Off-shell effective energy theory: A unified treatment of the Hubbard model from $d = 1$ to $d = \infty$

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Here we propose an exact formalism, off-shell effective energy theory (OET), which provides a thermodynamic description of a generic quantum 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.

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 dimensionality, 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 [1] 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) [2–4], 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 nonperturbatively. 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 [5,6] 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 exact solution [7,8], while for $d = \infty$, dynamical mean-field theory (DMFT) [9–11] provides the solution using numerically exact, but computationally intensive methods [12,13]. 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 [14,15] has the minus sign problem [16,17], 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.

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

$$\rho(k, X) = \mathrm{argmin}_{\hat{\rho}} \{\langle k\hat{K} + \beta^{-1} \ln \hat{\rho} \rangle_{\hat{\rho}} | \langle \hat{X} \rangle_{\hat{\rho}} = X\}, \quad (1)$$

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 $\rho(k, X)$ 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

$$\tilde{\rho}(k, X, K) = \mathcal{C}\mathcal{P}(k, X)\rho_{\hat{K}}(K)\mathcal{P}(k, X), \quad (2)$$

where $\mathcal{C}$ is the normalization, $K \in \mathcal{M}_K$ with $\mathcal{M}_K = \{\langle \hat{K} \rangle_{\hat{\rho}} : \hat{\rho} \in \mathcal{L}\}$, $\rho_{\hat{K}}(K) = \mathcal{C}' \exp(\kappa \hat{K})$ satisfying $\langle \hat{K} \rangle_{\rho_{\hat{K}}(K)} = K$, where $\mathcal{C}'$ is the normalization and $\kappa \in \mathbb{R}$ parametrizes $\rho_{\hat{K}}(K)$. The exact projector $\mathcal{P}(k, X)$ is defined by requiring Eq. (2) 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 $\tilde{\rho}(k, X, K^\star) = \rho(k, X)$. We can solve for $\mathcal{P}(k, X)$ using the on-shell condition

$$\mathcal{P}(k, X) = \frac{1}{\sqrt{\rho_g}}[\sqrt{\rho_g}\rho(k, X)\sqrt{\rho_g}]^{1/2}\frac{1}{\sqrt{\rho_g}}, \quad (3)$$

where $\rho_g = \rho_{\hat{K}}(K^\star)$. Finally, the ground-state energy can be constructed as

$$\mathcal{E}(k, x) = \lim_{\beta \to \infty} \min_{K \in \mathcal{M}_K, X \in \mathcal{M}_X} \langle \hat{H} \rangle_{\tilde{\rho}(k, X, K)}. \quad (4)$$

It is useful to introduce the map $\Upsilon(k, X, K) = (\langle \hat{K} \rangle_{\tilde{\rho}(k, X, K)}, \langle \hat{X} \rangle_{\tilde{\rho}(k, X, K)})$, 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.

We now introduce the key approximation scheme, the CPE. The CPE amounts to choosing an appropriate $K^\star$ and Taylor series expanding $\tilde{\rho}(k, X, K)$ 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 $\mathcal{P}(k, X_c) = 1$ within the CPE. Expanding $\mathcal{P}(k, X)$ to zeroth order in k about 0 and $\rho_{\hat{K}}(K)$ to first order in K about K_c, we find $K^\star = K_c$ and we have

$$\mathcal{P}(k, X) \approx \mathcal{P}(0, X) = \sqrt{\rho_{\hat{X}}(X)\rho_{\hat{X}}^{-1}(X_c)}, \quad (5)$$

$$\rho_{\hat{K}}(K) \approx \rho_{\hat{K}}(K_c)(1 + \langle\langle \Delta\hat{K}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X_c)}^{-1}\Delta\hat{K}\Delta K), \quad (6)$$

where $\Delta\hat{K} = \hat{K} - K_c\hat{1}$, $\Delta K = K - K_c$, and $\langle\langle \hat{A}; \hat{B} \rangle\rangle_{\hat{\rho}} = \text{Tr}(\hat{A}\sqrt{\hat{\rho}}\hat{B}\sqrt{\hat{\rho}})$, where the latter is known as the *symmetric correlator* [18]. 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 $\tilde{\rho}(k, X, K)$, denoted $\bar{\rho}$ for brevity:

$$\langle \Delta\hat{K} \rangle_{\bar{\rho}} = \lambda[\langle \Delta\hat{K} \rangle_{\rho_{\hat{X}}(X)} + Z(\Delta X)\Delta K], \quad (7)$$

$$\langle \Delta\hat{X} \rangle_{\bar{\rho}} = \lambda\left(\Delta X + \frac{\langle\langle \Delta\hat{X}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X)}}{\langle\langle \Delta\hat{K}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X_c)}}\Delta K\right), \quad (8)$$

$$\lambda = \left(1 + \langle \Delta\hat{K} \rangle_{\rho_{\hat{X}}(X)}\langle\langle \Delta\hat{K}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X_c)}^{-1}\Delta K\right)^{-1}, \quad (9)$$

$$Z(\Delta X) = \langle\langle \Delta\hat{K}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X)}\langle\langle \Delta\hat{K}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X_c)}^{-1}, \quad (10)$$

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 $\bar{\Upsilon}(X, K) = (\langle \hat{K} \rangle_{\bar{\rho}}, \langle \hat{X} \rangle_{\bar{\rho}})$.

For a number of important Hamiltonians, including the Hubbard model and its generalizations, we notice that $\langle \Delta\hat{K} \rangle_{\rho_{\hat{X}}(X)} = 0$, which implies that $\langle\langle \Delta\hat{K}; \Delta\hat{K} \rangle\rangle_{\rho_{\hat{X}}(X)} = 0$, and we refer to this scenario as the *orthogonal response condition* (ORC) [18]. 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 nonperturbative 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 RCPE [18], 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

$$\mathcal{K} \leftrightarrow \mathcal{X}, \quad k \leftrightarrow x, \quad K \leftrightarrow X, \quad \hat{K} \leftrightarrow \hat{X}. \quad (11)$$

All equations within the $\mathcal{K}$ formalism will have a correspondence in $\mathcal{X}$ [18], 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 the RCPE within 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 [18], and simply use the crossover of an energy derivative (e.g., double occupancy, density, etc.) when switching is employed.

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

$$\hat{H} = \hat{H}_K + \hat{H}_X = \sum_m k_m \hat{K}_m + \sum_n x_n \hat{X}_n, \quad (12)$$

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 $\hat{H} = \mathbf{k} \cdot \hat{\mathbf{K}} + \mathbf{x} \cdot \hat{\mathbf{X}}$. We define the density matrix determined from $\mathbf{A}$ as $\rho_{\hat{A}}(\mathbf{A}) = \mathcal{C} \exp(\boldsymbol{\alpha} \cdot \hat{\mathbf{A}})$ satisfying $\langle \hat{\mathbf{A}} \rangle_{\rho_{\hat{A}}(\mathbf{A})} = \mathbf{A}$, where $\boldsymbol{\alpha}$ is a vector of real numbers, and the domain of $\rho_{\hat{A}}(\mathbf{A})$ is denoted $\mathcal{M}_{\hat{A}} = \{\langle \hat{\mathbf{A}} \rangle_{\hat{\rho}} : \hat{\rho} \in \mathcal{L}\}$. The ground-state energy can then be written as

$$\mathcal{E}(\mathbf{k}, \mathbf{x}) = \lim_{\beta \to \infty} \min_{\mathbf{K} \in \mathcal{M}_{\hat{K}}, \mathbf{X} \in \mathcal{M}_{\hat{X}}} \langle \hat{H} \rangle_{\tilde{\rho}(\mathbf{k}, \mathbf{X}, \mathbf{K})}. \quad (13)$$

We also define the map $\Upsilon(\mathbf{k}, \mathbf{X}, \mathbf{K}) = (\langle \hat{\mathbf{K}} \rangle_{\tilde{\rho}(\mathbf{k}, \mathbf{X}, \mathbf{K})}, \langle \hat{\mathbf{X}} \rangle_{\tilde{\rho}(\mathbf{k}, \mathbf{X}, \mathbf{K})})$, 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 $\hat{\rho}_c = \rho_{\hat{\mathbf{C}}}(\mathbf{C})$ 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

$$\hat{H} = \sum_{p\sigma} \epsilon_p \hat{n}_{p\sigma} + N\left(U\hat{d} - \sum_{\sigma} \mu_\sigma \hat{n}_\sigma\right), \qquad (14)$$

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 $\hat{n}_{j\sigma} = \hat{a}_{j\sigma}^\dagger \hat{a}_{j\sigma}$, $\mu_\sigma = \mu + h(\delta_{\uparrow\sigma} - \delta_{\downarrow\sigma})$, and $\hat{d} = (1/N)\sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}$. To connect with Eq. (12), we identify $\hat{\mathbf{K}} = (\dots, \hat{n}_{p\sigma}, \dots)$, $\hat{\mathbf{X}} = (\hat{d}, \hat{n}_\uparrow, \hat{n}_\downarrow)$, and $\hat{\mathbf{C}} = (\hat{n}_\uparrow, \hat{n}_\downarrow)$. For a given constraint $(n_\uparrow, n_\downarrow)$, we parametrize $\mathbf{K} \in \mathcal{M}_K$ 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 $\Delta n_{p\sigma} \in [-n_\sigma, 1 - n_\sigma]$ with the constraint $\sum_p \Delta n_{p\sigma} = 0$; and for brevity, we denote $\Delta\mathbf{n} = (\dots, \Delta n_{p\sigma}, \dots)$.

We begin by presenting the CPE for both the $\mathcal{K}$ and $\mathcal{X}$ formalisms [18], where the $\mathcal{K}$ formalism yields

$$\bar{\Upsilon}_\mathcal{K}(\Delta\mathbf{n}, \Delta d) = (\mathbf{Z}_\mathcal{K}(\Delta d)\Delta\mathbf{n}, \Delta d), \qquad (15)$$

$$[\mathbf{Z}_\mathcal{K}(\Delta d)]_{p\sigma} = Z_\mathcal{K}^{(\sigma)}(\Delta d) = \mathcal{A}_\mathcal{K}^\sigma(\Delta d)/\mathcal{A}_\mathcal{K}^\sigma(0), \qquad (16)$$

$$\mathcal{A}_\mathcal{K}^\sigma(\Delta d) = \langle\langle \hat{a}_{j\sigma}^\dagger; \hat{a}_{j\sigma} \rangle\rangle_{\rho_{\hat{\mathbf{X}}}(\Delta d)}^2, \qquad (17)$$

where $\rho_{\hat{\mathbf{X}}}(\Delta d) = \bigotimes_j \rho_j(\Delta d)$ and

$$\rho_j(\Delta d) = \mathrm{diag}(p_0 + \Delta d, p_\downarrow - \Delta d, p_\uparrow - \Delta d, p_2 + \Delta d). \qquad (18)$$

The $\mathcal{X}$ formulation yields

$$\bar{\Upsilon}_\mathcal{X}(\Delta\mathbf{n}, \Delta d) = (\Delta\mathbf{n}, Z_\mathcal{X}(\Delta\mathbf{n})\Delta d), \qquad (19)$$

$$Z_\mathcal{X}(\Delta\mathbf{n}) = \mathcal{A}_\mathcal{X}(\Delta\mathbf{n})/\mathcal{A}_\mathcal{X}(\mathbf{0}), \qquad (20)$$

$$\mathcal{A}_\mathcal{X}(\Delta\mathbf{n}) = (1/N^4)\prod_\sigma \left|\sum_p \langle\langle \hat{a}_{p\sigma}^\dagger; \hat{a}_{p\sigma} \rangle\rangle_{\rho_{\hat{\mathbf{K}}}(\Delta\mathbf{n})}\right|^2, \qquad (21)$$

where $\rho_{\hat{\mathbf{K}}}(\Delta\mathbf{n}) = \bigotimes_{p\sigma} \rho_{p\sigma}(\Delta n_{p\sigma})$ and

$$\rho_{p\sigma}(\Delta n_{p\sigma}) = \mathrm{diag}(1 - n_\sigma - \Delta n_{p\sigma}, n_\sigma + \Delta n_{p\sigma}). \qquad (22)$$

The RCPE for the $\mathcal{K}$ formalism can be constructed as $\Upsilon_\mathcal{K}(\mathbf{k}, \mathbf{X}, \mathbf{K}) = (\mathcal{R}_\mathcal{K}(\mathbf{k}, \mathbf{Z}_\mathcal{K})\Delta\mathbf{n}, \Delta d)$ with $[\mathcal{R}_\mathcal{K}(\mathbf{k}, \mathbf{Z}_\mathcal{K})]_{p\sigma} = \gamma_0 (Z_\mathcal{K}^{(\sigma)})^{\gamma_1} + (1 - \gamma_0)(Z_\mathcal{K}^{(\sigma)})^{\gamma_2}$ and $\gamma_1 = 1$ and $\gamma_2 = 1/2$ [18]. Similarly, for the $\mathcal{X}$ formalism we have $\Upsilon_\mathcal{X}(\mathbf{x}, \mathbf{K}, \mathbf{X}) = (\Delta\mathbf{n}, \mathcal{R}_\mathcal{K}(\mathbf{x}, Z_\mathcal{X})\Delta d)$, where $\mathcal{R}_\mathcal{K}(\mathbf{x}, Z_\mathcal{X}) = \gamma_0(Z_\mathcal{X}^{(\sigma)})^{\gamma_1} + (1 - \gamma_0)(Z_\mathcal{X}^{(\sigma)})^{\gamma_2}$ 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 [18]. 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) of the $\mathcal{K}$ formalism, the classic Gutzwiller approximation (GA) [20–24] to the Hubbard model is rigorously recovered, providing a qualitative description of the

Fermi liquid phase, similar to slave bosons [25–27] and density matrix embedding theory [28–30]. 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 [31–36]. 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 [37–42] 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 [43–52].

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 [53] is used to solve the DMFT
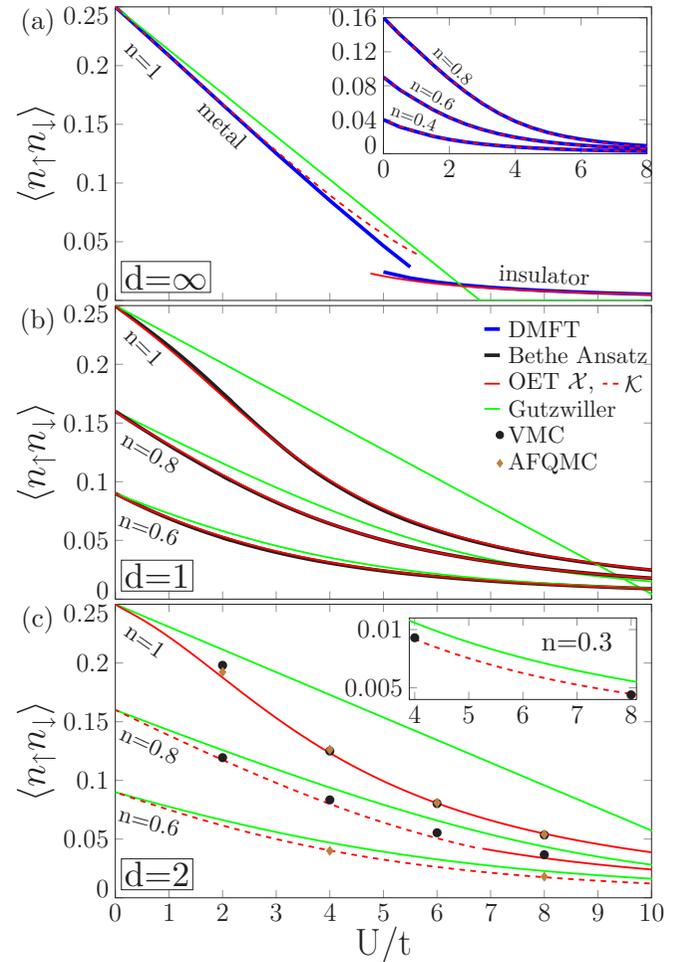

FIG. 1. Double occupancy for the Hubbard model in various dimensions. (a) The $d = \infty$ Bethe lattice for various dopings, solved within DMFT, GA, and OET. (b) The $d = 1$ lattice, solved within the BA, GA, and OET. (c) The $d = 2$ square lattice solved with GA, OET, and selected points using VMC and AFQMC [19].
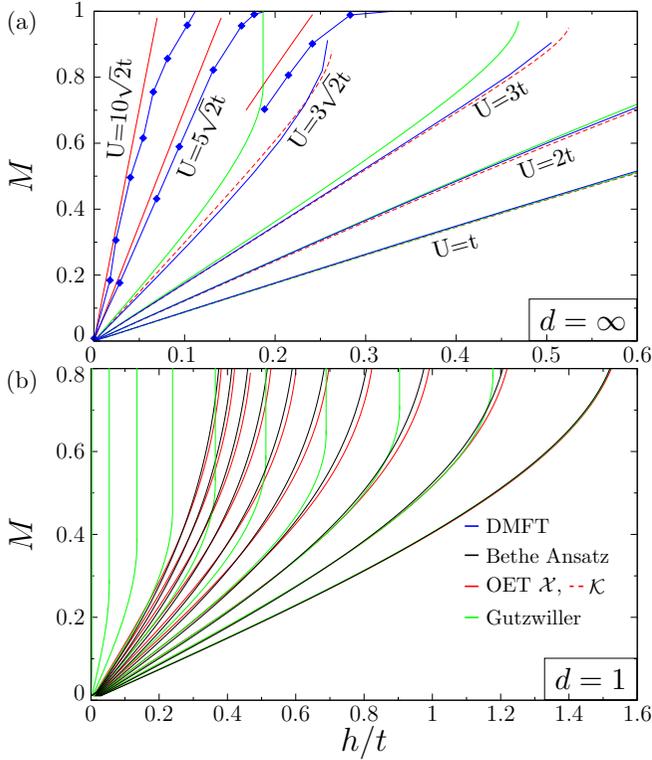
FIG. 2. Magnetization M vs magnetic field h for the Hubbard model in $d = \infty$ and $d = 1$. (a) The $d = \infty$ Bethe lattice solved within DMFT (insulating results from Ref. [9], denoted with points), GA, and OET. (b) The $d = 1$ lattice solved within the BA, GA, and OET for $U/t = 1, \ldots, 10$ (right to left).
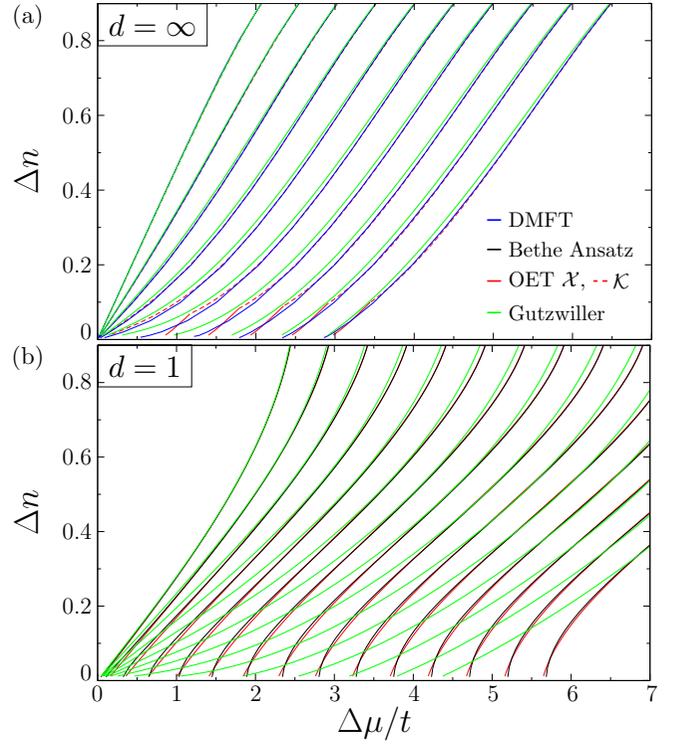

FIG. 3. The density ($\Delta n = n - 1$) as a function of chemical potential ($\Delta \mu = \mu - U/2$) for the Hubbard model in $d = \infty$ and $d = 1$. (a) The $d = \infty$ Bethe lattice solved within DMFT, GA, and OET for $U/t = 1, \ldots, 10$. (b) The $d = 1$ lattice solved with the BA, GA, and OET for $U/t = 1, \ldots, 16$.

impurity problem [9,54–56] as implemented in the "NRG Ljubljana" code [57]. In one dimension, we employ the exact BA solution [7,8], while in two dimensions we compare to variational quantum Monte Carlo (VMC) and auxiliary field quantum Monte Carlo (AFQMC) [19]. Additionally, we compare to the Gutzwiller approximation in all dimensions given that it is an efficient approach. We choose to present the double occupancy, density, and magnetization which are energy derivatives, providing a more sensitive comparison than solely evaluating the total energy. Additionally, total energies are presented for $n = 1$ in the Supplemental Material [18].

We begin by examining the double occupancy as a function of U/t for $d = \infty$ at half-filling [see Fig. 1(a)]. 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, showing excellent agreement with DMFT. We now turn to $d = 1$ and the $d = 2$ square lattice with nearest-neighbor hopping [see Figs. 1(b) and 1(c)]. In one dimension [Fig. 1(b)], 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 [18]. 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 [Fig. 1(c)].

We now turn to the magnetization under applied magnetic field and the density as a function of the chemical potential. For $d = \infty$, 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 Fig. 2(a)]. For $d = 1$, OET has excellent agreement over all parameters [see Fig. 2(b)]. In both $d = \infty$ and $d = 1$, Gutzwiller discontinuously polarizes for sufficiently large U. Now we consider the density as a function of the chemical potential in $d = \infty$ and $d = 1$ (Fig. 3). For $d = \infty$, the system opens a gap at a finite U, and the $\mathcal{K}$ and $\mathcal{X}$ ansatz can reasonably capture this behavior [Fig. 3(a)]. 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 [Fig. 3(b)]. Results for $d = 2$ can be found in Ref. [18].

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 $d = 1, 2$, and ∞. The success of our approach is based on four key ideas: the exact OET construction, a nonperturbative 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 to DFT+DMFT [12] and DFT+Gutzwiller [58], resulting in a highly efficient first-principles approach to the thermodynamics of strongly correlated materials in addition to molecules.

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