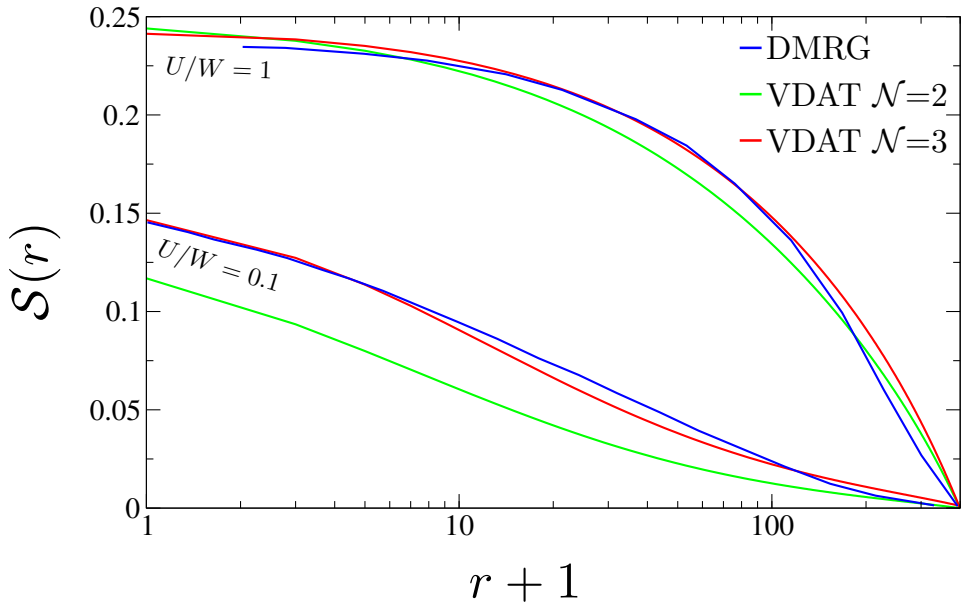

Figure 6.2: The unscreened spin $\mathcal{S}(r)$ vs. the distance from the impurity site for different values of U/W evaluated using VDAT and compared to published DMRG results[1].

Chapter 7

The Local Self-Consistent Approximation (LSA) and its application to Hubbard model

7.1 The Local Self-Consistent Approximation (LSA)

Another common scenario for models of interacting electrons is where the interaction is local, but not restricted to single subspace; prominent examples include the Hubbard model and the periodic Anderson impurity model. In such cases, it is natural to study an SPD where the interacting projectors are composed of disjoint local projectors, and we refer to such SPD as local disjoint SPD, denoted SPD-d. For example, in the Hubbard model with N sites, an SPD-d is

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right) \hat{P}_1 ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right) \hat{P}_{\mathcal{N}} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_{\mathcal{N}}, \quad \hat{P}_\tau = \prod_{i=1}^{N} \hat{P}_{i,\tau}, \quad \hat{\mathcal{P}}_\tau = \exp\left(\boldsymbol{\gamma}_\tau \cdot \hat{\boldsymbol{n}}\right) \hat{P}_\tau, \tag{7.1}$$

where $\hat{P}_{i,\tau}$ is an interacting projector restricted to the local Fock space of site i. We introduce the local self-consistent approximation (LSA) to evaluate this SPD, and the LSA is the discrete analogue of the dynamical mean-field theory (DMFT)[3]. The key idea for the LSA is the assumption that the discrete self-energy is local

$$\boldsymbol{\Sigma}_P\left(\boldsymbol{g}\right) = \oplus_{i=1}^{N} \boldsymbol{\Sigma}_{P_i}(\boldsymbol{g}_{ii}). \tag{7.2}$$

The self-consistent procedure can then be defined, beginning with an initial guess for the non-interacting discrete Green's function of the LDAM

$$\boldsymbol{\mathcal{G}}_i = \boldsymbol{g}_{0;ii}. \tag{7.3}$$

This defines our effective LDAM for site i, which can then be solved by computing the generating functional Z_i, yielding the self-energy operator $\boldsymbol{S}_i$ as

$$\boldsymbol{S}_i = \left(Z_i \mathbf{1} + \left(\frac{\partial Z_i}{\partial \boldsymbol{\mathcal{G}}_i^T} \right) (\hat{\mathbf{1}} - \boldsymbol{\mathcal{G}}_i) \right)^{-1} \left(Z_i \mathbf{1} - \left(\frac{\partial Z_i}{\partial \boldsymbol{\mathcal{G}}_i^T} \right) \boldsymbol{\mathcal{G}}_i \right). \tag{7.4}$$

In the absence of symmetry, one must solve a LDAM for each site, yielding the total self-energy operator for the system as

$$\boldsymbol{S} = \oplus_{i=1}^{N} \boldsymbol{S}_i. \tag{7.5}$$

The interacting discrete Green's function can then be constructed as

$$\boldsymbol{g} = \frac{\mathbf{1}}{\boldsymbol{g}_0 + (\mathbf{1} - \boldsymbol{g}_0)\, \boldsymbol{S}} \boldsymbol{g}_0. \tag{7.6}$$

Finally, we construct a new non-interacting discrete Green's function, yielding the updated LDAM

$$\boldsymbol{\mathcal{G}}_i = \boldsymbol{S}_i \frac{\mathbf{1}}{(\mathbf{1} + \boldsymbol{g}_{ii}\, (\boldsymbol{S}_i - \mathbf{1}))} \boldsymbol{g}_{ii}. \tag{7.7}$$

This entire procedure is then iterated until self-consistency is achieved. Upon achieving self-consistency, one has completed a single evaluation of the SPD-d. In order to obtain the ground state energy, one needs to minimize over the variational parameters. We later prove that the LSA is an exact evaluation of the SPD-d in infinite dimensions (see Section 7.2).

The preceding outline of the LSA is applied to a generic system without symmetry, and now we specify the LSA to the case of translation symmetry. We can begin with a guess for

the discrete non-interacting impurity Green's function $\boldsymbol{\mathcal{G}}_0$ as

$$\boldsymbol{\mathcal{G}} = \int d\epsilon D(\epsilon)\, \boldsymbol{g}_0(\epsilon) \tag{7.8}$$

This defines our effective LDAM for the crystal, which can then be solved by computing the generating functional Z, yielding the local self-energy operator $\boldsymbol{S}$ as

$$\boldsymbol{S}_{loc} = \left(Z\mathbf{1} + \left(\frac{\partial Z}{\partial \boldsymbol{\mathcal{G}}^T}\right)(\hat{\mathbf{1}} - \boldsymbol{\mathcal{G}})\right)^{-1} \left(Z\mathbf{1} - \left(\frac{\partial Z}{\partial \boldsymbol{\mathcal{G}}^T}\right)\boldsymbol{\mathcal{G}}\right). \tag{7.9}$$

We then use this self-energy to update the interacting discrete Green's function for each energy orbital as

$$\boldsymbol{g}(\epsilon) = \frac{\mathbf{1}}{\boldsymbol{g}_0(\epsilon) + (\mathbf{1} - \boldsymbol{g}_0(\epsilon))\, \boldsymbol{S}_{loc}} \boldsymbol{g}_0(\epsilon). \tag{7.10}$$

Then we get the new interacting local discrete Green's function as

$$\boldsymbol{g}_{loc} = \int d\epsilon D(\epsilon)\, \boldsymbol{g}(\epsilon). \tag{7.11}$$

Finally, we construct a new non-interacting discrete Green's function, yielding the updated LDAM as

$$\boldsymbol{\mathcal{G}} = \boldsymbol{S}_{loc} \frac{\mathbf{1}}{(\mathbf{1} + \boldsymbol{g}_{loc}(\boldsymbol{S}_{loc} - \mathbf{1}))} \boldsymbol{g}_{loc}. \tag{7.12}$$

7.2 A Proof that LSA is Exact in Infinite Dimensions

Here, we prove that the LSA exact evaluations the SPD-d in $d = \infty$. The main idea follows the cavity construction method used in proving that DMFT is exact in infinite dimensions[3]. We begin by considering the the non-interacting effective density matrix in the compound

space

$$\rho_{eff;0} = \hat{Q} \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}^{(1)}\right) ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}^{(\mathcal{N})}\right), \tag{7.13}$$

where

$$\exp\left(\boldsymbol{\gamma}_\tau \cdot \hat{\boldsymbol{n}}\right) = \exp(\sum_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma;\tau} \hat{n}^{(\tau)}_{\mathbf{k}\sigma}). \tag{7.14}$$

In the cavity construction, one selects a particular site in the lattice, denoted site i, and traces out all other sites. We can rewrite the non-interacting density matrix in the compound space in the following form

$$\rho_{eff;0} = \exp\left((\boldsymbol{v}_i + \boldsymbol{v}_b + \boldsymbol{v}_{ib}) \cdot \hat{\boldsymbol{N}}\right), \tag{7.15}$$

where v_i is a single-particle potential associated within site i, $\boldsymbol{v}_b$ is the single-particle potential of the remaining sites, and $\boldsymbol{v}_{ib}$ is the off-diagonal component of the single-particle potential between site i and the remaining sites. We can then construct the local density matrix for site i by tracing out all other sites

$$\hat{\rho}_{loc} = \mathrm{Tr}_{/i}\left(\exp\left((\boldsymbol{v}_i + \boldsymbol{v}_b + \boldsymbol{v}_{ib}) \cdot \hat{\boldsymbol{N}}\right) \prod_j \hat{P}_j\right) = \hat{\rho}_{loc;0} \hat{P}_i, \tag{7.16}$$

where

$$\hat{\rho}_{loc;0} = \mathrm{Tr}_{/i}\left(\exp\left((\boldsymbol{v}_i + \boldsymbol{v}_b + \boldsymbol{v}_{ib}) \cdot \hat{\boldsymbol{N}}\right) \prod_{j \neq i} \hat{P}_j\right). \tag{7.17}$$

Given the following identity for expanding the exponential of two general matrices

$$\begin{aligned} \exp(A+B) = \exp(A) + \int_0^1 d\lambda \exp(\lambda A) B \exp((1-\lambda)A) + \\ \int_0^1 d\lambda_1 \int_{\lambda_1}^1 d\lambda_2 \exp(\lambda_1 A) B \exp((\lambda_2 - \lambda_1)A) B \exp((1-\lambda_2)A) + \ldots \end{aligned} \tag{7.18}$$

and plugging in the following definitions

$$A = (\boldsymbol{v}_i + \boldsymbol{v}_b) \cdot \hat{\boldsymbol{N}} = A_i + A_b, \tag{7.19}$$

$$A_i = \boldsymbol{v}_i \cdot \hat{\boldsymbol{N}} = \sum_{\tau\tau'} \left(v^{\tau\tau'} a_i^{\dagger(\tau)} a_i^{(\tau')} + h.c. \right), \tag{7.20}$$

$$A_b = \boldsymbol{v}_b \cdot \hat{\boldsymbol{N}} = \sum_{j\neq i, j'\neq i, \tau\tau'} v_{jj'}^{\tau\tau'} a_j^{\dagger(\tau)} a_{j'}^{(\tau')}, \tag{7.21}$$

$$B = \boldsymbol{v}_{ib} \cdot \hat{\boldsymbol{N}} = \sum_{j\neq i, \tau\tau'} \left(t_j^{\tau\tau'} a_i^{\dagger(\tau)} a_j^{(\tau')} + h.c. \right), \tag{7.22}$$

we can then Taylor series expand $\hat{\rho}_{loc;0} = [\hat{\rho}_{loc;0}]^0 + [\hat{\rho}_{loc;0}]^1 + \ldots$, yielding

$$[\hat{\rho}_{loc;0}]^0 = \mathrm{Tr}_{/i} \left(\exp(A) \prod_{j\neq i} \hat{P}_j \right), \tag{7.23}$$

$$[\hat{\rho}_{loc;0}]^1 = \mathrm{Tr}_{/i} \left(\int_0^1 d\lambda_1 \exp(\lambda_1 A) \sum_{j_1\neq i, \tau\tau'} \left(t_{j_1}^{\tau\tau'} a_i^{\dagger(\tau)} a_{j_1}^{(\tau')} + h.c. \right) \exp((1-\lambda_1)A) \prod_{j\neq i} \hat{P}_j \right), \tag{7.24}$$

$$[\hat{\rho}_{loc;0}]^2 = \mathrm{Tr}_{/i} \Bigg(\int_0^1 d\lambda_1 \int_{\lambda_1}^1 d\lambda_2 \exp(\lambda_1 A) \sum_{j_1\neq i, \tau_1\tau_1'} \left(t_{j_1}^{\tau_1\tau_1'} a_i^{\dagger(\tau_1)} a_{j_1}^{(\tau_1')} + h.c. \right) \exp((\lambda_2 - \lambda_1)A) \tag{7.25}$$

$$\times \sum_{j_2\neq i, \tau_2\tau_2'} \left(t_{j_2}^{\tau_2\tau_2'} a_i^{\dagger(\tau_2)} a_{j_2}^{(\tau_2')} + h.c. \right) \exp((1-\lambda_2)A) \prod_{j\neq i} \hat{P}_j \Bigg), \tag{7.26}$$

where the cavity Green's function is defined as

$$G_{j_1 j_2}^{\tau_1\tau_2}(\lambda_1, \lambda_2) = \mathrm{Tr}_{/i} \Big(\exp(\lambda_1 A_b) a_{j_1}^{(\tau_1)} \exp((\lambda_2 - \lambda_1)A_b) a_{j_2}^{\dagger(\tau_2)} \exp((1-\lambda_2)A_b) \prod_{j\neq i} \hat{P}_j \Big). \tag{7.27}$$

The cavity Green's function is completely determined from the density matrix in the compound space of all sites not including i, defined as

$$\hat{\rho}_B = \exp(A_b) \prod_{j\neq i} \hat{P}_j. \tag{7.28}$$

In infinite dimensions, the single-particle density matrix computed under $\hat{\rho}_B$ is defined as

$$n_{B;jj'}^{\tau\tau'} = \mathrm{Tr}(\hat{\rho}_B a_j^{\dagger(\tau)} a_{j'}^{(\tau')}) \sim \left(\frac{1}{\sqrt{d}}\right)^{|j-j'|}, \tag{7.29}$$

where d is the dimension of the lattice. Similarly, Eq. 7.27 will scale in the same way. Analogous to the case of DMFT, the local effective density matrix $\hat{\rho}_{loc;0}$ only depends on $n_{B;jj'}^{\tau\tau'}$. To illustrate this, consider the second order contribution of

$$\begin{aligned}
&\mathrm{Tr}_{/i}\Big(\exp(\lambda_1 A) t_{j_1}^{\tau_1\tau_1'} a_i^{\dagger(\tau_1)} a_{j_1}^{(\tau_1')} \exp((\lambda_2-\lambda_1)A) t_{j_2}^{\tau_2\tau_2'} a_{j_2}^{\dagger(\tau_2)} a_i^{(\tau_2')} \exp((1-\lambda_2)A) \prod_{j\neq i} \hat{P}_j \Big) \\
&= t_{j_1}^{\tau_1\tau_1'} t_{j_2}^{\tau_2\tau_2'} G_{j_1 j_2}^{\tau_1'\tau_2}(\lambda_1,\lambda_2) \exp(\lambda_1 A_i) a_i^{\dagger(\tau_1)} \exp((\lambda_2-\lambda_1)A_i) a_i^{(\tau_2')} \exp((1-\lambda_2)A_i).
\end{aligned} \tag{7.30}$$

The total scaling of this term will be $d^{|j_1-i|} d^{|j_2-i|} d^{-\frac{1}{2}|j_1-i|} d^{-\frac{1}{2}|j_2-i|} d^{-\frac{1}{2}|j_1-j_2|} \sim 1$. Considering the fourth order contribution

$$\begin{aligned}
&t_{j_1}^{\tau_1\tau_1'} t_{j_2}^{\tau_2\tau_2'} t_{j_3}^{\tau_3\tau_3'} t_{j_4}^{\tau_4\tau_4'} G_{j_1 j_2 j_3 j_4}^{\tau_1'\tau_2\tau_3'\tau_4}(\lambda_1,\lambda_2,\lambda_3,\lambda_4) \times \\
&\exp(\lambda_1 A_i) a_i^{\dagger(\tau_1)} \exp((\lambda_2-\lambda_1)A_i) a_i^{(\tau_2')} \exp((\lambda_3-\lambda_2)A_i) a_i^{\dagger(\tau_3)} \\
&\exp((\lambda_4-\lambda_3)A_i) a_i^{(\tau_4')} \exp((1-\lambda_4)A_i)
\end{aligned} \tag{7.31}$$

the scaling for one of the connected portions is

$$\begin{aligned}
&d^{|j_1-i|} d^{|j_2-i|} d^{|j_3-i|} d^{|j_4-i|} d^{-\frac{1}{2}|j_1-i|} d^{-\frac{1}{2}|j_2-i|} d^{-\frac{1}{2}|j_3-i|} d^{-\frac{1}{2}|j_4-i|} d^{-\frac{1}{2}|j_1-j_2|} d^{-\frac{1}{2}|j_2-j_3|} d^{-\frac{1}{2}|j_3-j_4|} \\
&\sim d^{-\frac{1}{2}|j_2-j_3|} \to 0
\end{aligned} \tag{7.32}$$

and all other connected diagrams will scale to zero. The same result holds for higher orders. This proves that the we could replace the projector from other sites as non-interacting

projectors. Thus, we could replace the operator

$$\prod_{j\neq i} \hat{P}_j \to \exp\left(\Sigma_{B;i}\hat{N}\right), \tag{7.33}$$

where $\Sigma_{B;i}$ is a single-particle potential within the sites not containing i. We proceed by plugging in for $\hat{\rho}_{loc;0}$

$$\begin{aligned}
\hat{\rho}_{loc;0} &= \mathrm{Tr}_{/i}\left(\hat{\rho}_{eff;0}\exp\left(\Sigma_{B;i}\hat{N}\right)\right) && (7.34)\\
&= \mathrm{Tr}_{/i}\left(\hat{\rho}_{eff;0}\exp\left(\left(\Sigma_{B;i}+\Sigma_{loc;i}\right)\hat{N}\right)\exp\left(-\Sigma_{loc;i}\right)\right) && (7.35)\\
&= \mathrm{Tr}_{/i}\left(\hat{\rho}^{\star}_{eff}\exp\left(-\Sigma_{loc;i}\hat{N}\right)\right), && (7.36)
\end{aligned}$$

where $\Sigma_{loc;i}$ is the self-energy for the discrete time impurity model for a given $\hat{\rho}_{loc;0}$ and thus is a single-particle potential within the site i; and $\hat{\rho}^{\star}_{eff}$ is a non-interacting density matrix that has the same single-particle density matrix as $\hat{\rho}_{eff}$.

Finally, we prove that $\Sigma_{B;i}$ is local to site i. To see this, we notice that the above construction can be applied to every site i, and thus we have $\Sigma = \Sigma_{B;i} + \Sigma_{loc;i}$ for every site i. Therefore, we can solve for $\Sigma_{B;i} = \sum_{j\neq i}\Sigma_{loc;j}$, proving the LSA self-consistency condition, analogous to DMFT.

7.3 SPD for the Hubbard Model

In this section, we apply VDAT to the Hubbard model

$$\hat{H} = \hat{H}_0 + \hat{V}, \qquad \hat{H}_0 = \sum_{ij\sigma} t_{ij}\hat{a}^{\dagger}_{i\sigma}\hat{a}_{j\sigma}, \qquad \hat{V} = U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = U\sum_i \hat{d}_i. \tag{7.37}$$

We employ the SPD-d

$$\hat{\rho} = \exp\left(\boldsymbol{\gamma}_1 \cdot \hat{\boldsymbol{n}}\right) \hat{P}_1 ... \exp\left(\boldsymbol{\gamma}_{\mathcal{N}} \cdot \hat{\boldsymbol{n}}\right) \hat{P}_{\mathcal{N}} = \hat{\mathcal{P}}_1 ... \hat{\mathcal{P}}_{\mathcal{N}}, \quad \hat{P}_\tau = \exp\left(\hat{V}_\tau\right), \quad \hat{\mathcal{P}}_\tau = \exp\left(\boldsymbol{\gamma}_\tau \cdot \hat{\boldsymbol{n}}\right) \hat{P}_\tau, \tag{7.38}$$

where

$$\hat{P}_\tau = \prod_i \left(\left(1 - \mu_\tau - \frac{1}{4} u_\tau\right) \hat{1} + \mu_\tau \left(\hat{a}^\dagger_{i\uparrow} \hat{a}_{i\uparrow} + \hat{a}^\dagger_{i\downarrow} \hat{a}_{i\downarrow}\right) + u_\tau \hat{a}^\dagger_{i\uparrow} \hat{a}_{i\uparrow} \hat{a}^\dagger_{i\downarrow} \hat{a}_{i\downarrow} \right) \tag{7.39}$$

and

$$\exp\left(\boldsymbol{\gamma}_\tau \cdot \hat{\boldsymbol{n}}\right) = \prod_{\mathbf{k}\sigma} (1 + h(w_{\mathbf{k}\sigma}(\eta_{1\sigma;\tau}, \eta_{2\sigma;\tau}, \eta_{3\sigma;\tau}, \eta_{4\sigma;\tau})) \Delta \hat{n}_{\mathbf{k}\sigma}) \tag{7.40}$$

and

$$w_{\mathbf{k}\sigma}(\eta_1, \eta_2, \eta_3, \eta_4) = \eta_1 \theta(\epsilon_{\mathbf{k}\sigma} - \eta_2) + \eta_3 f(\epsilon_{\mathbf{k}\sigma} - \eta_2, \eta_4) + \eta_2 \tag{7.41}$$

where $f(x, \alpha) = \text{sign}(x)(1 - \exp(-\alpha|x|))/(1 - \exp(-\alpha))$, $h(x)$ is defined in Eq. 6.30, and $\Delta n_{\mathbf{k}\sigma}$ is defined in Eq. 6.31. We have parameterized the non-interacting projector using four independent variables $\eta_{i\sigma}$ for each spin. In principle, there can be a variational parameter for each $\mathbf{k}\sigma$, but in practice this massive flexibility is simply not needed.

The LSA for $\mathcal{N} = 2$

To understand how the LSA works, we study the case of $\mathcal{N} = 2$, which is equivalent to the Gutzwiller approximation. We focus on half-filling for clarity. The SPD-d is

$$\hat{\rho} = \exp\left(\sum_i u \Delta \hat{d}_i\right) \exp\left(\sum_\epsilon \gamma_{\epsilon\sigma} \hat{n}_{\epsilon\sigma}\right) \exp\left(\sum_i u \Delta \hat{d}_i\right). \tag{7.42}$$

Thus, the non-interacting discrete Green function for a given $\epsilon\sigma$ is

$$\boldsymbol{g}_0 = \begin{pmatrix} \frac{\exp(\epsilon_1+\epsilon_2)}{1+\exp(\epsilon_1+\epsilon_2)} & \frac{\exp(\epsilon_1)}{1+\exp(\epsilon_1+\epsilon_2)} \\ -\frac{\exp(\epsilon_2)}{1+\exp(\epsilon_1+\epsilon_2)} & \frac{\exp(\epsilon_1+\epsilon_2)}{1+\exp(\epsilon_1+\epsilon_2)} \end{pmatrix} = \frac{1}{2n_2n_1 - n_1 - n_2 + 1} \begin{pmatrix} n_1n_2 & -n_1(n_2-1) \\ (n_1-1)n_2 & n_1n_2 \end{pmatrix}, \tag{7.43}$$

where $\epsilon_1 = 0$, $\epsilon_2 = \gamma_{\epsilon\sigma}$, $n_1 = \frac{1}{2}$, and $n_2 = \frac{1}{1+\exp(-\epsilon_2)}$. One can clearly see it is better to use n_2 instead of ϵ_2 to parameterize the density matrix (see Section 3.4). We denote $n_2 = n_{\epsilon\sigma} = \frac{1}{1+\exp(-\gamma_{\epsilon\sigma})}$ as the independent variational parameters. Therefore,

$$\boldsymbol{g}_{0;\epsilon\sigma} = \begin{pmatrix} n_{\epsilon\sigma} & (1-n_{\epsilon\sigma}) \\ -n_{\epsilon\sigma} & n_{\epsilon\sigma} \end{pmatrix}, \tag{7.44}$$

and as a result we choose the following initial guess for the noninteracting discrete Green's function of the LDAM

$$\boldsymbol{\mathcal{G}_\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{7.45}$$

Following the same procedure as in the Anderson model, we could express the interacting local discrete Green function as

$$\boldsymbol{g}_{loc,\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{1-16\Delta \mathrm{d}^2} \\ -\frac{1}{2}\sqrt{1-16\Delta \mathrm{d}^2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}z(d) \\ -\frac{1}{2}z(d) & \frac{1}{2} \end{pmatrix}. \tag{7.46}$$

The self-energy operator can then be written as

$$\boldsymbol{S}_{loc;\sigma} = \left(\boldsymbol{\mathcal{G}}_\sigma^{-1} - 1\right)^{-1} \left(\boldsymbol{g}_{loc;\sigma}^{-1} - 1\right) = \begin{pmatrix} \frac{2z}{z^2+1} & \frac{2}{z^2+1} - 1 \\ 1 - \frac{2}{z^2+1} & \frac{2z}{z^2+1} \end{pmatrix} \tag{7.47}$$

and

$$\boldsymbol{S}_{loc} = \begin{pmatrix} \frac{2z}{z^2+1} & \frac{2}{z^2+1} - 1 & 0 & 0 \\ 1 - \frac{2}{z^2+1} & \frac{2z}{z^2+1} & 0 & 0 \\ 0 & 0 & \frac{2z}{z^2+1} & \frac{2}{z^2+1} - 1 \\ 0 & 0 & 1 - \frac{2}{z^2+1} & \frac{2z}{z^2+1} \end{pmatrix}. \tag{7.48}$$

Then

$$\boldsymbol{g}_{\epsilon\sigma} = \frac{\mathbf{1}}{\mathbf{1} + \left(\boldsymbol{g}_{0;\epsilon\sigma}^{-1} - \mathbf{1}\right) \boldsymbol{S}_{loc;\sigma}} = \begin{pmatrix} n_{\epsilon\sigma} & (1 - n_{\epsilon\sigma})\, z \\ -n_{\epsilon\sigma} z & \left(n_{\epsilon\sigma} - \frac{1}{2}\right) z^2 + \frac{1}{2} \end{pmatrix} \tag{7.49}$$

Then we can update the new interacting local discrete Green's function as

$$\boldsymbol{g}'_{loc;\sigma} = \int d\epsilon D\left(\epsilon\right) \boldsymbol{g}_{\epsilon\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} z \\ \frac{1}{2} z & \frac{1}{2} \end{pmatrix} \tag{7.50}$$

$$\boldsymbol{\mathcal{G}}'_{\sigma} = \boldsymbol{S}_{loc;\sigma} \frac{\mathbf{1}}{\left(\mathbf{1} + \boldsymbol{g}'_{loc;\sigma} \left(\boldsymbol{S}_{loc;\sigma} - \mathbf{1}\right)\right)} \boldsymbol{g}'_{loc;\sigma} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \boldsymbol{\mathcal{G}}_{\sigma}. \tag{7.51}$$

which proves that self-consistency has been achieved in the first iteration, demonstrating why self-consistency is not needed in the Gutzwiller approximation.

Now, we consider a more general case for an arbitrary density. We start with

$$\boldsymbol{\mathcal{G}}_{\sigma} = \begin{pmatrix} n & 1 - n \\ -n & n \end{pmatrix}, \tag{7.52}$$

where we assume spin symmetry. Then we use the local projectors

$$P_1^{(1)} = \left(1 - \mu - \frac{1}{4} u\right) I^{(1)} + \mu \left(\hat{n}_{\uparrow}^{(1)} + \hat{n}_{\downarrow}^{(1)}\right) + u \hat{n}_{\uparrow}^{(1)} \hat{n}_{\downarrow}^{(1)}, \tag{7.53}$$

$$P_2^{(2)} = \left(1 - \mu - \frac{1}{4} u\right) I^{(2)} + \mu \left(\hat{n}_{\uparrow}^{(2)} + \hat{n}_{\downarrow}^{(2)}\right) + u \hat{n}_{\uparrow}^{(2)} \hat{n}_{\downarrow}^{(2)} \tag{7.54}$$

and the local effective density matrix

$$\hat{\rho}_{eff} = \hat{\rho}_{eff;0} \hat{P}_1^{(1)} \hat{P}_2^{(2)}, \tag{7.55}$$

where $\hat{\rho}_{eff;0}$ is determined from

$$\boldsymbol{\mathcal{G}} = \begin{pmatrix} n & 0 & 1-n & 0 \\ 0 & n & 0 & 1-n \\ -n & 0 & n & 0 \\ 0 & -n & 0 & n \end{pmatrix}, \tag{7.56}$$

where we use the time index major scheme (see Section 3.4). Then

$$\begin{aligned} \left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \right\rangle_{\hat{\rho}_{eff;0}} =& \frac{1}{16} \left(8n^2+1\right) u^2 + \frac{1}{2} u \left(\mu + 4(\mu+1)n^2 - 2\mu n - 1\right) + \\ & \mu(\mu + 2n(\mu(n-1)+2) - 2) + 1. \end{aligned} \tag{7.57}$$

We can compute the density matrix as

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(1)} \hat{a}_\uparrow^{(1)} \right\rangle_{\hat{\rho}_{eff;0}} = \frac{1}{16} n \left(16\mu^2 n + 8\mu n(3u+4) + u(8n(u+4)+u-8) + 16\right), \tag{7.58}$$

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(1)} \hat{a}_\uparrow^{(2)} \right\rangle_{\hat{\rho}_{eff;0}} = \frac{1}{16} (n-1)(u-4)(\mu(8n-4) + (4n-1)u + 4), \tag{7.59}$$

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(2)} \hat{a}_\uparrow^{(1)} \right\rangle_{\hat{\rho}_{eff;0}} = \frac{1}{16} n(u-4)(\mu(8n-4) + (4n-1)u + 4), \tag{7.60}$$

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(2)} \hat{a}_\uparrow^{(2)} \right\rangle_{\hat{\rho}_{eff;0}} = \frac{1}{16} n \left(16\mu^2 n + 8\mu n(3u+4) + u(8n(u+4)+u-8) + 16\right), \tag{7.61}$$

$$\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(2)} \hat{a}_\uparrow^{(2)} \hat{a}_\downarrow^{(2)} \hat{a}_\downarrow^{(2)} \right\rangle_{\hat{\rho}_{eff;0}} = \frac{1}{16} n^2 (4\mu + 3u + 4)^2. \tag{7.62}$$

The first step is that we can determine μ for a given u such that

$$\frac{\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(2)} \hat{a}_\uparrow^{(2)} \right\rangle_{\hat{\rho}_{eff;0}}}{\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \right\rangle_{\hat{\rho}_{eff;0}}} = n. \tag{7.63}$$

Thus, we could solve

$$\mu = \frac{\pm\sqrt{n^2u^2 - 64n^4u + 192n^3u - 200n^2u + 16n^2 - 2nu^2 + 80nu - 32n + u^2 - 8u + 16} - 4n^2u + 5nu - 4n - u + 4}{4\left(2n^2 - 3n + 1\right)}. \tag{7.64}$$

Both solutions should produce the same expectation values, and we can pick either of them. Then, for the diagonal part we have

$$\frac{\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(1)} \hat{a}_\uparrow^{(1)} \right\rangle_{\hat{\rho}_{eff;0}}}{\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \right\rangle_{\hat{\rho}_{eff;0}}} = n, \qquad \frac{\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \hat{a}_\uparrow^{(2)} \hat{a}_\uparrow^{(2)} \right\rangle_{\hat{\rho}_{eff;0}}}{\left\langle \hat{P}_1^{(1)} \hat{P}_2^{(2)} \right\rangle_{\hat{\rho}_{eff;0}}} = n \tag{7.65}$$

and for the off-diagonal part

$$\frac{\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\hat{a}_\uparrow^{(1)}\hat{a}_\uparrow^{(2)}\right\rangle_{\hat{\rho}_{eff;0}}}{\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\right\rangle_{\hat{\rho}_{eff;0}}} =$$

$$\left((1-2n)^2(u-4)\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}\right)\Big/\Big($$

$$8(8(n-1)n+1)u+4nu\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}+$$

$$16n\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}-u^2-16\Big), \tag{7.66}$$

$$\frac{\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\hat{a}_\uparrow^{(2)}\hat{a}_\uparrow^{(1)}\right\rangle_{\hat{\rho}_{eff;0}}}{\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\right\rangle_{\hat{\rho}_{eff;0}}} =$$

$$\left((1-2n)^2n(u-4)\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}\right)\Big/\Big($$

$$(n-1)\Big(8(8(n-1)n+1)u+4nu\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}+$$

$$16n\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}-u^2-16\Big)\Big) \tag{7.67}$$

$$\frac{\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\hat{a}_\uparrow^{(2)}\hat{a}_\uparrow^{(2)}\hat{a}_\downarrow^{(2)}\hat{a}_\downarrow^{(2)}\right\rangle_{\hat{\rho}_{eff;0}}}{\left\langle \hat{P}_1^{(1)}\hat{P}_2^{(2)}\right\rangle_{\hat{\rho}_{eff;0}}} =$$

$$-\left(n^2\left(2(n-2)n(u+4)-\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}+2u+8\right)^2\right)\Big/\Big($$

$$(n-1)^2\Big(8(8(n-1)n+1)u+4nu\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}+$$

$$16n\sqrt{(n-1)^2(u(-64(n-1)n+u-8)+16)}-u^2-16\Big)\Big) \tag{7.68}$$

Then we can get the interacting local discrete Green's function by solving for u as a function of n and d

$$\boldsymbol{g}_{loc;\sigma}=\begin{pmatrix} n & (1-n)\,z \\ -nz & n \end{pmatrix}, \qquad z\,(n,d)=\frac{\left(\sqrt{(1-2n+d)}+\sqrt{d}\right)\sqrt{n-d}}{\sqrt{n\,(1-n)}}. \tag{7.69}$$

So we get

$$\boldsymbol{S}_{loc;\sigma} = \begin{pmatrix} \frac{z}{-nz^2+n+z^2} & \frac{1}{-nz^2+n+z^2} - 1 \\ \frac{n-nz^2}{(n-1)z^2-n} & \frac{z}{-nz^2+n+z^2} \end{pmatrix}, \qquad \boldsymbol{g}_{0;\epsilon\sigma} = \begin{pmatrix} n_{\epsilon\sigma} & 1-n_{\epsilon\sigma} \\ -n_{\epsilon\sigma} & n_{\epsilon\sigma} \end{pmatrix}. \tag{7.70}$$

Finally, we have

$$\boldsymbol{g}_{\epsilon\sigma} = \frac{\mathbf{1}}{\mathbf{1} + \left(\boldsymbol{g}_{0;\epsilon\sigma}^{-1} - \mathbf{1}\right) \boldsymbol{S}_{loc;\sigma}} = \begin{pmatrix} n_{\epsilon\sigma} & z - zn_{\epsilon\sigma} \\ -zn_{\epsilon\sigma} & z^2 n_{\epsilon\sigma} - nz^2 + n \end{pmatrix}. \tag{7.71}$$

Once again, we see that self-consistency has already been achieved. One can also see that this analysis can be generalized to the multi-band case, and recover the Gutzwilller approximation exactly in general. Consider

$$\hat{\rho}_{loc} = \hat{\rho}_{loc;0} \hat{P}_1^{(1)} \hat{P}_2^{(2)}, \tag{7.72}$$

where $\hat{P}_1 = \hat{P}_2 = \hat{p}$ in the physical space due to the constraint of the SPD being symmetric. We notice that $\hat{\rho}_{loc;0}$ is the effective density matrix of an SPD (this is not true for $\mathcal{N} > 2$ in general). Therefore, we can map the compound system back the the original system and compute the renormalization of the off-diagonal part of the discrete Green's function as

$$\frac{\mathrm{Tr}\left(\hat{p}\hat{a}_{n\sigma}^\dagger \exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}\right) \hat{p}\hat{a}_{n\sigma}\right)}{\mathrm{Tr}\left(\hat{a}_{n\sigma}^\dagger \exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}\right) \hat{a}_{n\sigma}\right)} = \frac{\mathrm{Tr}\left(\hat{p} \exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}/2\right) \hat{a}_{n\sigma}^\dagger \exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}/2\right) \hat{p}\hat{a}_{n\sigma}\right)}{\mathrm{Tr}\left(\exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}/2\right) \hat{a}_{n\sigma}^\dagger \exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}/2\right) \hat{a}_{n\sigma}\right)} \tag{7.73}$$

$$= \frac{\mathrm{Tr}\left(\sqrt{\hat{\rho}_{loc}}\hat{a}_{n\sigma}^\dagger \sqrt{\hat{\rho}_{loc}}\hat{a}_{n\sigma}\right)}{\mathrm{Tr}\left(\sqrt{\hat{\rho}_{loc;0}}\hat{a}_{n\sigma}^\dagger \sqrt{\hat{\rho}_{loc;0}}\hat{a}_{n\sigma}\right)}, \tag{7.74}$$

where we assume that $\boldsymbol{v}_0$ is a diagonal matrix in the basis of spin orbitals, and thus we can move the $\hat{a}_{n\sigma}^\dagger$ while only acquiring a trivial factor, and $\hat{p}$ commutes with $\exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}\right)$. Additionally, we require

$$\frac{\mathrm{Tr}\left(\hat{p} \exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}\right) \hat{p}\right)}{\mathrm{Tr}\left(\exp\left(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}\right)\right)} = 1 \tag{7.75}$$

in order to satisy the normalization of the density matrix. Alternatively, if $\hat{p}$ does not

commute with $\exp(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}})$, we must evaluate

$$\frac{\mathrm{Tr}\left(\hat{T}^\dagger \hat{a}^\dagger \hat{T} a\right)}{\mathrm{Tr}\left(\hat{T}_0^\dagger \hat{a}^\dagger \hat{T}_0 \hat{a}\right)}, \tag{7.76}$$

where $\hat{T}_0 = \exp(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}/2)$ and $\hat{T} = \exp(\boldsymbol{v}_0 \cdot \hat{\boldsymbol{n}}/2)\,\hat{p}$ and normalization requires $\mathrm{Tr}\left(\hat{T}^\dagger \hat{T}\right) = \mathrm{Tr}\left(\hat{T}_0^\dagger \hat{T}_0\right)$.

7.4 Results for the $d = \infty$ Hubbard model

Here we present the results for the $d = \infty$ Hubbard model on the Bethe lattice, where VDAT within the LSA exactly evaluates the SPD-d for a given $\mathcal{N}$. It should be emphasized that the computed ground state energy within VDAT is a rigorous upper bound for the exact ground state energy, and we can compare to the numerically exact dynamical mean-field theory (DMFT) results obtained using the numerical renormalization group (NRG) method as the impurity solver[27]. We begin by examining the double occupancy as a function of U/t (see Figure 7.1), where we present VDAT results for $\mathcal{N} = 3$. We do not explore $\mathcal{N} = 2$, as this reproduces the Gutzwiller approximation (see Section 7.2), and these results are presented in Section 8.5. For half-filling, shown in red, we see that VDAT is very close to the DMFT solutions (points), reliably capturing the Mott metal-insulator transition. DMFT shows that the discontinuity in the double occupancy is removed upon doping, and is relatively sensitive for small doping around half-filling. We can see that VDAT clearly captures this behavior as the doping changes from 1 to 0.99 to 0.98 to 0.95 to 0.9. Capturing this delicate behavior is highly nontrivial. We can also proceed to much larger doping (see Figure 7.2), where VDAT once again reliably describes the DMFT solution.

All VDAT results discussed thus far have been for $\mathcal{N} = 3$, and it is interesting to consider $\mathcal{N} = 4$ to better understand the convergence of the VDAT. Therefore, we study the double occupancy as a function of U/t at half filling for $\mathcal{N} = 3$ and 4 (see Figure 7.3). We see that

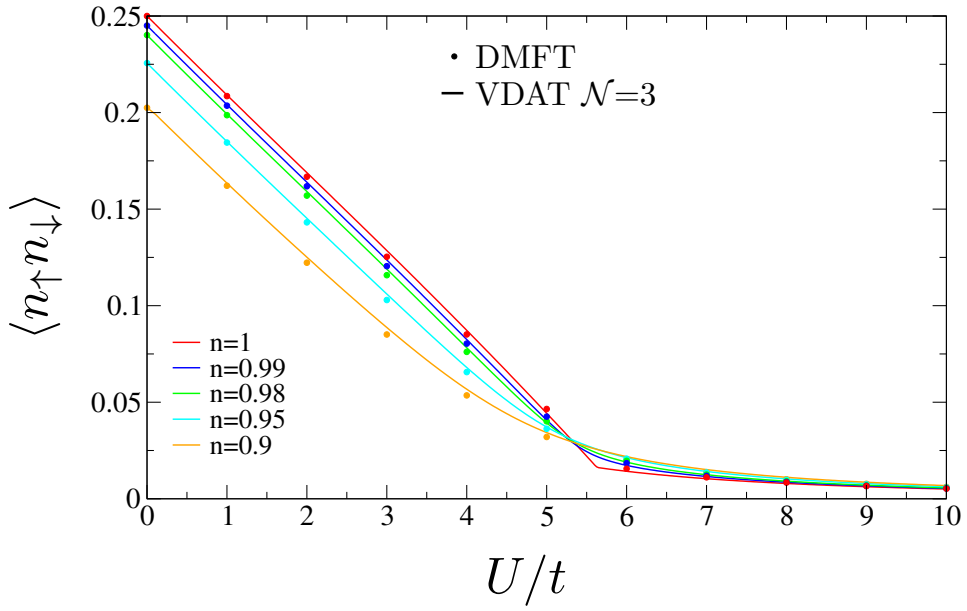

Figure 7.1: The double occupancy vs. U/t in the $d = \infty$ Hubbard model on the Bethe lattice evaluated using VDAT($\mathcal{N} = 3$) (lines) and compared to DMFT (points). Densities of 1, 0.99, 0.98, 0.95, and 0.9 are evaluated.

$\mathcal{N} = 4$ has a smaller error for all values of U/t, as it must, and the error for large U/t is nearly zero, while the error is substantially reduced for small U/t.

We now proceed to study the density as a function of the chemical potential, which characterizes the energetics and the band gap (see Figure 7.4). Here we compare to both DMFT and the Gutzwiller approximation (i.e. $\mathcal{N} = 2$). We see that VDAT $\mathcal{N} = 3$ does a reasonable job at capturing the DMFT results, but has nontrivial errors for large U/t near half filling, and $\mathcal{N} = 4$ would likely be needed to correct this, though we have not performed such calculations yet.

Finally, we consider the density distribution in momentum space, characterized by the band energy (see Figure 7.5). Here we consider VDAT results at various U/t at half filling for $\mathcal{N} = 3$ and 4, and compare to DMFT. For small U/t and large U/t, as in the insulating state, we see that $\mathcal{N} = 3$ already performs very well. Alternatively, there are nontrivial errors for intermediate values of U/t. However, increasing to $\mathcal{N} = 4$ substantially improves the results.

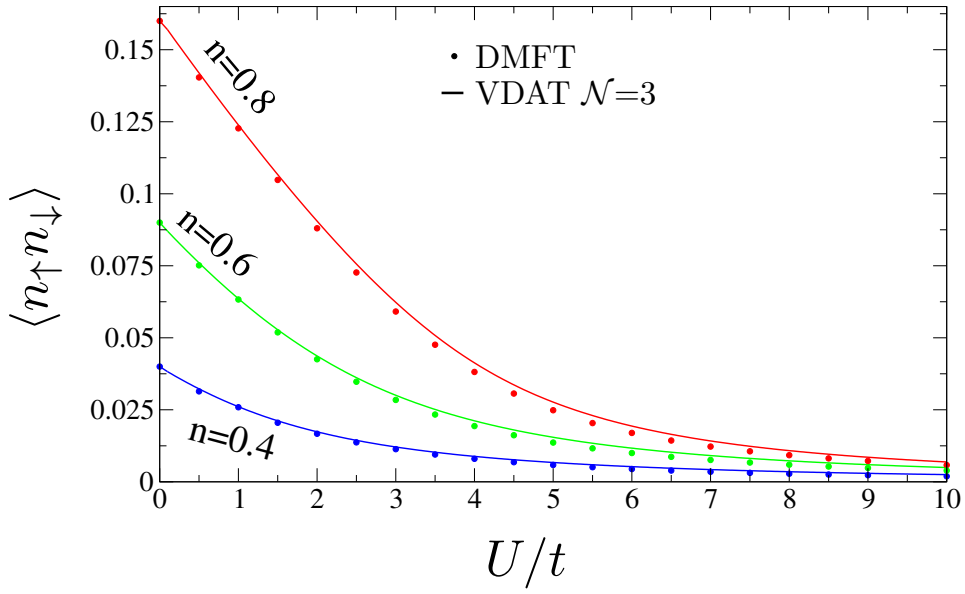

Figure 7.2: The double occupancy vs. U/t in the $d = \infty$ Hubbard model on the Bethe lattice evaluated using VDAT($\mathcal{N} = 3$) (lines) and compared to DMFT (points). Densities of 0.8, 0.6, and 0.4 are evaluated.

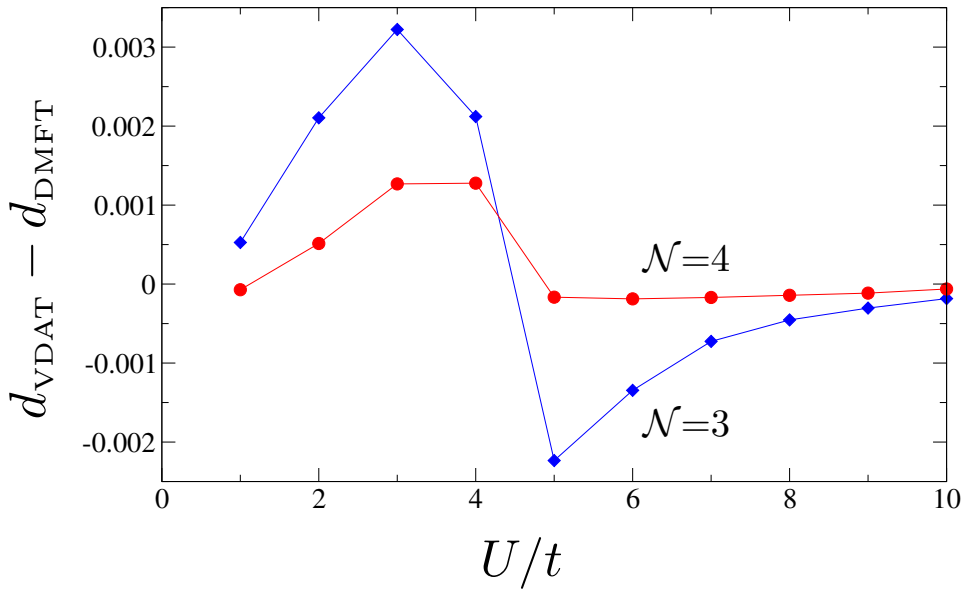

Figure 7.3: The difference in the double occupancy between VDAT and DMFT vs. U/t in the $d = \infty$ Hubbard model on the Bethe lattice. VDAT is evaluated using both $\mathcal{N} = 3$ and $\mathcal{N} = 4$.

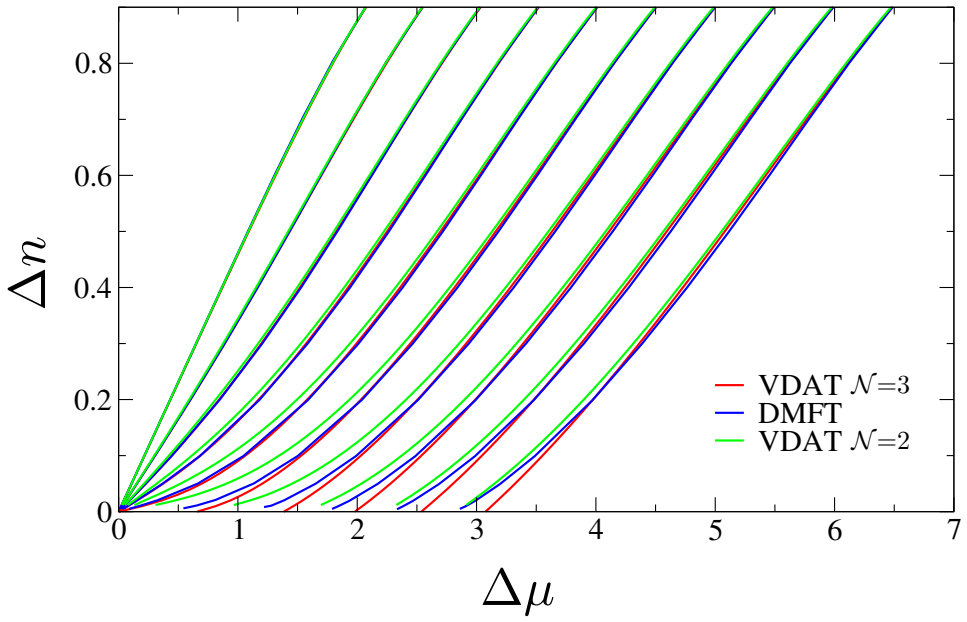

Figure 7.4: The density ($\Delta n = n-1$) as a function of chemical potential ($\Delta\mu = \mu - U/2$) for the d=∞ Hubbard model on the Bethe lattice solved using DMFT, GA, and VDAT($\mathcal{N}=3$) for $U/t = 1, .., 10$.

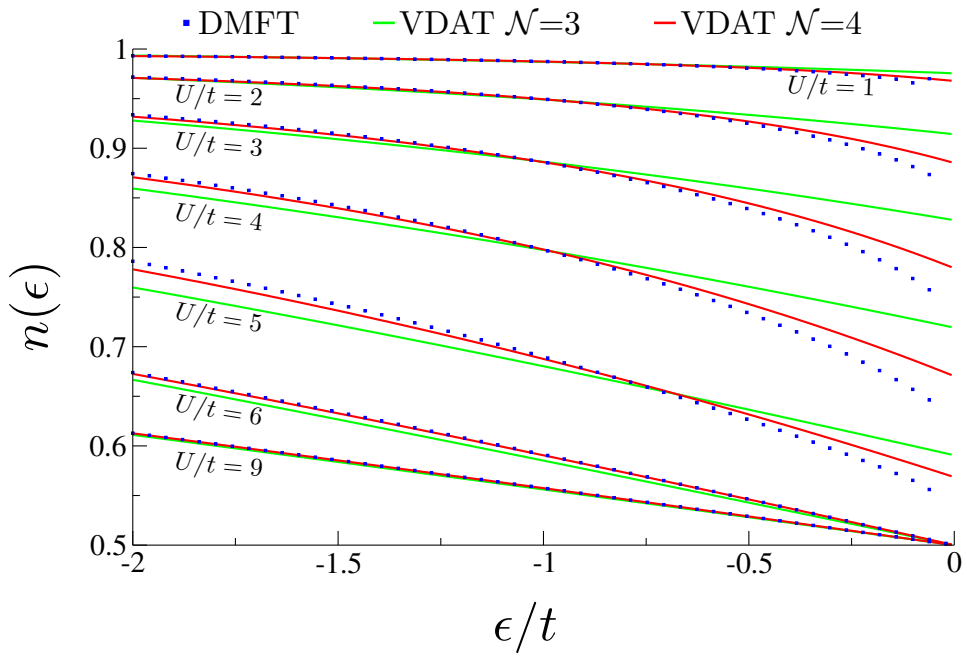

Figure 7.5: The density distribution vs. energy for the d=∞ Hubbard model on the Bethe lattice for various values of U/t evaluated using VDAT($\mathcal{N}=3,4$) and DMFT.

Chapter 8

Off-shell Effective Energy Theory

8.1 An Exact Approach to Correct the SPD

As we have seen, the SPD provide a systematic way to construct a variational density matrix that approximates the exact ground state density matrix, and the VDAT provides a general formalism to evaluate the SPD via a discrete action and its corresponding discrete Green's function. One could view this line of development as a true ab initio method as, in principle, one would approach the exact result with sufficient computational resources. However, there is another very different type of theory, which is also coined with the terminology ab initio, which go under the name of effective energy theories; such as density functional theory (DFT). These types of theories are based on the constrained search or Legendre transformation of the energy. The central idea is that for a given Hamiltonian, we can divide it into internal and external parts, and the energy of the internal part could be expressed a functional of the external observables; and this functional captures all the information for this class of Hamiltonians. We demonstrate this problem with the following Hamiltonian

$$\hat{H} = \hat{H}_0 + f\hat{A}, \tag{8.1}$$

where $\hat{H}_0$ is the internal part and f is the external potential and $\hat{A}$ is the external operator. Then we can define the effective energy as

$$E(A) = \min_{\hat{\rho}} \left\{ \left\langle \hat{H}_0 \right\rangle_{\hat{\rho}} | \mathrm{Tr}\left(\hat{\rho}\hat{A}\right) = A \right\}. \tag{8.2}$$

Now, imagine we have also a variational density matrix $\hat{\rho}(\gamma_1, ..\gamma_N)$, which could be taken as the SPD, and we can then perform the same procedure using the variational density matrix as

$$E_{appr}(A) = \min_{\{\gamma\}} \left\{ \left\langle \hat{H}_0 \right\rangle_{\hat{\rho}(\gamma_1,..\gamma_N)} \left| \mathrm{Tr}\left(\hat{\rho}(\gamma_1, ..\gamma_N)\hat{A}\right) = A \right. \right\}. \tag{8.3}$$

We can further introduce

$$\mathcal{A}(\gamma_1, ..\gamma_N) = \mathrm{Tr}\left(\hat{\rho}(\gamma_1, ..\gamma_N)\hat{A}\right). \tag{8.4}$$

By solving the equation

$$\mathcal{A}(\gamma_1, ..\gamma_N) = A, \tag{8.5}$$

we can eliminate one variational parameter, substituting A in place of γ_1, for example. Using the energy functional we then have

$$\mathcal{E}(A, \gamma_2, ..\gamma_N) = \mathrm{Tr}\left(\hat{\rho}(A, \gamma_2, ..\gamma_N)\hat{H}_0\right) \tag{8.6}$$

and we can minimize over $\gamma_2, ..\gamma_N$ for a given A, resulting in

$$\gamma_i = g_i(A), \qquad i = 2, \ldots, N. \tag{8.7}$$

Thus, we could correct the energy functional as

$$\mathcal{E}^*(A, \gamma_2, ..\gamma_N) = \mathcal{E}(A, \gamma_2, ..\gamma_N) + \Delta E(A), \tag{8.8}$$

where the correction is given as

$$\Delta E\left(A\right)=E\left(A\right)-\mathcal{E}\left(A,g_{2}\left(A\right),..,g_{N}\left(A\right)\right), \tag{8.9}$$

which explicitly depends on A and implicitly depends on $\hat{H}_{0}$. In practice, we could use an approximate form $\Delta\tilde{E}$ where

$$\Delta\tilde{E}\left(A,\gamma_{2},..\gamma_{N}\right)\geq\Delta E\left(A\right) \tag{8.10}$$

and the equal sign is taken at

$$\gamma_{i}=g_{i}\left(A\right). \tag{8.11}$$

We refer to this general form

$$\mathcal{E}^{*}\left(A,\gamma_{2},..\gamma_{N}\right)=\mathcal{E}\left(A,\gamma_{2},..\gamma_{N}\right)+\Delta\tilde{E}\left(A,\gamma_{2},..\gamma_{N}\right) \tag{8.12}$$

as an off-shell effective energy functional, where off-shell means that in addition to the physical observable A, we also have variational parameters γ_{i}. One can view the off-shell effective energy functional as a combination of the variational principle and the effective energy theory.

Notice that in the first formulation of OET[28], we used the exact projector to construct the OET ansatz. While that construction is different from what we have outlined above, the final forms are the same. We explore the latter in the next section.

8.2 Motivation for OET

Computing the ground state properties of quantum Hamiltonians requires the search of an exponentially large space of wave functions. To formally resolve the issue of large dimension-

ality, one can use effective energy approaches, which partition the Hamiltonian of a given class into some external and internal components; where each component consists of operators and corresponding coupling constants. The constrained search[29] can then be used to define the energy of the internal contribution in terms of the internal coupling constants and the expectation values of the external operators. For example, in density functional theory (DFT)[30–32], the internal component is the kinetic and interaction energy, and the external component is the coupling between the density and the external potential; and the resulting energy functional depends on the density and the coupling constants of the kinetic and interaction energy. The ground state wave function is then fully determined from the corresponding external expectation values and internal couplings, but such a construction is only useful if robust approximations can be formulated.

Here we introduce off-shell effective energy theory (OET), which employs a wave function ansatz determined from the internal coupling constants and *both* the internal and external expectation values. Unlike the usual effective energy theories, such as DFT, an arbitrary set of expectation values will not generally correspond to any ground state within the class of Hamiltonians; but OET will yield the exact ground state when minimizing the total energy over all expectation values. OET opens a new avenue for developing novel approximations. We introduce the central point expansion (CPE), which is an expansion of the OET ansatz in terms of the internal couplings and the internal expectation values, while treating the external expectation values non-perturbatively. The CPE can then be renormalized (RCPE) using the standard expansion of the energy in terms of the external expectation values. Finally, we exploit the possibility of inverting the role of internal and external components, yielding a dual formulation of our theory; which will be critical for an accurate description of the Hamiltonian over all parameter space.

We apply OET to the single band Hubbard model, which is a canonical model of interacting Fermions[5, 33] with many practical applications, and this will provide a stringent benchmark of the OET within RCPE. For d=1, the Bethe Ansatz (BA) efficiently provides the ex-

act solution[11, 13]; while for d=∞, dynamical mean-field theory (DMFT)[3, 34, 35] provides the solution using numerically exact, but computationally intensive methods[10, 36]. For an arbitrary dimension, there are powerful but expensive methods which might provide reliable solutions, though each typically has severe limitations (e.g. quantum Monte-Carlo[37, 38] has the minus sign problem[39, 40], etc.). Our approach yields favorable agreement with the aforementioned approaches over all parameter space for the single band Hubbard model in d=1, 2, and ∞, which is remarkable for a single formalism.

8.3 Exact projector approach to construct OET

We begin by considering an arbitrary Hamiltonian which has been partitioned into two parts, $\hat{H} = k\hat{K} + x\hat{X}$, where each contribution can be exactly solved. Though this is not the most general scenario that we consider, it illustrates all key features of the theory. We begin by choosing $k\hat{K}$ as the internal component and $x\hat{X}$ as the external component; and this choice is referred to as the $\mathcal{K}$ formulation. The effective energy theory then yields the density matrix at a given temperature as

$$\hat{\rho}(k, X) = \underset{\hat{\rho}}{\operatorname{argmin}}\{\langle k\hat{K} + \beta^{-1} \ln \hat{\rho}\rangle_{\hat{\rho}} | \langle \hat{X}\rangle_{\hat{\rho}} = X\}, \tag{8.13}$$

where $X \in \mathcal{M}_{\hat{X}}$, with $\mathcal{M}_{\hat{X}} = \{\langle \hat{X}\rangle_{\hat{\rho}} : \hat{\rho} \in \mathcal{L}\}$ and $\mathcal{L}$ is the Liouville space of all possible density matrices; and we use the notation $\langle \hat{A}\rangle_{\hat{\rho}} = \mathrm{Tr}(\hat{A}\hat{\rho})$. The function $\hat{\rho}(k, X)$ provides the formal solution to $\hat{H}$ for arbitrary values of k and x. Our main strategy is to introduce a trial density matrix using the OET ansatz

$$\tilde{\hat{\rho}}(k, X, K) = \mathcal{C}\hat{\mathcal{P}}(k, X)\hat{\rho}_{\hat{K}}(K)\hat{\mathcal{P}}(k, X), \tag{8.14}$$

where $\mathcal{C}$ is the normalization, $K \in \mathcal{M}_K$ with $\mathcal{M}_K = \{\langle \hat{K}\rangle_{\hat{\rho}} : \hat{\rho} \in \mathcal{L}\}$, $\hat{\rho}_{\hat{K}}(K) = \mathcal{C}' \exp(\kappa\hat{K})$ satisfying $\langle \hat{K}\rangle_{\hat{\rho}_{\hat{K}}(K)} = K$, where $\mathcal{C}'$ is the normalization and $\kappa \in \mathbb{R}$ parameterizes $\hat{\rho}_{\hat{K}}(K)$.

The exact projector $\hat{\mathcal{P}}(k,X)$ is defined by requiring Eq. 8.14 to satisfy the on-shell condition: for any $k \in \mathbb{R}$ and $X \in \mathcal{M}_{\hat{X}}$ there exists a $K^\star \in \mathcal{M}_K$ such that $\tilde{\hat{\rho}}(k,X,K^\star) = \hat{\rho}(k,X)$. We can solve for $\hat{\mathcal{P}}(k,X)$ using the on-shell condition

$$\hat{\mathcal{P}}(k,X) = \frac{1}{\sqrt{\rho_g}} \left(\sqrt{\rho_g}\hat{\rho}(k,X)\sqrt{\rho_g}\right)^{1/2} \frac{1}{\sqrt{\rho_g}}, \tag{8.15}$$

where $\rho_g = \hat{\rho}_{\hat{K}}(K^\star)$. Finally, the ground state energy can be constructed as

$$\mathcal{E}(k,x) = \lim_{\beta\to\infty} \min_{K\in\mathcal{M}_K, X\in\mathcal{M}_X} \langle \hat{H} \rangle_{\tilde{\hat{\rho}}(k,X,K)}. \tag{8.16}$$

It is useful to introduce the map $\Upsilon(k,X,K) = (\langle \hat{K} \rangle_{\tilde{\hat{\rho}}(k,X,K)}, \langle \hat{X} \rangle_{\tilde{\hat{\rho}}(k,X,K)})$, which is the essential quantity needed to execute the theory. Our formalism has recast the exact solution of the Hamiltonian to a form which will prove to be amenable to approximations.

8.4 Central Point Approximation and its correction

We now introduce the key approximation scheme: the central point expansion (CPE). The CPE amounts to choosing an appropriate $K^\star$ and Taylor series expanding $\tilde{\hat{\rho}}(k,X,K)$ in k and K about some *central point*. Here we choose the central point $\hat{\rho}_c \equiv \mathcal{C}\hat{1}$, where $\mathcal{C}$ is the normalization, which yields $(K_c, X_c) = (\langle \hat{K} \rangle_{\hat{\rho}_c}, \langle \hat{X} \rangle_{\hat{\rho}_c})$, and we choose $K^\star$ such that $\hat{\mathcal{P}}(k,X_c) = 1$ within the CPE. Expanding $\hat{\mathcal{P}}(k,X)$ to zeroth order in k about 0 and $\hat{\rho}_{\hat{K}}(K)$ to first order in K about K_c, we find $K^\star = K_c$ and we have

$$\hat{\mathcal{P}}(k,X) \approx \hat{\mathcal{P}}(0,X) = \sqrt{\hat{\rho}_{\hat{X}}(X)\hat{\rho}^{-1}_{\hat{X}}(X_c)}, \tag{8.17}$$

$$\hat{\rho}_{\hat{K}}(K) \approx \hat{\rho}_{\hat{K}}(K_c)(1 + \langle\!\langle \Delta\hat{K}; \Delta\hat{K} \rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{X}}(X_c)} \Delta\hat{K}\Delta K), \tag{8.18}$$

where $\Delta\hat{K} = \hat{K} - K_c\hat{1}$, $\Delta K = K - K_c$, and $\langle\!\langle \hat{A}; \hat{B} \rangle\!\rangle_{\hat{\rho}} = \mathrm{Tr}(\hat{A}\sqrt{\hat{\rho}}\hat{B}\sqrt{\hat{\rho}})$, where the latter is known as the *symmetric correlator*[41]. To evaluate the ground state properties we only

need to evaluate $\Delta\hat{K}$ and $\Delta\hat{X} = \hat{X} - X_c\hat{1}$ under the CPE approximated $\tilde{\bar{\rho}}(k, X, K)$, denoted $\bar{\tilde{\rho}}$ for brevity

$$\langle\Delta\hat{K}\rangle_{\bar{\tilde{\rho}}} = \lambda\Big(\langle\Delta\hat{K}\rangle_{\hat{\rho}_{\hat{X}}(X)} + Z(\Delta X)\Delta K\Big), \tag{8.19}$$

$$\langle\Delta\hat{X}\rangle_{\bar{\tilde{\rho}}} = \lambda\Big(\Delta X + \frac{\langle\!\langle\Delta\hat{X};\Delta\hat{K}\rangle\!\rangle_{\hat{\rho}_{\hat{X}}(X)}}{\langle\!\langle\Delta\hat{K};\Delta\hat{K}\rangle\!\rangle_{\hat{\rho}_{\hat{X}}(X_c)}}\Delta K\Big), \tag{8.20}$$

$$\lambda = \Big(1 + \langle\Delta\hat{K}\rangle_{\hat{\rho}_{\hat{X}}(X)}\langle\!\langle\Delta\hat{K};\Delta\hat{K}\rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{X}}(X_c)}\Delta K\Big)^{-1}, \tag{8.21}$$

$$Z(\Delta X) = \langle\!\langle\Delta\hat{K};\Delta\hat{K}\rangle\!\rangle_{\hat{\rho}_{\hat{X}}(X)}\langle\!\langle\Delta\hat{K};\Delta\hat{K}\rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{X}}(X_c)}, \tag{8.22}$$

where $\Delta X = X - X_c$. The preceding expectation values approximate the map $\Upsilon(k, X, K)$, and given that $k = 0$ within the CPE, we use a distinct symbol $\bar{\Upsilon}(X, K) = (\langle\hat{K}\rangle_{\bar{\tilde{\rho}}}, \langle\hat{X}\rangle_{\bar{\tilde{\rho}}})$.

For a number of important Hamiltonians, including the Hubbard model and its generalizations, we notice that $\langle\Delta\hat{K}\rangle_{\hat{\rho}_{\hat{X}}(X)} = 0$, which implies that $\langle\!\langle\Delta\hat{X};\Delta\hat{K}\rangle\!\rangle_{\hat{\rho}_{\hat{X}}(X)} = 0$, and we refer to this scenario as the *orthogonal response condition* (ORC)[41]. For Hamiltonians with a given partition that satisfy the ORC, the CPE satisfies the exact condition $\bar{\Upsilon}(\Delta K, 0) = (\Delta K, 0)$, and has the form $\bar{\Upsilon}(\Delta K, \Delta X) = (Z(\Delta X)\Delta K, \Delta X)$; all subsequent discussions of the CPE will presume the ORC. The CPE will provide a reliable solution for $\Delta X \ll \Delta K$ and may provide reasonable solutions for $\Delta X \approx \Delta K$.

Though the CPE has a non-perturbative structure in X, in addition to the favorable characteristics outlined above, it does not have the correct second order expansion coefficient in ΔX. Therefore, we introduce the *renormalized central point expansion* (RCPE)[41], which maintains the form of $\bar{\Upsilon}$ but replaces $Z \to \mathcal{R}(Z)$. Here we introduce perhaps the simplest scheme where $\mathcal{R}(Z) = \gamma_0 Z^{\gamma_1} + (1-\gamma_0)Z^{\gamma_2}$ and γ_1, γ_2 are chosen from an asymptotic analysis while γ_0 is chosen to reproduce perturbation theory to second order. It should be emphasized that $\mathcal{R}$ has no free parameters.

The $\mathcal{K}$ formalism takes $k\hat{K}$ as internal and $x\hat{X}$ as external, as previously defined. Alternatively, we can invert internal and external to create a *dual formulation*, which we refer to

as the $\mathcal{X}$ formulation; and this can be obtained by the substitutions

$$\mathcal{K} \leftrightarrow \mathcal{X}, \qquad k \leftrightarrow x, \qquad K \leftrightarrow X, \qquad \hat{K} \leftrightarrow \hat{X}. \tag{8.23}$$

All equations within the $\mathcal{K}$ formalism will have a correspondence in $\mathcal{X}$[41], and therefore a subscript of $\mathcal{K}$ or $\mathcal{X}$ will be introduced when necessary. The $\mathcal{X}$ formulation provides an opposite viewpoint of the physics, and exploring both $\mathcal{K}$ and $\mathcal{X}$ will provide a more robust description of the solution as each formulation will reproduce the exact second order expansion of the energy in the corresponding limit (e.g. using $\mathcal{K}$ for small x/k). There could be many schemes to choose between $\mathcal{K}$ and $\mathcal{X}$, and the total energy is a natural candidate. However, the RCPE may give energies that are lower than the exact solution in its dual regime (e.g. using $\mathcal{K}$ for large x/k), and thus using energy as a switching criteria will have to wait for approximations beyond the RCPE. Here we explore both $\mathcal{K}$ and $\mathcal{X}$ approaches over all parameter space[41], and simply use the crossover of an energy derivative (e.g. double occupancy, density, etc.) when switching is employed.

8.5 Application to the Hubbard model

Several simplifications were made in the above exposition of the OET formalism and its approximations. Now we consider a more general case applicable to many important Hamiltonians including Hubbard models. We begin by considering a Hamiltonian partitioned into two parts, where each portion is now resolved onto a set of commuting operators

$$\hat{H} = \hat{H}_K + \hat{H}_X = \sum_m k_m \hat{K}_m + \sum_n x_n \hat{X}_n, \tag{8.24}$$

where $[\hat{K}_m, \hat{K}_{m'}] = [\hat{X}_n, \hat{X}_{n'}] = 0$. A set of quantities $\{A_i\}$ (e.g. operators, expectation values, etc.) can be encoded as a vector, which is denoted as $\mathbf{A} = (A_1, A_2, \dots)$. For example, we have $\hat{H} = \boldsymbol{k} \cdot \hat{\mathbf{K}} + \boldsymbol{x} \cdot \hat{\mathbf{X}}$. We define the density matrix determined from $\mathbf{A}$ as

$\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A}) = \mathcal{C}\exp(\boldsymbol{\alpha}\cdot\hat{\mathbf{A}})$ satisfying $\langle\hat{\mathbf{A}}\rangle_{\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A})} = \mathbf{A}$, where $\boldsymbol{\alpha}$ is a vector of real numbers, and the domain of $\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A})$ is denoted $\mathcal{M}_{\hat{\mathbf{A}}} = \{\langle\hat{\mathbf{A}}\rangle_{\hat{\rho}} : \hat{\rho}\in\mathcal{L}\}$. The ground state energy can then be written as

$$\mathcal{E}(\boldsymbol{k},\boldsymbol{x}) = \lim_{\beta\to\infty}\min_{\mathbf{K}\in\mathcal{M}_{\hat{\mathbf{K}}},\mathbf{X}\in\mathcal{M}_{\hat{\mathbf{X}}}}\langle\hat{H}\rangle_{\tilde{\hat{\rho}}(\boldsymbol{k},\mathbf{X},\mathbf{K})}. \tag{8.25}$$

We also define the map $\Upsilon(\boldsymbol{k},\mathbf{X},\mathbf{K}) = (\langle\hat{\mathbf{K}}\rangle_{\tilde{\hat{\rho}}(\boldsymbol{k},\mathbf{X},\mathbf{K})}, \langle\hat{\mathbf{X}}\rangle_{\tilde{\hat{\rho}}(\boldsymbol{k},\mathbf{X},\mathbf{K})})$, which provides the complete solution to the Hamiltonian. In order to implement the CPE in general, we need to find the independent constraints between $\hat{\mathbf{K}}$ and $\hat{\mathbf{X}}$ (e.g. density), denoted as $\hat{\mathbf{C}}$, where $\hat{C}_i = \mathbf{A}_i\cdot\hat{\mathbf{K}} = \mathbf{B}_i\cdot\hat{\mathbf{X}}$. The central point will be chosen as $\hat{\rho}_c = \hat{\rho}_{\hat{\mathbf{C}}}(\mathbf{C})$ where $[\mathbf{C}]_i = \mathbf{A}_i\cdot\mathbf{K} = \mathbf{B}_i\cdot\mathbf{X}$.

Here we test our formalism on the single band Hubbard model

$$\hat{H} = \sum_{p\sigma}\epsilon_p\hat{n}_{p\sigma} + N(U\hat{d} - \sum_{\sigma}\mu_\sigma\hat{n}_\sigma), \tag{8.26}$$

where p labels a point in the first Brillouin Zone, N is the total number of sites in the lattice, $\hat{n}_\sigma = (1/N)\sum_j\hat{n}_{j\sigma}$ where j labels a real space lattice point and $\hat{n}_{j\sigma} = \hat{a}^\dagger_{j\sigma}\hat{a}_{j\sigma}$, $\mu_\sigma = \mu + h(\delta_{\uparrow\sigma} - \delta_{\downarrow\sigma})$, and $\hat{d} = (1/N)\sum_j\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}$. To connect with Eq. 8.24, we identify $\hat{\mathbf{K}} = (\ldots,\hat{n}_{p\sigma},\ldots)$, $\hat{\mathbf{X}} = (\hat{d},\hat{n}_\uparrow,\hat{n}_\downarrow)$, and $\hat{\mathbf{C}} = (\hat{n}_\uparrow,\hat{n}_\downarrow)$. For a given constraint $(n_\uparrow,n_\downarrow)$, we parameterize $\mathbf{K}\in\mathcal{M}_K$ and $\mathbf{X}\in\mathcal{M}_X$ using $\Delta d = d - n_\uparrow n_\downarrow$ and $\Delta n_{p\sigma} = n_{p\sigma} - n_\sigma$, where $\Delta d\in[-\min(p_0,p_2),\min(p_\uparrow,p_\downarrow)]$ with $p_0 = (1-n_\uparrow)(1-n_\downarrow)$, $p_\sigma = (1-n_{\bar{\sigma}})n_\sigma$, and $p_2 = n_\uparrow n_\downarrow$; and $\Delta n_{p\sigma}\in[-\hat{n}_\sigma, 1-\hat{n}_\sigma]$ with the constraint $\sum_p\Delta n_{p\sigma} = 0$; and for brevity, we denote $\Delta\mathbf{n} = (\ldots,\Delta n_{p\sigma},\ldots)$.

We begin by presenting the CPE for both the $\mathcal{K}$ and $\mathcal{X}$ formalisms[41], where the $\mathcal{K}$

formalism yields

$$\bar{\Upsilon}_{\mathcal{K}}(\Delta\mathbf{n},\Delta d)=(\mathbf{Z}_{\mathcal{K}}(\Delta d)\Delta\mathbf{n},\Delta d), \tag{8.27}$$

$$[\mathbf{Z}_{\mathcal{K}}(\Delta d)]_{p\sigma}=Z^{(\sigma)}_{\mathcal{K}}(\Delta d)=\mathcal{A}^{\sigma}_{\mathcal{K}}(\Delta d)/\mathcal{A}^{\sigma}_{\mathcal{K}}(0), \tag{8.28}$$

$$\mathcal{A}^{\sigma}_{\mathcal{K}}(\Delta d)=\langle\langle\hat{a}^{\dagger}_{j\sigma};\hat{a}_{j\sigma}\rangle\rangle^{2}_{\hat{\rho}_{\hat{\mathbf{X}}}(\Delta d)}, \tag{8.29}$$

where $\hat{\rho}_{\hat{\mathbf{X}}}(\Delta d)=\bigotimes_{j}\hat{\rho}_{j}(\Delta d)$ and

$$\hat{\rho}_{j}(\Delta d)=\mathrm{diag}(p_0+\Delta d,p_{\downarrow}-\Delta d,p_{\uparrow}-\Delta d,p_2+\Delta d). \tag{8.30}$$

The $\mathcal{X}$ formulation yields

$$\bar{\Upsilon}_{\mathcal{X}}(\Delta\mathbf{n},\Delta d)=(\Delta\mathbf{n},Z_{\mathcal{X}}(\Delta\mathbf{n})\Delta d), \tag{8.31}$$

$$Z_{\mathcal{X}}(\Delta\mathbf{n})=\mathcal{A}_{\mathcal{X}}(\Delta\mathbf{n})/\mathcal{A}_{\mathcal{X}}(\mathbf{0}), \tag{8.32}$$

$$\mathcal{A}_{\mathcal{X}}(\Delta\mathbf{n})=(1/N^4)\textstyle\prod_{\sigma}|\sum_{p}\langle\langle\hat{a}^{\dagger}_{p\sigma};\hat{a}_{p\sigma}\rangle\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})}|^2, \tag{8.33}$$

where $\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})=\bigotimes_{p\sigma}\hat{\rho}_{p\sigma}(\Delta n_{p\sigma})$ and

$$\hat{\rho}_{p\sigma}(\Delta n_{p\sigma})=\mathrm{diag}(1-n_{\sigma}-\Delta n_{p\sigma},n_{\sigma}+\Delta n_{p\sigma}). \tag{8.34}$$

The RCPE for the $\mathcal{K}$ formalism can be constructed as $\Upsilon_{\mathcal{K}}(\boldsymbol{k},\mathbf{X},\mathbf{K})=(\mathcal{R}_{\mathcal{K}}(\boldsymbol{k},\mathbf{Z}_{\mathcal{K}})\Delta\mathbf{n},\Delta d)$ with $[\mathcal{R}_{\mathcal{K}}(\boldsymbol{k},\mathbf{Z}_{\mathcal{K}})]_{p\sigma}=\gamma_0(Z^{(\sigma)}_{\mathcal{K}})^{\gamma_1}+(1-\gamma_0)(Z^{(\sigma)}_{\mathcal{K}})^{\gamma_2}$ and $\gamma_1=1$ and $\gamma_2=1/2$ [41]. Similarly, for the $\mathcal{X}$ formalism we have $\Upsilon_{\mathcal{X}}(\boldsymbol{x},\mathbf{K},\mathbf{X})=(\Delta\mathbf{n},\mathcal{R}_{\mathcal{X}}(\boldsymbol{x},Z_{\mathcal{X}})\Delta d)$, where $\mathcal{R}_{\mathcal{X}}(\boldsymbol{x},Z_{\mathcal{X}})=\gamma_0(Z^{(\sigma)}_{\mathcal{X}})^{\gamma_1}+(1-\gamma_0)(Z^{(\sigma)}_{\mathcal{X}})^{\gamma_2}$ and $\gamma_1=1$ when there is no short range magnetic order (i.e. paramagnetic state in $d{=}\infty$) while $\gamma_1=1/2$ otherwise; and $\gamma_2=1/4$ in all cases[41]. In both $\mathcal{K}$ and $\mathcal{X}$, γ_0 is uniquely determined from perturbation theory, thus there are no free parameters within the RCPE.

It should be noted that within the CPE (i.e. without renormalization), the classic

Gutzwiller approximation (GA)[6–8, 15, 20] to the Hubbard model is rigorously recovered, providing a qualitative description of the Fermi liquid phase; similar to slave Bosons[42–44] and DMET[45–47]. Therefore, the RCPE in the $\mathcal{K}$ formulation is a clear improvement of Gutzwiller and related approximations. Alternatively, the $\mathcal{X}$ formulation within the RCPE will be shown to provide a robust description of the Luttinger liquid and the Mott insulator, and we are not aware of a corresponding result; though a related approach has been explored in the Baeriswyl wave function and its extensions[21, 22, 48–51]. Furthermore, we note that the maps $\Upsilon_{\mathcal{K}}, \Upsilon_{\mathcal{X}}$ directly provide a description of the physical space of all $(\langle \Delta \hat{\mathbf{n}} \rangle_{\hat{\rho}}, \langle \Delta \hat{d} \rangle_{\hat{\rho}})$, yielding a concrete approximation that resolves the N-representability problem[52–57] in this class of Hamiltonians. Therefore, OET provides an alternative viewpoint to this problem, which is of strong interest in the field of quantum chemistry and solid state physics[58–67].

We now apply OET for the Hubbard model in d=1, 2, and ∞ over a broad range of t, U, and density; and we compare to exact or state-of-the-art methods. In infinite dimensions, DMFT is formally exact, and numerical renormalization group[68] is used to solve the DMFT impurity problem[3, 27, 69, 70] as implemented in the "NRG Ljubljana" code[71]. In one dimension, we employ the exact Bethe Ansatz (BA) solution[11, 13], while in two dimensions we compare to variational quantum Monte-Carlo (VMC) and Auxiliary Field Quantum Monte-Carlo (AFQMC) [2]. Additionally, we compare to the Gutzwiller approximation in all dimensions given that it is an efficient approach. We choose to study the double occupancy, density, and magnetization given that these are energy derivatives, and thus our results also imply total energies.

We begin by examining the double occupancy as a function of U/t for d=∞ at half-filling (see Figure 8.1a). The DMFT results are denoted by blue lines, while the Gutzwiller results are in green. Gutzwiller yields a qualitative description of the metallic phase, whereas the insulator is improperly described as a collection of atoms. The OET results are given in red, with a dashed line for $\mathcal{K}$ and solid for $\mathcal{X}$, showing favorable agreement with DMFT in both the metallic and insulating regimes. The inset illustrates OET for doped cases,

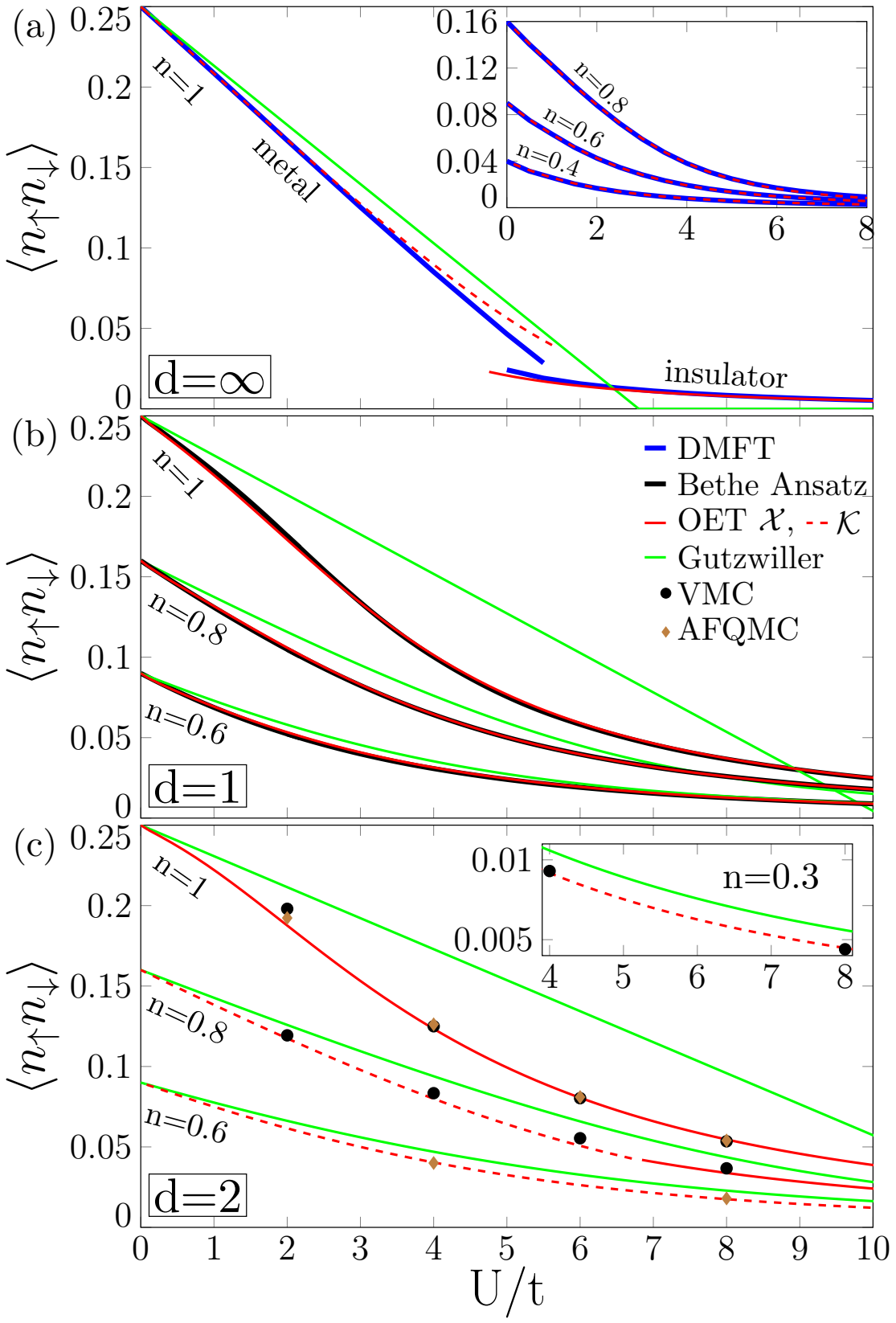

Figure 8.1: Double occupancy for the Hubbard model in various dimensions. (a) The d=∞ Bethe lattice for various dopings, solved within DMFT, GA, and OET. (b) The d=1 lattice, solved within the BA, GA, and OET. (c) The d=2 square lattice solved with GA, OET, and selected points using VMC and AFQMC [2].

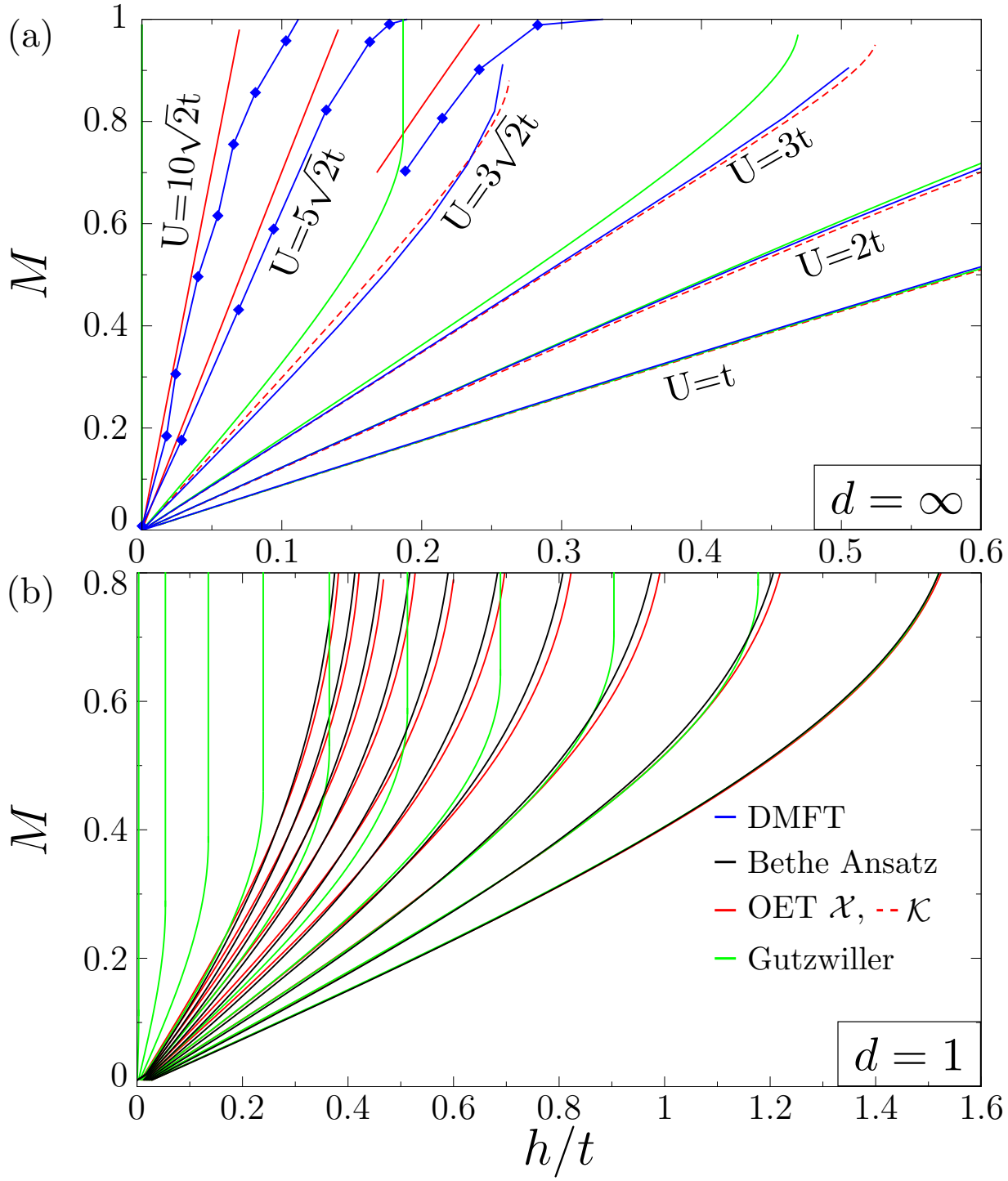

Figure 8.2: Magnetization M vs. magnetic field h for the Hubbard model in d=∞ and d=1. (a) The d=∞ Bethe lattice solved within DMFT (insulating results from Ref. [3], denoted with points), GA, and OET. (b) The d=1 lattice solved within the BA, GA, and OET for $U/t = 1, .., 10$ (right to left).

showing excellent agreement with DMFT. We now turn to d=1 and the d=2 square lattice with nearest neighbor hopping (see Figure 8.1b, c). In one dimension (Figure 8.1b), the OET $\mathcal{X}$ formulation shows remarkable agreement with the BA, both at half filling and for doped cases, and the $\mathcal{K}$ formulation is found not to be necessary[41]. In two dimensions, OET is also in good agreement with the VMC and AFQMC results, both at half filling and for the doped cases; and here continuity is used to switch between the $\mathcal{K}$ and $\mathcal{X}$ formulations (Figure 8.1c).

We now turn to the magnetization under applied magnetic field and the density as a function of the chemical potential. For d=∞, OET precisely captures the magnetization in the metallic regime, and is in reasonable agreement with the insulating DMFT results, though the latter have not been recomputed with precise modern methods (see Figure 8.2a). For d=1, OET has excellent agreement over all parameters (see Figure 8.2b). In both d=∞ and d=1, Gutzwiller discontinuously polarizes for sufficiently large U. Now we consider the density as a function of the chemical potential for $U/t = 1, \ldots, 10$ in d=∞ and d=1 (Figure 8.3). For d=∞, the system opens a gap at a finite U, and the $\mathcal{K}$ and $\mathcal{X}$ ansatz can reasonably capture this behavior (Figure 8.3a). For d=1, it is well known that any finite U opens a gap, and this property is captured using the $\mathcal{X}$ formulation, yielding favorable agreement over all parameters (Figure 8.3b). Results for d=2 can be found in Ref. [41].

In summary, we have developed an exact formalism (i.e. OET) and a generic approximation scheme (i.e. RCPE) for solving the ground state of quantum Hamiltonians. Our approach is proven to be efficient and globally robust for the one band Hubbard model in d=1, 2, ∞. The success of our approach is based on four key ideas: the exact OET construction, a non-perturbative form given by the CPE, a perturbative correction given by the RCPE, and the combination of the dual forms $\mathcal{K}$ and $\mathcal{X}$. Our approach can be straightforwardly applied to a multitude of important quantum Hamiltonians. Furthermore, our entire formalism can be generalized to finite temperature, and this will be presented in a forthcoming paper. Finally, OET can straightforwardly be combined with DFT, similar

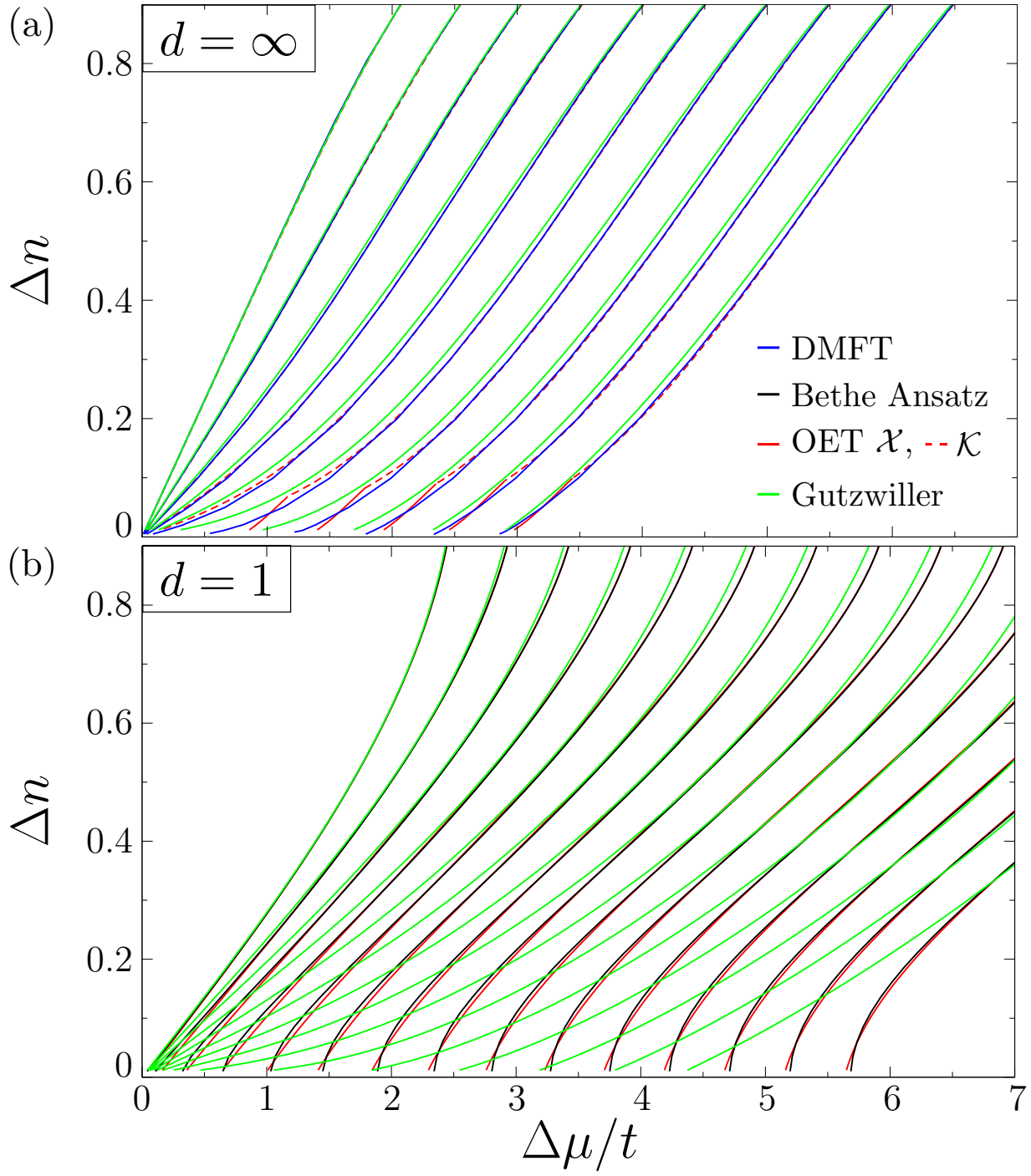

Figure 8.3: The density ($\Delta n = n - 1$) as a function of chemical potential ($\Delta\mu = \mu - U/2$) for the Hubbard model in d=∞ and d=1. (a) The d=∞ Bethe lattice solved within DMFT, GA, and OET for $U/t = 1, .., 10$. (b) The d=1 lattice solved with the BA, GA, and OET for $U/t = 1, .., 16$.

to DFT+DMFT[36] and DFT+Gutzwiller[18], resulting in a highly efficient first-principles approach to the thermodynamics of strongly correlated materials in addition to molecules.

8.6 Details for OET

Orthogonal Response Condition (ORC)

Here we define the orthogonal response condition (ORC) and prove that Hubbard-like models satisfy this condition. We begin by reviewing the relevant notation. A set of quantities $\{\hat{A}_i\}$ (e.g. operators, expectation values, etc) can be encoded as a vector, which is denoted as $\hat{\mathbf{A}} = (\hat{A}_1, \hat{A}_2, \dots)$, and we denote the vector space it spans as $\mathcal{O}_{\hat{\mathbf{A}}}$.. The Liouville space for all density matrices is $\mathcal{L}$, and the expectation value of the operator $\hat{A}$ for density matrix $\hat{\rho}$ is $\langle \hat{A} \rangle_{\hat{\rho}} = \mathrm{Tr}(\hat{A}\hat{\rho})$. The expectation value of $\hat{\mathbf{A}} = (\hat{A}_1, \hat{A}_2, \dots)$ is given by $\langle \hat{\mathbf{A}} \rangle_{\hat{\rho}}$. We define an $\hat{\mathbf{A}}$-generated density matrix $\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A}) = \mathcal{C} \exp(\boldsymbol{\alpha} \cdot \hat{\mathbf{A}})$ satisfying $\langle \hat{\mathbf{A}} \rangle_{\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A})} = \mathbf{A}$ where $\mathcal{C}$ is the normalization and $\boldsymbol{\alpha}$ is a real vector; and we denote the domain of $\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A})$ as $\mathcal{M}_{\hat{\mathbf{A}}} = \{\langle \hat{\mathbf{A}} \rangle_{\hat{\rho}} : \hat{\rho} \in \mathcal{L}\}$. Finally, the subspace of $\mathcal{L}$ for all $\hat{\rho}_{\hat{\mathbf{A}}}(\mathbf{A})$ is $\mathcal{L}_{\hat{\mathbf{A}}}$. The preceding definitions will be applied to $\hat{\mathbf{K}}$-generated, $\hat{\mathbf{X}}$-generated, and $\hat{\mathbf{C}}$-generated density matrices.

Next we consider two sets of operators $\hat{\mathbf{K}}$ and $\hat{\mathbf{X}}$ having a set of $\hat{n}_C$ independent constraint operators $\hat{\mathbf{C}}$, where $\hat{C}_i = \mathbf{A}_i \cdot \hat{\mathbf{K}} = \mathbf{B}_i \cdot \hat{\mathbf{X}}$. We define the orthogonal space $\mathcal{O}^{\perp}_{\hat{\mathbf{K}}}(\mathbf{C}) = \{\hat{v} \in \mathcal{O}_{\hat{\mathbf{K}}} : \langle \hat{v} \rangle_{\rho_{\hat{\mathbf{C}}}(\mathbf{C})} = 0\}$ (with a similar definition for $\mathcal{O}^{\perp}_{\hat{\mathbf{X}}}(\mathbf{C})$). The ORC are the following:

1. $\left[\hat{K}_m, \hat{K}_{m'}\right] = \left[\hat{X}_n, \hat{X}_{n'}\right] = 0.$
2. For any $\hat{\tilde{\rho}} \in \mathcal{L}_{\hat{\mathbf{K}}}$, $\langle \hat{\mathbf{X}} \rangle_{\hat{\rho}} = \langle \hat{\mathbf{X}} \rangle_{\rho_{\hat{\mathbf{C}}}(\langle \hat{\mathbf{C}} \rangle_{\hat{\rho}})}$.
3. For any $\hat{\tilde{\rho}} \in \mathcal{L}_{\hat{\mathbf{X}}}$, $\langle \hat{\mathbf{K}} \rangle_{\hat{\rho}} = \langle \hat{\mathbf{K}} \rangle_{\rho_{\hat{\mathbf{C}}}(\langle \hat{\mathbf{C}} \rangle_{\hat{\rho}})}$.

Five useful corollaries follow from the ORC.

1. $\left[\hat{C}_i, \hat{K}_m\right] = \left[\hat{C}_i, \hat{X}_n\right] = 0.$
2. Given any $\hat{\tilde{\rho}}_\ell \in \mathcal{L}_{\hat{\mathbf{K}}}$ for $\ell = 1, 2$, if $\langle \hat{\mathbf{C}} \rangle_{\hat{\tilde{\rho}}_1} = \langle \hat{\mathbf{C}} \rangle_{\hat{\tilde{\rho}}_2}$ then $\langle \hat{\mathbf{X}} \rangle_{\hat{\tilde{\rho}}_1} = \langle \hat{\mathbf{X}} \rangle_{\hat{\tilde{\rho}}_2}$; therefore $\langle \hat{X} \rangle_{\hat{\tilde{\rho}}_1} = \langle \hat{X} \rangle_{\hat{\tilde{\rho}}_2}$ for any $\hat{X} \in \mathcal{O}_{\hat{\mathbf{X}}}$.

3. Given any $\hat{\hat{\rho}}_\ell \in \mathcal{L}_{\hat{\mathbf{X}}}$ for $\ell = 1, 2$, if $\langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}_1} = \langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}_2}$ then $\langle \hat{\mathbf{K}} \rangle_{\hat{\hat{\rho}}_1} = \langle \hat{\mathbf{K}} \rangle_{\hat{\hat{\rho}}_2}$; therefore $\langle \hat{K} \rangle_{\hat{\hat{\rho}}_1} = \langle \hat{K} \rangle_{\hat{\hat{\rho}}_2}$ for any $\hat{K} \in \mathcal{O}_{\hat{\mathbf{K}}}$.
4. For any $\hat{\rho} \in \mathcal{L}_{\hat{\mathbf{K}}}$, any $\hat{X}_\perp \in \mathcal{O}^\perp_{\hat{\mathbf{X}}}(\mathbf{C})$ and $\hat{K}_\perp \in \mathcal{O}^\perp_{\hat{\mathbf{K}}}(\mathbf{C})$ with $\mathbf{C} = \langle \hat{\mathbf{C}} \rangle_{\hat{\rho}}$, we have $\langle \hat{X}_\perp \rangle_{\hat{\rho}} = 0$ and $\langle \hat{K}_\perp \hat{X}_\perp \rangle_{\hat{\rho}} = 0$.
5. For any $\hat{\rho} \in \mathcal{L}_{\hat{\mathbf{X}}}$, any $\hat{K}_\perp \in \mathcal{O}^\perp_{\hat{\mathbf{K}}}(\mathbf{C})$ and $\hat{X}_\perp \in \mathcal{O}^\perp_{\hat{\mathbf{X}}}(\mathbf{C})$ with $\mathbf{C} = \langle \hat{\mathbf{C}} \rangle_{\hat{\rho}}$, we have $\langle \hat{K}_\perp \rangle_{\hat{\rho}} = 0$ and $\langle \hat{X}_\perp \hat{K}_\perp \rangle_{\hat{\rho}} = 0$.

Corollary 1 naturally follows from ORC 1. Corollary 2 and 3 naturally follow from ORC 2 and 3. Corollary 4 can be proven as follows: for the given $\hat{\rho}$, we have $\langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}} = \langle \hat{\mathbf{C}} \rangle_{\rho_{\hat{\mathbf{C}}}(\langle \hat{\mathbf{C}} \rangle_{\hat{\rho}})}$; therefore, $\langle \hat{X}_\perp \rangle_{\hat{\rho}} = \langle \hat{X}_\perp \rangle_{\rho_{\hat{\mathbf{C}}}(\langle \hat{\mathbf{C}} \rangle_{\hat{\rho}})} = 0$. Now consider a $\hat{K}_\perp \in \mathcal{O}^\perp_{\hat{\mathbf{K}}}(\mathbf{C})$: we define $\hat{\rho}(\alpha) = \mathcal{C}(\alpha) \exp\left(\ln\left(\rho_{\hat{\mathbf{C}}}(\langle \hat{\mathbf{C}} \rangle_{\hat{\rho}}) \right) + \alpha \hat{K}_\perp \right)$ and thus $\mathrm{Tr}\left(\frac{d}{d\alpha} \hat{\rho}(\alpha) \hat{X}_\perp \right) = 0$, which gives $\mathrm{Tr}(\hat{\rho} \hat{K}_\perp \hat{X}_\perp) = 0$ for $\alpha = 0$. This completes the proof for Corollary 4, and Corollary 5 follows in a similar fashion.

Now we show that the ORC conditions are satisfied for the N orbital Hubbard model, with a local Fock space at site j spanned from the basis $\{|\hat{n}_1 \hat{n}_2 \dots \hat{n}_{2N}; j\rangle\}$. We first focus on proving the second assertion. Given that $\hat{\hat{\rho}} \in \mathcal{L}_{\hat{\mathbf{K}}}$ has a non-interacting form, and using Wick's theorem, an arbitrary entry of the local reduced density matrix $\hat{\hat{\rho}}^{(j)}$ of site j is given by $\langle |\hat{n}_1 \hat{n}_2 \dots \hat{n}_{2N}; j\rangle \langle n'_1 n'_2 \dots n'_{2N}; j| \rangle_{\hat{\hat{\rho}}} = \prod_{\ell=1}^N \delta_{\hat{n}_\ell \hat{n}'_\ell} \nu_\ell(\hat{n}_\ell)$ where $\nu_\ell(1) = \langle \hat{a}^\dagger_{j\ell} \hat{a}_{j\ell} \rangle_{\hat{\hat{\rho}}}$ and $\nu_\ell(0) = \langle \hat{a}_{j\ell} \hat{a}^\dagger_{j\ell} \rangle_{\hat{\hat{\rho}}}$, indicating that $\hat{\hat{\rho}}^{(j)}$ is completely determined from $\langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}}$. Thus, $\langle \hat{\mathbf{X}} \rangle_{\hat{\hat{\rho}}}$ is also completely determined from $\langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}}$. This proves the second assertion.

For the third assertion, given that $\hat{\hat{\rho}} \in \mathcal{L}_{\hat{\mathbf{X}}}$ has an atomic form, its local reduced density matrix $\hat{\hat{\rho}}^{(q)}$ for a given $q = (p, \eta, \sigma)$, where p is the k-point index, η is the band index, and σ is the spin index, is completely determined by $\langle \hat{n}_q \rangle_{\hat{\rho}}$. For a given (η, σ), all $\langle \hat{n}_{p\eta\sigma} \rangle_{\hat{\rho}}$ are equal, which is determined from $\langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}}$. Thus, $\langle \hat{\mathbf{K}} \rangle_{\hat{\hat{\rho}}}$ is also completely determined from $\langle \hat{\mathbf{C}} \rangle_{\hat{\hat{\rho}}}$. This proves the third assertion.

Central Point Expansion (CPE)

In this section, we derive the key equations of the CPE for a general Hamiltonian $\hat{H} = \boldsymbol{k}\cdot\hat{\mathbf{K}} + \boldsymbol{x}\cdot\hat{\mathbf{X}}$ where $\hat{\mathbf{K}}$ and $\hat{\mathbf{X}}$ obey the constraint $\hat{\mathbf{C}}$ and satisfy the ORC. We first focus on the $\mathcal{K}$ formalism. For a given constraint $\mathbf{C}$, we define the central point $\hat{\rho}_c \equiv \rho_{\hat{\mathbf{C}}}(\mathbf{C})$ which yields $(\mathbf{K}_c, \mathbf{X}_c) = (\langle\hat{\mathbf{K}}\rangle_{\hat{\rho}_c}, \langle\hat{\mathbf{X}}\rangle_{\hat{\rho}_c})$. We begin with the OET ansatz

$$\tilde{\hat{\rho}}(\boldsymbol{k}, \mathbf{X}, \mathbf{K}) = \mathcal{C}\hat{\mathcal{P}}(\boldsymbol{k}, \mathbf{X})\hat{\rho}_{\hat{K}}(\mathbf{K})\hat{\mathcal{P}}(\boldsymbol{k}, \mathbf{X}), \tag{8.35}$$

where

$$\hat{\mathcal{P}}(\boldsymbol{k}, \mathbf{X}) = \frac{1}{\sqrt{\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}^\star)}}\left(\sqrt{\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}^\star)}\hat{\rho}(\boldsymbol{k}, \mathbf{X})\sqrt{\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}^\star)}\right)^{1/2}\frac{1}{\sqrt{\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}^\star)}}, \tag{8.36}$$

and we choose $\mathbf{K}^\star$ such that $\hat{\mathcal{P}}(\boldsymbol{k}, \mathbf{X}_c) = 1$. The CPE is the following truncated Taylor series

$$\hat{\mathcal{P}}(\boldsymbol{k}, \mathbf{X}) \approx \hat{\mathcal{P}}(\mathbf{0}, \mathbf{X}) = \sqrt{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X})\hat{\rho}^{-1}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}, \tag{8.37}$$

$$\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}) \approx \hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)(1 + \Delta\hat{\mathbf{K}}\langle\!\langle\Delta\hat{\mathbf{K}}; \Delta\hat{\mathbf{K}}\rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\Delta\mathbf{K}), \tag{8.38}$$

given that $\mathbf{K}^\star = \mathbf{K}_c$ from $\hat{\mathcal{P}}(\mathbf{0}, \mathbf{X}_c) = 1$ and $\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c) = \hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}_c)$. Equation 8.37 naturally follows from setting $\boldsymbol{k} = \mathbf{0}$, while Eq. 8.38 can be proven by parameterizing $\rho_{\hat{\mathbf{K}}}(\mathbf{K}) = \hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)\exp(\boldsymbol{\kappa}\cdot\Delta\hat{\mathbf{K}}) \approx \hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)(\hat{1} + \boldsymbol{\kappa}\cdot\Delta\hat{\mathbf{K}})$ using $\boldsymbol{\kappa}$, which can be determined from

$$\Delta\mathbf{K} = \langle\Delta\hat{\mathbf{K}}\rangle_{\rho_{\hat{\mathbf{K}}}(\mathbf{K})} = \langle(\boldsymbol{\kappa}\cdot\Delta\hat{\mathbf{K}})\Delta\hat{\mathbf{K}}\rangle_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)} \tag{8.39}$$

$$= \mathrm{Tr}\left(\Delta\hat{\mathbf{K}}\sqrt{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\Delta\hat{\mathbf{K}}\sqrt{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\right)\boldsymbol{\kappa} = \langle\!\langle\Delta\hat{\mathbf{K}}; \Delta\hat{\mathbf{K}}\rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\boldsymbol{\kappa}. \tag{8.40}$$

Solving for $\boldsymbol{\kappa}$, we have

$$\boldsymbol{\kappa} = \langle\!\langle\Delta\hat{\mathbf{K}}; \Delta\hat{\mathbf{K}}\rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\Delta\mathbf{K}. \tag{8.41}$$

Substituting into the expression for the density matrix, we have

$$\tilde{\hat{\rho}}(\mathbf{0},\mathbf{X},\mathbf{K}) \approx \mathcal{C}\hat{\mathcal{P}}(\mathbf{0},\mathbf{X})\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{K}_c)(1+\Delta\hat{\mathbf{K}}\langle\langle\Delta\hat{\mathbf{K}};\Delta\hat{\mathbf{K}}\rangle\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\Delta\mathbf{K})\hat{\mathcal{P}}(\mathbf{0},\mathbf{X}), \tag{8.42}$$

where $\mathcal{C}$ is determined to be 1. Finally, we have

$$\langle\Delta\hat{\mathbf{K}}\rangle_{\tilde{\hat{\rho}}(\mathbf{0},\mathbf{X},\mathbf{K})} \approx \langle\langle\Delta\hat{\mathbf{K}};\Delta\hat{\mathbf{K}}\rangle\rangle_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X})}\langle\langle\Delta\hat{\mathbf{K}};\Delta\hat{\mathbf{K}}\rangle\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{X}}}(\mathbf{X}_c)}\Delta\mathbf{K}, \tag{8.43}$$

$$\langle\Delta\hat{\mathbf{X}}\rangle_{\tilde{\hat{\rho}}(\mathbf{0},\mathbf{X},\mathbf{K})} \approx \Delta\mathbf{X}, \tag{8.44}$$

where we note that $\Delta\hat{\mathbf{K}} \in \mathcal{O}^{\perp}_{\hat{\mathbf{K}}}(\mathbf{C})$ and $\Delta\hat{\mathbf{X}} \in \mathcal{O}^{\perp}_{\hat{\mathbf{X}}}(\mathbf{C})$ and we have used corollaries four and five of the ORC. When minimizing the energy we require that $[\mathbf{C}]_i = \mathbf{A}_i \cdot \mathbf{K} = \mathbf{B}_i \cdot \mathbf{X}$ for all constraints.

Having derived the general formulas of CPE, we now insert the notation for the case of the Hubbard model.

$$\hat{\mathcal{P}}(\mathbf{0},\Delta d) = \sqrt{\hat{\rho}^{-1}_{\hat{\mathbf{X}}}(0)\hat{\rho}_{\hat{\mathbf{X}}}(\Delta d)}, \tag{8.45}$$

$$\tilde{\hat{\rho}}(\mathbf{0},\Delta\mathbf{n},\Delta d) \approx \hat{\mathcal{P}}(\mathbf{0},\Delta d)(\hat{1}+\Delta\hat{\mathbf{n}}\langle\langle\Delta\hat{\mathbf{n}};\Delta\hat{\mathbf{n}}\rangle\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{X}}}(0)}\Delta\mathbf{n})\hat{\rho}_{\hat{\mathbf{X}}}(0)\hat{\mathcal{P}}(\mathbf{0},\Delta d), \tag{8.46}$$

$$\langle\Delta\hat{\mathbf{n}}\rangle_{\tilde{\hat{\rho}}(\mathbf{0},\Delta\mathbf{n},\Delta d)} \approx \langle\langle\Delta\hat{\mathbf{n}};\Delta\hat{\mathbf{n}}\rangle\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{X}}}(0)}\langle\langle\Delta\hat{\mathbf{n}};\Delta\hat{\mathbf{n}}\rangle\rangle_{\hat{\rho}_{\hat{\mathbf{X}}}(\Delta d)}\Delta\mathbf{n}, \tag{8.47}$$

$$\langle\Delta\hat{d}\rangle_{\tilde{\hat{\rho}}(\mathbf{0},\Delta\mathbf{n},\Delta d)} \approx \Delta d. \tag{8.48}$$

Evaluating the symmetric correlator, we find

$$\langle\langle\Delta\hat{n}_{p\sigma};\Delta\hat{n}_{p'\sigma'}\rangle\rangle_{\hat{\rho}_{\hat{\mathbf{X}}}(\Delta d)} = \delta_{\sigma\sigma'}\left(\delta_{pp'}\mathcal{A}^{\sigma}_{\mathcal{K}}(\Delta d) - \frac{1}{N}\mathcal{A}^{\sigma}_{\mathcal{K}}(\Delta d)\right) + \frac{1}{N}\left(\langle\hat{n}_{\sigma}\hat{n}_{\sigma'}\rangle_{\hat{\rho}_{\hat{\mathbf{X}}}(0)} - n_{\sigma}n_{\sigma'}\right), \tag{8.49}$$

where

$$\mathcal{A}^{\sigma}_{\mathcal{K}}(\Delta d) = \langle\langle\hat{a}^{\dagger}_{j\sigma};\hat{a}_{j\sigma}\rangle\rangle^{2}_{\hat{\rho}_{\hat{\mathbf{X}}}(\Delta d)}. \tag{8.50}$$

Given $\sum_p \Delta n_{p\sigma} = 0$, we find

$$\langle \Delta \hat{n}_{p\sigma} \rangle_{\tilde{\hat{\rho}}(\mathbf{0},\Delta\mathbf{n},\Delta d)} = \frac{\mathcal{A}^{\sigma}_{\mathcal{K}}(\Delta d)}{\mathcal{A}^{\sigma}_{\mathcal{K}}(0)} \Delta n_{p\sigma} = Z^{(\sigma)}_{\mathcal{K}}(\Delta d) \Delta n_{p\sigma}. \tag{8.51}$$

Now we turn our attention to the $\mathcal{X}$ formalism. We start with the CPE, where

$$\hat{\mathcal{P}}(0, \Delta\mathbf{n}) = \sqrt{\hat{\rho}^{-1}_{\hat{\mathbf{K}}}(\mathbf{0}) \hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})}, \tag{8.52}$$

$$\tilde{\hat{\rho}}(0, \Delta d, \Delta\mathbf{n}) = \hat{\mathcal{P}}(0, \Delta\mathbf{n})(\hat{1} + \Delta\hat{d} \langle\!\langle \Delta\hat{d}; \Delta\hat{d} \rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{0})} \Delta d) \hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{0}) \hat{\mathcal{P}}(0, \Delta\mathbf{n}), \tag{8.53}$$

$$\langle \Delta\hat{d} \rangle_{\tilde{\hat{\rho}}(0,\Delta d,\Delta\mathbf{n})} = \langle\!\langle \Delta\hat{d}; \Delta\hat{d} \rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})} \langle\!\langle \Delta\hat{d}; \Delta\hat{d} \rangle\!\rangle^{-1}_{\hat{\rho}_{\hat{\mathbf{K}}}(\mathbf{0})} \Delta d = \frac{\mathcal{A}_{\mathcal{X}}(\Delta\mathbf{n})}{\mathcal{A}_{\mathcal{X}}(\mathbf{0})} \Delta d = Z_{\mathcal{X}}(\Delta\mathbf{n}) \Delta d, \tag{8.54}$$

$$\langle \Delta\hat{\mathbf{n}} \rangle_{\tilde{\hat{\rho}}(0,\Delta d,\Delta\mathbf{n})} = \Delta\mathbf{n}, \tag{8.55}$$

where

$$\begin{aligned} \mathcal{A}_{\mathcal{X}}(\Delta\mathbf{n}) = \frac{1}{N^3} \sum_{p_1 p_2 p_3 p_4} \Big(& \delta_{p_1+p_2, p_3+p_4} \langle\!\langle \hat{a}^{\dagger}_{p_1\uparrow}; \hat{a}_{p_1\uparrow} \rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})} \langle\!\langle \hat{a}^{\dagger}_{p_2\downarrow}; \hat{a}_{p_2\downarrow} \rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})} \times \\ & \langle\!\langle \hat{a}^{\dagger}_{p_3\uparrow}; \hat{a}_{p_3\uparrow} \rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})} \langle\!\langle \hat{a}^{\dagger}_{p_4\downarrow}; \hat{a}_{p_4\downarrow} \rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})} \Big) \end{aligned} \tag{8.56}$$

$$\approx \prod_{\sigma} \left| \frac{1}{N} \sum_{p} \langle\!\langle \hat{a}^{\dagger}_{p\sigma}; \hat{a}_{p\sigma} \rangle\!\rangle_{\hat{\rho}_{\hat{\mathbf{K}}}(\Delta\mathbf{n})} \right|^2, \tag{8.57}$$

where the latter approximation is exact in infinite dimensions.

Renormalized Central Point Expansion (RCPE) for $\mathcal{K}$ and $\mathcal{X}$ in the Hubbard Model

We begin by considering the $\mathcal{K}$ formulation, where the map $\Upsilon_{\mathcal{K}}(\boldsymbol{k}, \mathbf{X}, \mathbf{K})$ clearly depends on $\boldsymbol{k}$ while the CPE produces a map $\bar{\Upsilon}_{\mathcal{K}}(\mathbf{X}, \mathbf{K})$ which is independent of $\boldsymbol{k}$. This occurs because within the CPE we have $\hat{\mathcal{P}}_{\mathcal{K}}(\boldsymbol{k}, \mathbf{X}) \approx \hat{\mathcal{P}}_{\mathcal{K}}(\mathbf{0}, \mathbf{X})$. To obtain $\boldsymbol{k}$ dependence, one

should expand $\hat{\mathcal{P}}_{\mathcal{K}}(\boldsymbol{k}, \mathbf{X})$ beyond zeroth order in $\boldsymbol{k}$, though this is nontrivial and therefore we pursue the simplest approach forward in this work. We propose a correction ansatz $[\mathcal{R}_{\mathcal{K}}(\boldsymbol{k}, \mathbf{Z}_{\mathcal{K}})]_{p\sigma} = R^{(\sigma)}_{\mathcal{K}}(Z^{(\sigma)}_{\mathcal{K}})$, where $R^{(\sigma)}_{\mathcal{K}}$ is a single variable scalar function that has several key properties.

1. $R^{(\sigma)}_{\mathcal{K}}(1) = 1$. This is required by $\Upsilon_{\mathcal{K}}(\boldsymbol{k}, \Delta\mathbf{n}, 0) = (\Delta\mathbf{n}, 0)$.
2. $R^{(\sigma)}_{\mathcal{K}}(0) = 0$. This is required by $\Upsilon_{\mathcal{K}}(\boldsymbol{k}, \Delta\mathbf{n}, -\hat{n}_\uparrow\hat{n}_\downarrow) = (\mathbf{0}, -\hat{n}_\uparrow\hat{n}_\downarrow)$ given $\hat{n}_\uparrow + \hat{n}_\downarrow = 1$.
3. $\frac{\partial R^{(\sigma)}_{\mathcal{K}}(Z)}{\partial Z}|_{Z=1} = \alpha^{(\sigma)}_{\mathcal{K}}$ is completely determined from weak coupling perturbation theory, and depends on the constraint $\hat{n}_\sigma$ (see Figure 8.4).
4. We require $\lim_{Z\to 0} R^{(\sigma)}_{\mathcal{K}}(Z) \propto \sqrt{Z}$ such that we have the correct saddle point structure in the atomic limit.

In order to fulfill the above requirements, we propose a two term ansatz.

$$R^{(\sigma)}_{\mathcal{K}}(Z) = \gamma^{(\sigma)}_0 Z^{\gamma_1} + (1 - \gamma^{(\sigma)}_0) Z^{\gamma_2}, \tag{8.58}$$

where $\gamma_1 = 1$ and $\gamma_2 = 1/2$, and using the third condition, we have

$$\gamma^{(\sigma)}_0\gamma_1 + \gamma_2\left(1 - \gamma^{(\sigma)}_0\right) = \alpha^{(\sigma)}_{\mathcal{K}} \quad \rightarrow \quad \gamma^{(\sigma)}_0 = \frac{\alpha^{(\sigma)}_{\mathcal{K}} - \gamma_2}{\gamma_1 - \gamma_2}. \tag{8.59}$$

The total energy is written as

$$\mathcal{E}_{\mathcal{K}} = \min_{\substack{\hat{n}_\sigma\in[0,1] \\ \Delta n_{p\sigma}\in[-\hat{n}_\sigma, 1-\hat{n}_\sigma] \\ \Delta d\in[\Delta d_{\min}, \Delta d_{\max}]}} \left(\frac{1}{N}\left(\sum_{p\sigma}\epsilon_p\left(R^{(\sigma)}_{\mathcal{K}}(Z^{(\sigma)}_{\mathcal{K}}(\Delta d))\Delta n_{p\sigma} + \hat{n}_\sigma\right)\right) + U\left(\Delta d + \hat{n}_\uparrow\hat{n}_\downarrow\right) - \sum_\sigma \mu_\sigma \hat{n}_\sigma\right) \tag{8.60}$$

where we require $\sum_p \Delta n_{p\sigma} = 0$ and we have

$$\Delta d_{\min} = -\min\left(\left(1-n_\uparrow\right)\left(1-n_\downarrow\right), n_\uparrow n_\downarrow\right), \quad \Delta d_{\max} = \min\left(\left(1-n_\uparrow\right) n_\downarrow, n_\uparrow\left(1-n_\downarrow\right)\right). \tag{8.61}$$

For a given $\hat{n}_\sigma$ and Δd, one can analytically find the saddle point of $\Delta n_{p\sigma}$, which is denoted as $\Delta n^\star_{p\sigma}$. Finally, the energy can then be written as

$$\begin{aligned}\mathcal{E}_{\mathcal{K}} = \min_{\substack{\hat{n}_\sigma\in[0,1] \\ \Delta d\in[\Delta d_{\min},\Delta d_{\max}]}} \Bigg(\frac{1}{N}\left(\sum_{p\sigma}\epsilon_p\left(R^{(\sigma)}_{\mathcal{K}}(Z^{(\sigma)}_{\mathcal{K}}(\Delta d))\Delta n^\star_{p\sigma}(n_\sigma,\Delta d)+\hat{n}_\sigma\right)\right). \\ + U\left(\Delta d+\hat{n}_\uparrow\hat{n}_\downarrow\right) - \sum_\sigma \mu_\sigma \hat{n}_\sigma\Bigg)\end{aligned} \tag{8.62}$$

The above expression can be minimized by analytically constructing the gradient and numerically minimizing.

The above presentation completes the $\mathcal{K}$ formulation of the RCPE, and the only remaining task is to compute the $\alpha_{\mathcal{K}}$ from weak coupling perturbation theory. The second order coefficient of the energy expansion in U is

$$E^{(2)} = \frac{1}{N^3}\sum_{p_1p_2p_3p_4}\delta_{p_1+p_3,p_2+p_4}\frac{\hat{n}_{p_1\uparrow}\hat{n}_{p_3\downarrow}\left(1-\hat{n}_{p_2\uparrow}\right)\left(1-\hat{n}_{p_4\downarrow}\right)}{\epsilon_{p_2\uparrow}+\epsilon_{p_4\downarrow}-\epsilon_{p_1\uparrow}-\epsilon_{p_3\downarrow}}, \tag{8.63}$$

and in $d=\infty$ this reduces to

$$E^{(2)} = \frac{1}{N^4}\sum_{p_1p_2p_3p_4}\frac{\hat{n}_{p_1\uparrow}\hat{n}_{p_3\downarrow}\left(1-\hat{n}_{p_2\uparrow}\right)\left(1-\hat{n}_{p_4\downarrow}\right)}{\epsilon_{p_2\uparrow}+\epsilon_{p_4\downarrow}-\epsilon_{p_1\uparrow}-\epsilon_{p_3\downarrow}}. \tag{8.64}$$

Within the CPE, the second order coefficient of the total energy is

$$E^{(2)}_{\mathrm{CPE}} = \frac{\hat{n}_\uparrow(1-\hat{n}_\uparrow)\hat{n}_\downarrow(1-\hat{n}_\downarrow)}{\sum_\sigma(E^{(0)}_\sigma/(\hat{n}_\sigma(1-\hat{n}_\sigma)))}, \tag{8.65}$$

where

$$E_\sigma^{(0)} = \int_{-\infty}^{\mu_\sigma} d\epsilon D(\epsilon)\,\epsilon, \qquad \int_{-\infty}^{\mu_\sigma} d\epsilon D(\epsilon) = n_\sigma. \tag{8.66}$$

Finally, the correction coefficient is given as

$$\alpha_{\mathcal{K}} = \frac{E^{(2)}_{\mathrm{CPE}}}{E^{(2)}}. \tag{8.67}$$

The numerical values of $\alpha_{\mathcal{K}}$ for d=1, 2, ∞ are given in Figure 8.4.

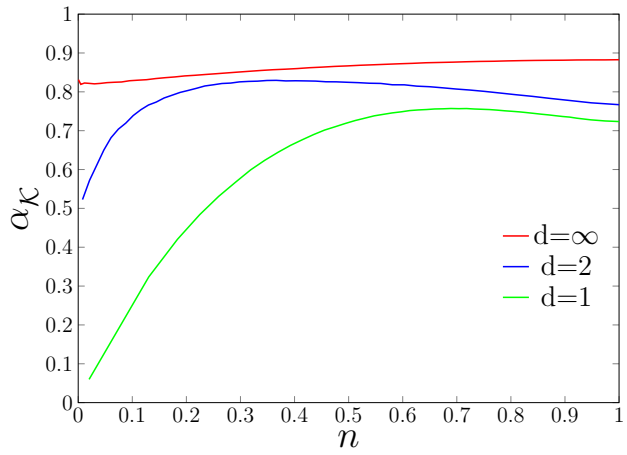

Figure 8.4: A plot of $\alpha_{\mathcal{K}}$ as a function of total density for d=1, 2, ∞ (under zero magnetic field).

Now we turn to the $\mathcal{X}$ formulation, where we have $\mathcal{R}_{\mathcal{X}}(\boldsymbol{x}, Z_{\mathcal{X}}) = R_{\mathcal{X}}(Z_{\mathcal{X}})$, and $R_{\mathcal{X}}$ has the corresponding properties.

1. $R_{\mathcal{X}}(1) = 1$. This is required by $\Upsilon_{\mathcal{X}}(\boldsymbol{x}, \Delta d, \mathbf{0}) = (\Delta d, \mathbf{0})$.
2. $R_{\mathcal{X}}(0) = 0$. This is required by $\Upsilon_{\mathcal{X}}(\boldsymbol{x}, \Delta d, \Delta\mathbf{n}_o) = (0, \Delta\mathbf{n}_o)$, where $\Delta\mathbf{n}_o$ corresponds to the noninteracting distribution.
3. $\frac{\partial R_{\mathcal{X}}}{\partial Z}|_{Z=1} = \alpha_{\mathcal{X}}$ is completely determined from the second order strong coupling expansion, and depends on the constraint $\hat{n}_\sigma$. Therefore, we denote $\alpha_{\mathcal{X}}(n, m)$, where n is the total density and m is the magnetization.

4. If the formalism can be adiabatically connected to the noninteracting limit, we require $\lim_{Z\to 0} R_{\mathcal{X}}(Z) \propto Z^{1/4}$ such that we have the correct saddle point structure in the noninteracting limit.

As in the $\mathcal{K}$ formulation, we use the two term ansatz.

$$R_{\mathcal{X}}(Z) = \gamma_0 Z^{\gamma_1} + (1-\gamma_0) Z^{\gamma_2}, \tag{8.68}$$

where we set $\gamma_1 = 1$ when there is no short range magnetic order (i.e. paramagnetic state in $d = \infty$) and $\gamma_1 = 1/2$ for short or long range antiferromagnetic order; and $\gamma_2 = 1/4$ in all cases. Using the third condition, we have

$$\gamma_0\gamma_1 + \gamma_2(1-\gamma_0) = \alpha_{\mathcal{X}} \quad \rightarrow \quad \gamma_0 = \frac{\alpha_{\mathcal{X}} - \gamma_2}{\gamma_1 - \gamma_2}. \tag{8.69}$$

The value of $\alpha_{\mathcal{X}}(1,0)$ (i.e. half filling, zero magnetization) is obtained by solving the Heisenberg model,

$$\alpha_{\mathcal{X}}(1,0) = \frac{1}{(1 - 4\langle \hat{S}_i \cdot \hat{S}_j \rangle)}, \tag{8.70}$$

and the results are tabulated in various cases in Table 8.1. For the value of $\alpha_{\mathcal{X}}(n,m)$ at non-integer filling, it is necessary to solve the $t-J$ model, and this is a non-trivial task in its own right for $d > 1$. Therefore, we adopt a simple approximation instead:

$$\alpha_{\mathcal{X}}(n,0) = \frac{1}{4} + (\frac{1}{4} - \alpha_{\mathcal{X}}(1,0))n^{\beta_d}, \quad \alpha_{\mathcal{X}}(1,m) = \alpha_{\mathcal{X}}(1,0) + (\alpha_{\mathcal{X}}(1,1) - \alpha_{\mathcal{X}}(1,0))m^2, \tag{8.71}$$

where we approximate $\alpha_{\mathcal{X}}(1,1) = 1/2$ and $\beta_d = 1$ for $d = 1, 2$; and we approximate $\alpha_{\mathcal{X}}(1,1) = 1$ and $\beta_d = 8$ for $d = \infty$.

Type	$-\langle S_i \cdot S_j \rangle$	$\alpha_{\mathcal{X}}(1,0)$
d=1	$-\left(\ln(2)-\frac{1}{4}\right)$	$1/(4\ln 2)$
d=2	0.352	0.415
d=∞	0	1

Table 8.1: Nearest neighbor spin correlation in the Heisenberg model and the correction $\alpha_{\mathcal{X}}$ for the Hubbard model. The d=2 spin correlation was obtained by linearly extrapolating the QMC data in Ref. [4] to zero temperature.

The total energy can then be written as

$$\mathcal{E}_{\mathcal{X}} = \min_{\substack{\hat{n}_\sigma \in [0,1] \\ \Delta n_{p\sigma} \in [-\hat{n}_\sigma, 1-\hat{n}_\sigma] \\ \Delta d \in [\Delta d_{\min}, \Delta d_{\max}]}} \left(\frac{1}{N} \sum_{p\sigma} \epsilon_p n_{p\sigma} + U \Big(R_{\mathcal{X}}\big(Z_{\mathcal{X}}(\Delta \mathbf{n})\big) \Delta d + \hat{n}_\uparrow \hat{n}_\downarrow \Big) - \sum_\sigma \mu_\sigma \hat{n}_\sigma \right). \quad (8.72)$$

The minimization of the above equation follows analogously to the minimization of Eq. **??**.

Finally, we address a subtle issue when applying the CPE within the $\mathcal{X}$ formalism for non-integer filling. In the large U limit, CPE in the $\mathcal{X}$ formulation dictates $\Delta\mathbf{n} = 0$, meaning that the system has zero kinetic energy; but the exact solution to the $U = \infty$ Hubbard model dictates that the kinetic energy is nonzero. This indicates that we need an improved starting point for our CPE expansion, and perhaps the simplest choice is:

$$n_{p\sigma} = \begin{cases} 1 & \epsilon_p \le m \\ \frac{n_\sigma}{n_\uparrow + n_\downarrow} + \Delta n_{p\sigma} & \epsilon_p > m \end{cases} \quad \text{for} \quad n_\uparrow + n_\downarrow > 1, \quad (8.73)$$

$$n_{p\sigma} = \begin{cases} \frac{n_\sigma}{n_\uparrow + n_\downarrow} + \Delta n_{p\sigma} & \epsilon_p \le m \\ 0 & \epsilon_p > m \end{cases} \quad \text{for} \quad n_\uparrow + n_\downarrow < 1, \quad (8.74)$$

where m is determined from

$$n_\uparrow + n_\downarrow > 1, \qquad 2\int_\infty^m d\epsilon D(\epsilon) + \int_m^\infty d\epsilon D(\epsilon) = 1 + \int_\infty^m d\epsilon D(\epsilon) = n_\uparrow + n_\downarrow, \quad (8.75)$$

$$n_\uparrow + n_\downarrow < 1, \qquad \int_\infty^m d\epsilon D(\epsilon) = 1 - \int_m^\infty d\epsilon D(\epsilon) = n_\uparrow + n_\downarrow. \quad (8.76)$$

These revised $\Delta\mathbf{n}$ can be directly utilized as usual, except that $\Delta n_{p\sigma} \in [\frac{-n_\sigma}{n_\uparrow+n_\downarrow}, 1-\frac{n_\sigma}{n_\uparrow+n_\downarrow}]$ and is only defined in the region where $\epsilon_p > m$ for $n_\uparrow + n_\downarrow > 1$ and $\epsilon_p \leq m$ for $n_\uparrow + n_\downarrow < 1$; in addition to satisfying the same constraint $\sum_p \Delta n_{p\sigma} = 0$.

Summary of results for $\mathcal{K}$ and $\mathcal{X}$

Here we provide a complete catalogue of results for the $\mathcal{K}$ and $\mathcal{X}$ formalisms, including all results for d=2 which were suppressed in the main text due to space constraints. Here we do not switch between formulations, instead showing each separately over the entire range of parameter space. We also provide the total energy for n=1 in all cases.

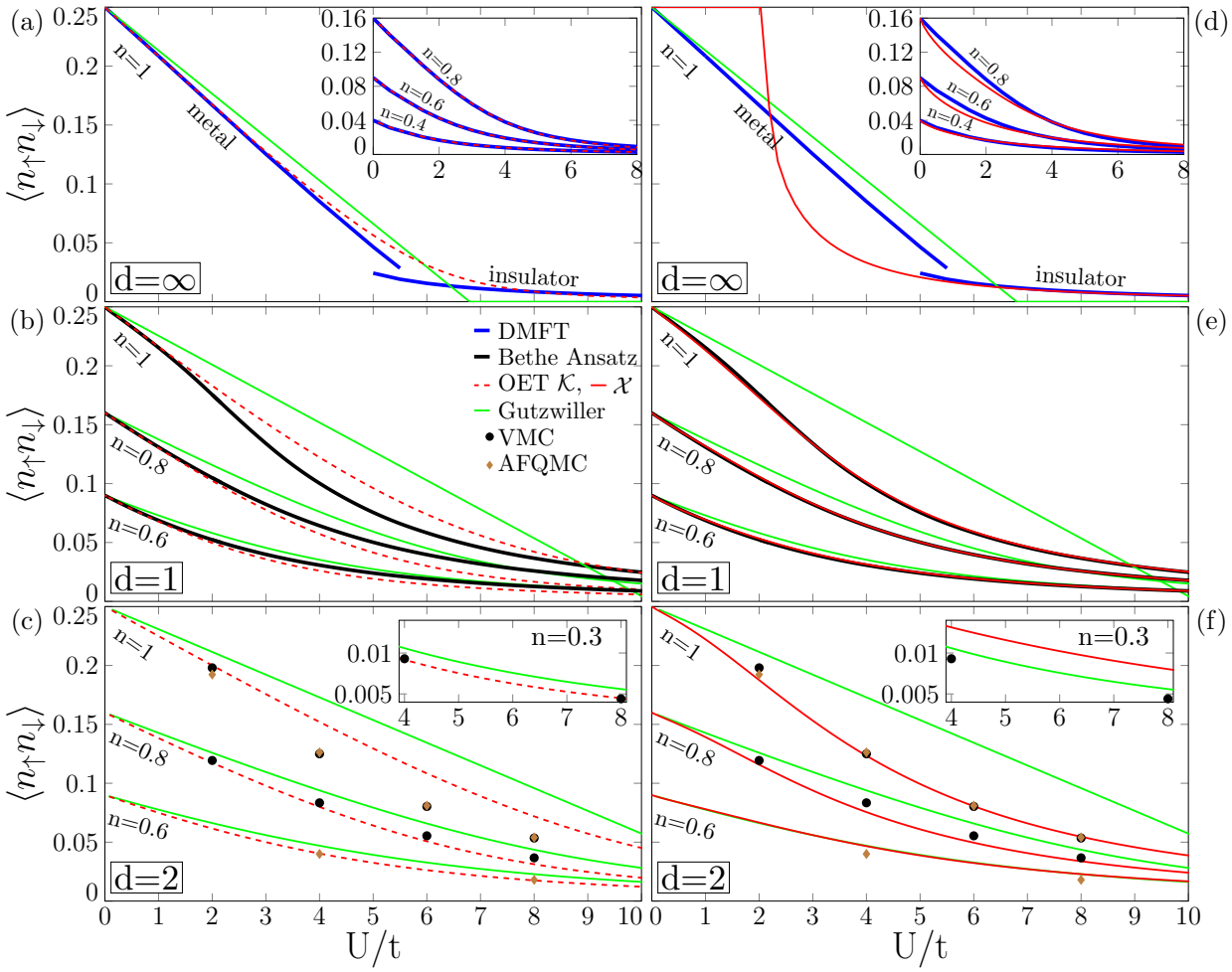

Figure 8.5: Double occupancy for the Hubbard model in various dimensions. (a,d) The d=∞ Bethe lattice for various dopings, solved within DMFT, GA, and OET within $\mathcal{K}$ (a) and $\mathcal{X}$ (d). (b,e) The d=1 lattice, solved within Bethe Ansatz, GA, and OET within $\mathcal{K}$ (b) and $\mathcal{X}$ (e). (c,f) The d=2 square lattice solved within GA, selected points using VMC and AFQMC [2], and OET within $\mathcal{K}$ (c) and $\mathcal{X}$ (f).

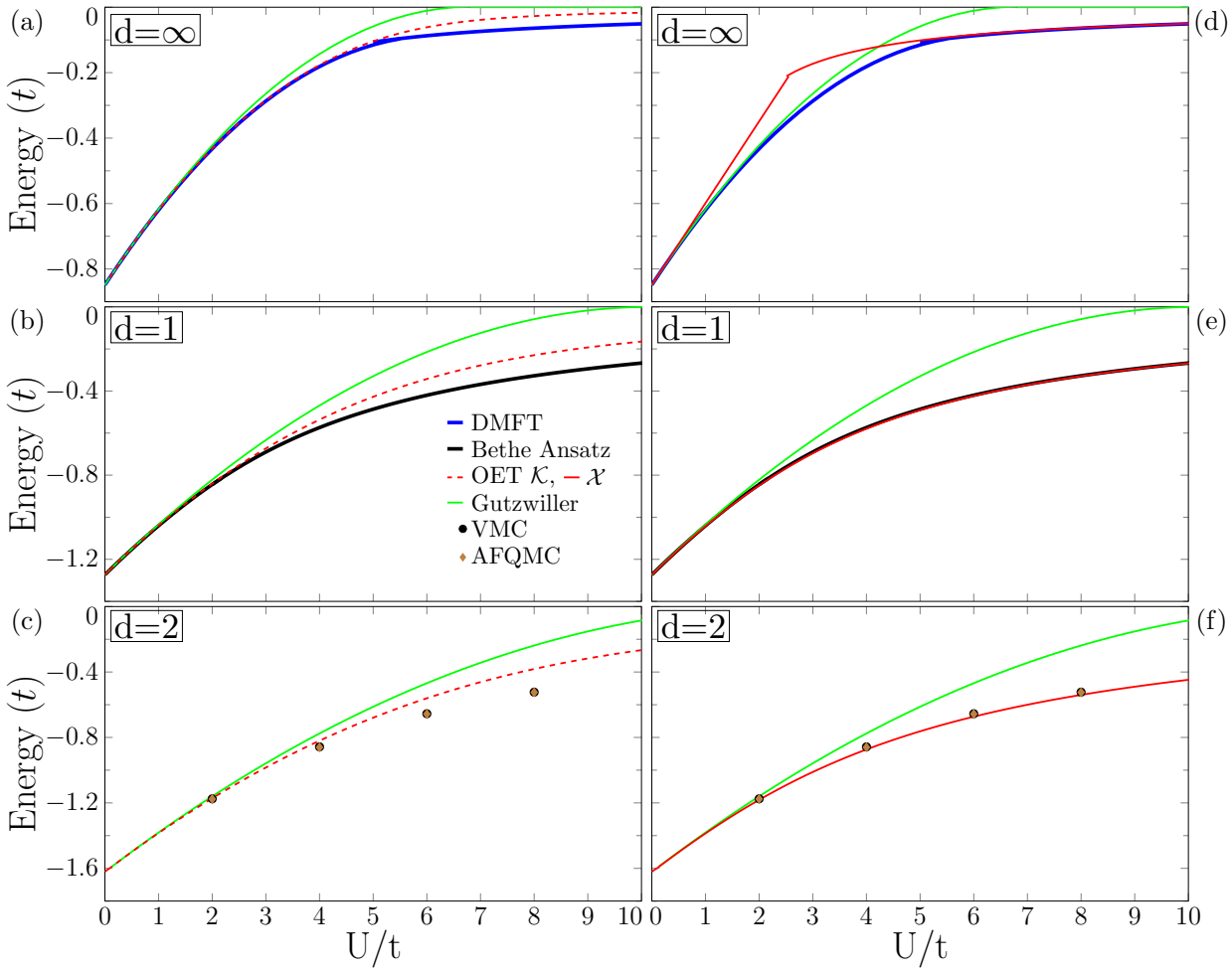

Figure 8.6: Total energy for the Hubbard model in various dimensions for n=1. (a,d) The d=∞ Bethe lattice solved within DMFT, GA, and OET within $\mathcal{K}$ (a) and $\mathcal{X}$ (d). (b,e) The d=1 lattice, solved within Bethe Ansatz, GA, and OET within $\mathcal{K}$ (b) and $\mathcal{X}$ (e). (c,f) The d=2 square lattice solved within GA, selected points using VMC and AFQMC [2], and OET within $\mathcal{K}$ (c) and $\mathcal{X}$ (f).

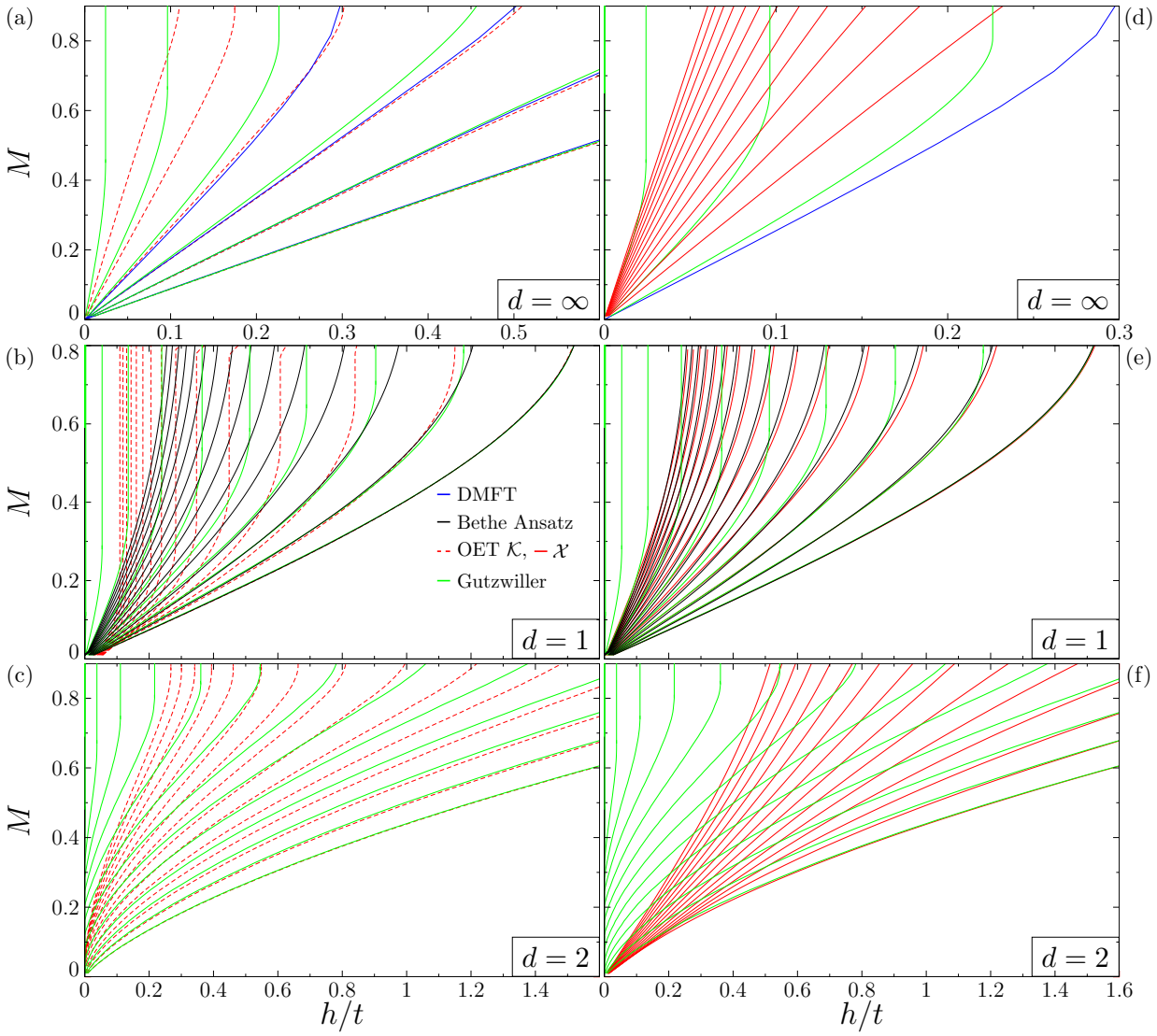

Figure 8.7: Magnetization M vs. applied field h for the Hubbard model in various dimensions. (a,d) The d=∞ Bethe lattice solved within DMFT (insulating results from Ref. [3]), GA, and OET within $\mathcal{K}$ (panel a, U/t =1,..,6) and $\mathcal{X}$ (panel d, U/t=4,..,16). (b,e) The d=1 lattice for $U/t = 1, .., 16$ (right to left) solved within the Bethe Ansatz, GA, and OET within $\mathcal{K}$ (b) and $\mathcal{X}$ (e). (c,f) The d=2 lattice for $U/t = 1, .., 16$ (right to left) solved within the GA and OET within $\mathcal{K}$ (c) and $\mathcal{X}$ (f).

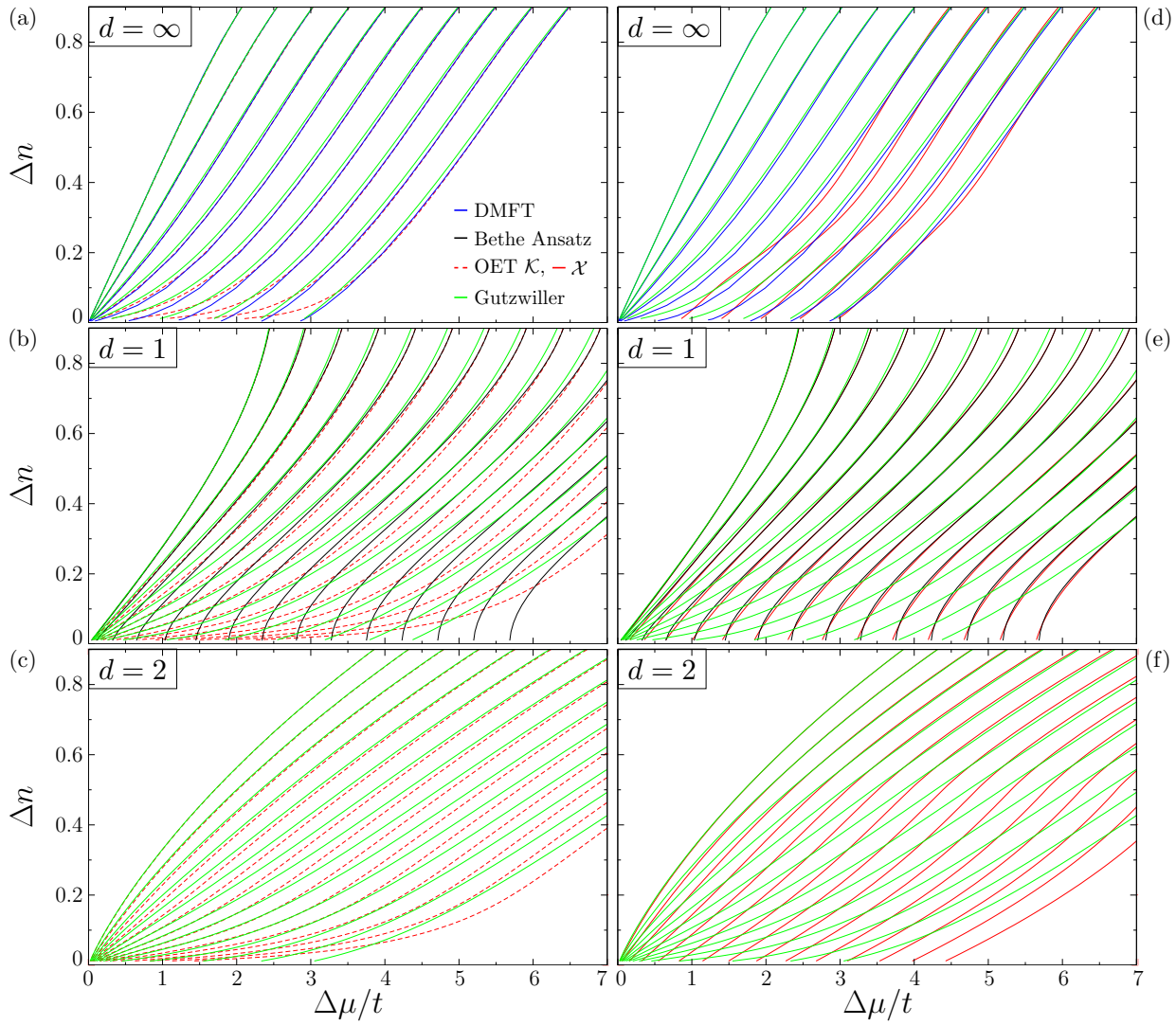

Figure 8.8: The density ($\Delta n = n - 1$) as a function of chemical potential ($\Delta\mu = \mu - U/2$) for the Hubbard model in various dimensions. (a,d) The d=∞ Bethe lattice for $U/t = 1, .., 10$ (left to right) solved within DMFT, GA, and OET within $\mathcal{K}$ (a) and $\mathcal{X}$ (d). (b,e) The d=1 lattice for $U/t = 1, .., 16$ (right to left) solved within the Bethe Ansatz, GA, and OET within $\mathcal{K}$ (b) and $\mathcal{X}$ (e). (c,f) The d=2 lattice for $U/t = 1, .., 16$ (right to left) solved within the GA and OET within $\mathcal{K}$ (c) and $\mathcal{X}$ (f).

Chapter 9

Summary and Outlook

In this thesis, we have presented two distinct but related theories. The variational discrete action theory (VDAT) combines two important paradigms in many body physics: the variational principle and diagrammatic techniques based on Green's functions. The basic idea is to use discrete time Green's function to study a variational density matrix known as the sequential product density matrix (SPD), resulting in a completely analogous mathematical structure to the usual many-body Green's functions. VDAT inherits the advantages from both the variational principle and many-body Green's functions: a rigorous upper bound for the total energy and a systematic improvement characteristic of perturbation theory. The time discretization number $\mathcal{N}$ plays an important role in fine tuning the balance of computational cost of accuracy. In this thesis, we used VDAT to study both the Anderson Impurity model on the ring and the Hubbard model in $d = \infty$, showing excellent results in both cases. There are many possible future directions for the VDAT formalism, given that many ideas from both variational and Green's function paradigms can be readily generalized to the VDAT formalism. For example, variational quantum Monte-Carlo, GW, and the coupled-cluster approach can all clearly be generalized to the VDAT formalism. We believe that VDAT will be useful for exploring both model Hamiltonians and real materials. Furthermore, it is likely that VDAT will be competitive with the most advanced many-body techniques in the context of model Hamiltonians, such as the two dimensional Hubbard model. Furthermore, it is highly likely that VDAT will find applications in other areas of physics, such as nuclear physics.

In the second part of the thesis, we proposed the Off-Shell Effective Energy Theory

(OET), which can be viewed as theoretical framework that allows one to construct exact energy functionals from a variational density matrix ansatz. The OET encapsulates and extrapolates precise results from other methods such as perturbation theory or VDAT. We demonstrated that an appropriately parameterized OET yields remarkable results for the one band Hubbard model in $d = 1, 2, \infty$. OET is a flexible formalism, and offers many approaches to parameterizing the correction to the energy function, such as machine learning, etc. OET will likely be an important tool to efficiently study strongly correlated materials.

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[41] See Supplemental Material at [URL will be inserted by publisher] for the defintion and derivations of the orthogonal response conditions (ORC); derivation of the CPE and RCPE for $\mathcal{K}$ and $\mathcal{X}$; and complete results for $\mathcal{K}$ and $\mathcal{X}$ in the Hubbard model.

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