Systematic $1/d$ Corrections to the Infinite-Dimensional Limit of Correlated Lattice Electron Models

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We present a self-consistent treatment of Hubbard-like lattice models at large, but finite, spatial dimensions d. This involves a systematic expansion in powers of $1/d$ about the limit $d = \infty$. The first-order corrections can be obtained by self-consistent solution of coupled one- and two-impurity models. We calculate the leading corrections to properties of the Falicov-Kimball model. The infinite-dimensional limit seems to describe this particular model remarkably well even for $d = 2$.

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The limit of large spatial dimensions d [1] has been used extensively to study models of correlated lattice fermions [2]. The local approximation, which maps a lattice problem onto a single-impurity model supplemented by a self-consistency condition that simulates the role of the lattice, is exact at $d = \infty$ [3]. This provides a dynamical mean-field theory which captures much of the rich physics of correlated lattice models [4–7]. The local approximation cannot, however, address the existence of instabilities towards unconventional superconductivity [4], or fully probe the competition between correlation and magnetism in heavy-fermion compounds. To date, attempts to recover the effects of spatial fluctuations through systematic expansion about the limit $d = \infty$ have succeeded only in a few special cases: the Gutzwiller variational approach [8], the motion of a single hole in the $J = 0$ t-J model [9], and the spinless-fermion model [10]. Extension to the Hubbard Hamiltonian and related models, containing full many-body effects, has proved elusive.

In this paper we present a systematic theory of $1/d$ corrections for all Hubbard-like models, in the form of an effective cluster expansion. At leading order in $1/d$, the local approximation is replaced by a mapping onto coupled single- and two-impurity models. As a first step towards implementing this theory, we have explicitly obtained leading $1/d$ corrections for the Falicov-Kimball Hamiltonian, a restricted model to which a simplified version of this method can be applied. Only small deviations are found from the local approximation, even for $d = 2$. For larger values of the on-site Coulomb interaction, nonanalyticities develop within the simplified scheme. We expect $1/d$ corrections to have a much greater effect in the Hubbard and periodic Anderson Hamiltonians, models which are more relevant for the issues mentioned above.

We take as our generic model the Hubbard Hamiltonian on a d-dimensional hypercubic lattice

$$\mathcal{H} = -\frac{t^*}{\sqrt{d}} \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \qquad (1)$$

Here the nearest-neighbor hopping is scaled so that the kinetic energy has a suitable $d \to \infty$ limit. This implies [1,11] that in real space the bare ($U = 0$) propagator $G_{ij\sigma}^{(0)}$ is proportional to $d^{-\|i-j\|/2}$, where $\|i - j\|$ is the smallest number of nearest-neighbor hops between sites i and j. To leading order, the fully dressed single-particle lattice Green's function $G_{ij\sigma}$ has the same d dependence.

A concise formulation of $1/d$ corrections employs the Luttinger-Ward functional $\Phi[G_{ij\sigma}]$—the sum of all vacuum-to-vacuum skeleton diagrams—in terms of which the self-energy is

$$\Sigma_{ij\sigma}(i\omega_n) = \frac{\delta \Phi}{\delta G_{ji\sigma}(i\omega_n)} . \qquad (2)$$

Any two vertices i and j within a closed skeleton diagram can be connected by four paths having no line in common. For example, the diagram in Fig. 1 contains two paths going directly from i to j, and two going via site k. After summation over intermediate sites, each path contributes to a given diagram at least the same power of $1/d$ as $G_{ij\sigma}$. Even after summation over all equivalent sites j, the diagram is suppressed by a factor of at least $1/d^{\max}$, where max is the greatest intersite distance in that diagram. Thus, to order $1/d^n$, all diagrams containing intersite distances greater than n are negligible. This has two consequences for the self-energies: by virtue of Eq. (2),

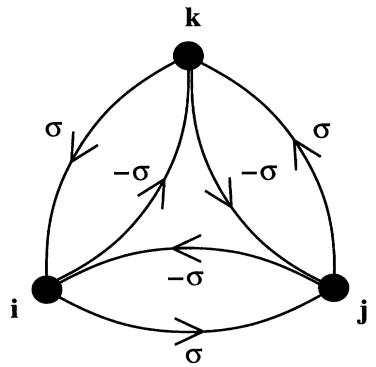

FIG. 1. A typical diagram in the expansion of the Luttinger-Ward functional, $\Phi[G_{ij\sigma}]$. Lines represent fully dressed Green's functions, circles indicate on-site Coulomb interactions.

one need consider only those $\Sigma_{ij\sigma}$ with $\|i - j\| \leq n$; furthermore, the remaining self-energies reduce to functionals solely of $G_{kl\sigma}$ with $\|k - l\| \leq n$. Hence, *summation of all skeleton diagrams with no intersite distance greater than n constitutes a systematic approximation scheme correct to order* $1/d^n$. An equivalent classification can be deduced directly from the diagrammatic representation of the self-energies [12].

Let us focus on first-order corrections in $1/d$. Then, Φ reduces to all possible skeleton diagrams that are either purely local, or involve just a *single* pair of nearest-neighbor sites. Consequently, we can write

$$\Phi[G] = \sum_{\langle i,j\rangle,\sigma} \Phi_{\text{2-imp}}[G_{ii\sigma}, G_{ij\sigma}, G_{ji\sigma}, G_{jj\sigma}] - (2d - 1)\sum_{i,\sigma} \Phi_{\text{1-imp}}[G_{ii\sigma}], \tag{3}$$

where $\Phi_{\text{1-imp}}$ and $\Phi_{\text{2-imp}}$ are the generating functionals for one and two Hubbard impurities, respectively. The second term in Eq. (3) prevents overcounting of purely local diagrams. $\Phi_{\text{1-imp}}$ and $\Phi_{\text{2-imp}}$, respectively, can be generated from the one- and two-impurity actions

$$S_{\text{1-imp}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^\dagger_{1\sigma}(\tau)\mathcal{G}^{(0)-1}_{\text{1-imp},\sigma}(\tau - \tau')c_{1\sigma}(\tau') + U\int_0^\beta d\tau\, c^\dagger_{1\uparrow}(\tau)c_{1\uparrow}(\tau)c^\dagger_{1\downarrow}(\tau)c_{1\downarrow}(\tau), \tag{4a}$$

$$S_{\text{2-imp}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{i,j=1}^{2}\sum_\sigma c^\dagger_{i\sigma}(\tau)[\mathcal{G}^{(0)-1}_{\text{2-imp},\sigma}(\tau - \tau')]_{ij}c_{j\sigma}(\tau') + U\sum_{i=1}^{2}\int_0^\beta d\tau\, c^\dagger_{i\uparrow}(\tau)c_{i\uparrow}(\tau)c^\dagger_{i\downarrow}(\tau)c_{i\downarrow}(\tau). \tag{4b}$$

The site indices 1 and 2 label a specific pair of nearest-neighbor lattice sites. $\mathcal{G}^{(0)}_{\text{1-imp},\sigma}(\tau - \tau')$ and $\mathcal{G}^{(0)}_{\text{2-imp},\sigma}(\tau - \tau')$, the latter being a 2×2 matrix, represent the "bare" propagators. These are to be chosen so that, when dressed with the impurity self-energies, they coincide with the corresponding lattice Green's functions

$$\mathcal{G}^{(0)\,-1}_{\text{1-imp},\sigma}(i\omega_n) = G^{-1}_{11\sigma}(i\omega_n) + \Sigma^{\text{1-imp}}_\sigma(i\omega_n), \tag{5a}$$

$$[\mathcal{G}^{(0)\,-1}_{\text{2-imp},\sigma}(i\omega_n)] = [G^{-1}_\sigma(i\omega_n)]_{ij} + \Sigma^{\text{2-imp}}_{ij\sigma}(i\omega_n). \tag{5b}$$

Here our 2×2 matrix notation has been extended to G_σ, i.e., $[G_\sigma(i\omega_n)]_{ij} \equiv G_{ij\sigma}(i\omega_n)$.

Solution of the impurity problems allows one to extract the impurity self-energies from the lattice propagators. Then a functional derivative of Eq. (3) relates the lattice and impurity self-energies. In the paramagnetic phase all spin dependence drops out and just two lattice self-energies remain: the on-site $\Sigma_0(z)$ and nearest-neighbor $\Sigma_1(z)$ self-energies. These can be written

$$\Sigma_0(i\omega_n) = \Sigma^{\text{1-imp}}(i\omega_n) + 2d\left[\Sigma^{\text{2-imp}}_{11}(i\omega_n) - \Sigma^{\text{1-imp}}(i\omega_n)\right], \tag{6a}$$

$$\Sigma_1(i\omega_n) = \Sigma^{\text{2-imp}}_{11}(i\omega_n). \tag{6b}$$

Similar relations hold for phases with long-range order.

A self-consistent loop can be closed by expressing the full Green's functions in terms of the lattice self-energies. This relation will depend on the specific phase under consideration. For the spatially homogeneous phase, solution of the lattice Dyson's equation yields

$$G_{ij\sigma}(z) = \frac{1}{1 + \Sigma_1(z)/t}\, G^{(0)}_{ij\sigma}\left(\frac{z - \Sigma_0(z) + \mu}{1 + \Sigma_1(z)/t}\right). \tag{7}$$

The bare $G^{(0)}_{ij\sigma}$ functions (corresponding to a chemical potential $\mu = 0$) must be taken to be the actual d-dimensional propagators, or unphysical results will emerge. This is because on a hypercubic lattice, the bare propagators have nonanalytic corrections in $1/d$ that cannot be treated within perturbation theory in $1/d$ [11]. The self-consistency requirement is enforced numerically according to the following iteration scheme:

$$\Sigma^{\text{imp}} \xrightarrow{\text{Eqs. (6)}} \Sigma^{\text{latt}} \xrightarrow{\text{Eq. (7)}} G_{\text{latt}} \xrightarrow{\text{Eqs. (5)}} \mathcal{G}^{(0)}_{\text{imp}} \xrightarrow[\text{actions}]{\text{Solve imp.}} \Sigma^{\text{imp}}. \tag{8}$$

The above constitutes a self-consistent theory, correct to order $1/d$, *which by construction is thermodynamically conserving.* It can be extended to describe phases with long-range order, as well as other related models [12]. An equivalent theory has been formulated independently by Georges and Kotliar [13].

Among the steps entering Eq. (8), solution of the impurity actions is by far the most complicated, since it requires the solution of one- and two-impurity Anderson-like models. Application of the above formulation of $1/d$ corrections to any correlated lattice model therefore requires a large-scale numerical effort. In what follows we focus on the Falicov-Kimball model, for which a simplified version of the $1/d$ treatment can be implemented.

In the Falicov-Kimball Hamiltonian [14],

$$\mathcal{H} = -\frac{t^*}{\sqrt{d}}\sum_{\langle i,j\rangle} d^\dagger_i d_j + E_f\sum_i f^\dagger_i f_i + U\sum_i f^\dagger_i f_i d^\dagger_i d_i, \tag{9}$$

itinerant d fermions interact with localized f fermions via an on-site Coulomb interaction U. (This can be regarded as a variant of the Hubbard model in which one spin species is tied down.) The two fermion species share a joint chemical potential μ and are thermodynamically correlated, leading to long-range ordered phases. Most notably, in the symmetric case $E_f = 0$, $\mu = U/2$, a checkerboard decomposition of the f particles occurs, with a finite critical temperature T_c for any $d \geq 2$ [15].

The localized nature of the f fermions in the Falicov-Kimball model permits a greatly simplified treatment of

$1/d$ corrections. Expanding in terms of fully dressed d propagators and *bare* f propagators, we can still obtain a classification in powers of $1/d$ based on the greatest intersite distance within a diagram, and hence derive impurity mappings similar to Eqs. (4). Now, however, just as for $d = \infty$ [16], bare f propagators enter the impurity actions, and the self-consistency equation applies only to the d propagators. As an important consequence, solution of the impurity actions no longer requires heavy computation. The d-fermion lattice Green's function $G_{ij}(z)$ is calculated by integrating out the f particles and expressing the one- and two-impurity d propagators as

$$\mathcal{G}_{1\text{-imp}}(i\omega_n) = \sum_{\gamma=0,1} w_\gamma [\mathcal{G}^{(0)-1}_{1\text{-imp}}(i\omega_n) - \gamma U]^{-1}, \tag{10a}$$

$$\mathcal{G}_{2\text{-imp}}(i\omega_n) = \sum_{\gamma,\delta=0,1} p_{\gamma\delta} \left[\mathcal{G}^{(0)-1}_{2\text{-imp}}(i\omega_n) - U \begin{pmatrix} \gamma & 0 \\ 0 & \delta \end{pmatrix} \right]^{-1}. \tag{10b}$$

Here γ and δ represent the f-occupancy number on sites 1 and 2, respectively; w_γ and $p_{\gamma\delta}$ are probabilities for the different f configurations in each impurity action. Different Matsubara frequencies $i\omega_n = i(2n + 1)T$ are coupled only through the probabilities, which are expressed as sums over all $i\omega_n$ [16]. Apart from this, Eqs. (10) implement the impurity-solution step of Eq. (8) in a purely algebraic manner. Once Eq. (8) has been iterated and the probabilities w_γ and $p_{\gamma\delta}$ determined, the same sequence can be used to calculate $G_{ij}(z)$ for an arbitrary complex z. A special feature of the resulting equations is that they are purely local in z.

Although this simplified treatment is correct to order $1/d$, it is no longer thermodynamically conserving. It also neglects certain diagrams retained within the general scheme. For example, the f self-energy diagram in Fig. 2 is formally $O(1/d^2)$, yet it enters the general treatment at order $1/d$ since the part containing site k can be absorbed into a dressed f propagator. By contrast, the d self-energy diagram obtained by swapping f and d lines in Fig. 2 enters both formulations at first order. The simplified scheme thus treats d and f fermions on different footings. This also leads to the locality in z of Eqs. (10).

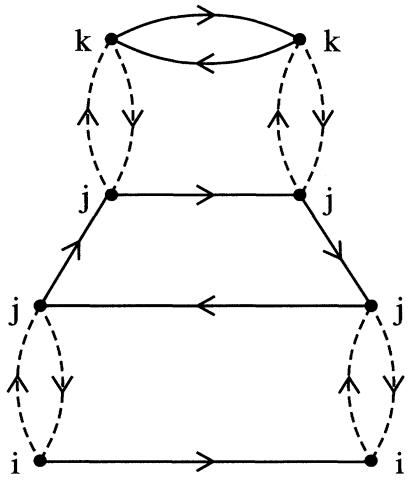

FIG. 2. An f self-energy diagram for the Falicov-Kimball model which is included in the general treatment of $1/d$ corrections but is omitted under the simplified scheme. Solid and dashed lines represent bare f and d propagators, respectively. Sites i and k are distinct nearest neighbors of j. There is summation over j and k for fixed i.

We believe that this locality is responsible for the appearance of unphysical solutions to Eqs. (8). Let us focus on the spatially homogeneous phase ($T > T_c$) of the symmetric model ($E_f = 0$, $\mu = U/2$). As U exceeds a critical value U_c ($\approx 1.85t^*$ for $d = 2$), a patch develops around $z = 0$—growing with increasing U—within which two distinct solutions for $G_{ij}(z)$ can be found. Both solutions are nonanalytic along the real axis: they violate the spectral sum rule and the Kramers-Kronig relation, although the spectral function remains nonnegative. Analyticity is restored for z well above the real axis. We note that similar difficulties were encountered in attempts to go beyond the single-site mapping (coherent potential approximation) for disordered systems [17].

We concentrate on $U < U_c$, for which one can confirm numerically that the single solution that emerges is Herglotz: it fulfills both the spectral sum rule and the constraints of the spectral representation, and shows the correct asymptotic behavior $G_{ii}(z) \sim 1/z$ for $|z| \to \infty$. Figure 3 depicts the itinerant density of states in the homogeneous phase of the symmetric Falicov-Kimball

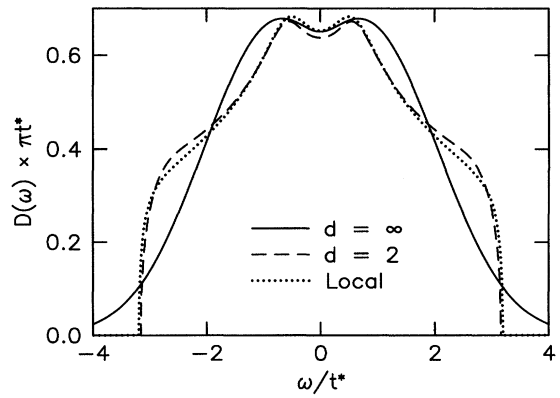

FIG. 3. The density of states for itinerant d fermions in the symmetric Falicov-Kimball model, with $U/t^* = 1.5$ and $T/t^* = 0.1$. The dotted line corresponds to the local approximation for $d = 2$.

model for $d = 2, \infty$, with $U/t^* = 1.5$ and $T/t^* = 0.1$. The results of the local approximation—a single-impurity mapping, using the true d dependence of $G_{ij}^{(0)}$—are shown for comparison. Deviations from the local approximation practically vanish for $U/t^* \lesssim 1$. This is to be expected, at least in weak coupling, since corrections to the local approximation appear first at order U^4 for the Falicov-Kimball model (compared to only U^2 for the Hubbard model). It is somewhat surprising, however, that the deviations remain so small even for $U/t^* = 1.5$.

The checkerboard decomposition of the symmetric Falicov-Kimball model can be treated using three effective impurity actions: a two-impurity action, and separate one-impurity actions for the inequivalent sublattices A and B. One must determine five self-energies ($\Sigma_A^{1\text{-imp}}$, $\Sigma_B^{1\text{-imp}}$, $\Sigma_{AA}^{2\text{-imp}}$, $\Sigma_{BB}^{2\text{-imp}}$, and $\Sigma_{AB}^{2\text{-imp}} \equiv \Sigma_{BA}^{2\text{-imp}}$) plus independent probabilities $w_{A\gamma}$ and $w_{B\gamma}$ for the one-impurity f configurations on the two sublattices. The critical temperature T_c is the highest temperature at which a broken-symmetry solution $w_{A\gamma} \neq w_{B\gamma}$ appears.

Figure 4 plots T_c versus U for $d = 2$ and ∞. Within the range of U shown, Herglotz solutions for G_{ij} can be found both above and below the transition temperature (although multiple solutions may develop once T is lowered deep into the broken-symmetry phase). Deviations from the $d = \infty$ curve are remarkably small for $d = 2$. However, the effect of $1/d$ corrections is always to depress T_c relative to the local approximation, as is characteristic of fluctuations about a mean-field theory.

We expect $1/d$ corrections to be more significant for fully interacting models in which a small many-body energy scale appears at $d = \infty$ in addition to the bare scales in the Hamiltonian. For instance, since the Hubbard model maps onto one- and two-impurity Anderson models, the solution must reflect a competition between an on-site Kondo effect and an intersite RKKY interaction. This should capture the interesting physics that is missed at $d = \infty$.

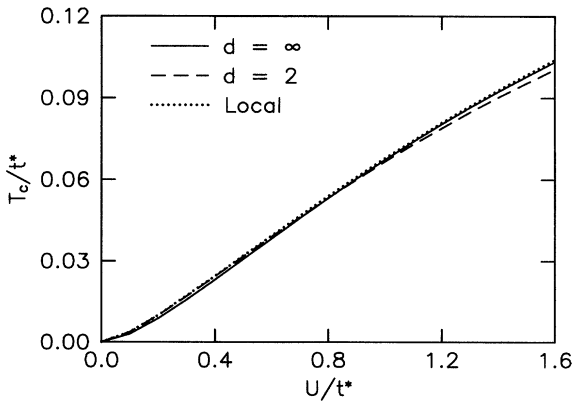

FIG. 4. The critical temperature for the checkerboard decomposition of the symmetric Falicov-Kimball model versus the strength of the Coulomb interaction. The dotted line shows the local approximation for $d = 2$.

In summary, we have presented a self-consistent expansion about the limit of infinite spatial dimensions for all Hubbard-like models. Implementation of leading-order $1/d$ corrections within a simplified scheme, specific to the Falicov-Kimball model, reveals nonanalytic Green's functions above some critical value of U. Below this value, solutions are Herglotz for all $T > T_c$ and into the broken-symmetry phase. Even for $d = 2$, the properties of the symmetric Falicov-Kimball model are modified only slightly, compared to the local approximation. It remains to be seen whether the appearance of multiple solutions is removed within the full expansion scheme.

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