Local approach to the one-band Hubbard model: Extension of the coherent-potential approximation

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We present a simple scheme to extend the earlier single-site coherent-potential-approximation (CPA) theories by utilizing connections of the CPA solution with the exact solution of the Falicov-Kimball model in infinite dimensions, and with the single-impurity Anderson-type models. We study the local spectral density of the model at $n = 1$; in the metallic regime, this exhibits a narrow Abrikosov-Suhl resonance and satellite peaks, which correspond, respectively, to the quasiparticle and Hubbard subband structures. This collective resonance disappears in the split-band (insulating) regime, where the CPA is found to be a good approximation. Comparisons are made with numerical works on finite-sized two-dimensional lattices, and good agreement is obtained.

I. INTRODUCTION

The physics of strongly correlated electrons in solids still contains many open questions. In this context, the limit of infinite dimensionality considered by several authors provided great insights. In this limit, due to the freezing of spatial fluctuations, a certain self-consistent mean-field theory becomes exact. In this limit, the action becomes purely local, and the bare Green's function of the local dynamics contains information about all other sites which have been integrated out. The momentum conservation is actually trivial in infinite dimensions, and only frequency conservation needs to be ensured in the skeleton expansion. The essential simplification in this limit is that the single-particle (sp) properties can be understood by looking at a single fixed lattice site. This has enabled workers to make an exact mapping of this model to a single-impurity Anderson model with a self-consistency condition.

The earlier coherent-potential-approximation (CPA)-like theories reproduce the Hubbard subband structures correctly as $U$ is raised, but are expected to do a bad job in the low-energy region, especially in the metallic state. Indeed, in the CPA, electronlike quasiparticles are unstable for all finite $U$; this is somewhat counterintuitive, since for small $U$, we expect a Fermi liquid with $Z < 1$. The drawback of the CPA is that it neglects the propagation of the opposite spin species; it freezes the down-spin configuration while looking at the propagation of an up spin. Strictly speaking, this is not true; it is a good approximation only in the split-band regime, where the local spin-fluctuation time $\tau d \ll \hbar/\Delta$, the mean hopping time, but is not good at longer time scales. Here, $\Delta$ is the bandwidth of noninteracting electrons in our model. In the language of the alloy analogy, the CPA replaces dynamical, annealed disorder by quenched, static disorder.

In this paper, we try to rectify the above-mentioned deficiency of the CPA. We make use of our earlier results: (1) the CPA solution for the Hubbard model is identical to the exact solution of the Falicov-Kimball model in infinite dimensions, (2) results identical to (1) above are obtained by looking at the local propagator of a single $d$ impurity hybridized with a conduction electron sea.

These connections enable us to look at the local dynamics of a $\sigma$-spin electron while the opposite spin species is also allowed to hop. In particular, we focus on the impurity density of states (DOS), which is just the full interacting density of states for the lattice, as is required by self-consistency. We study the local spectral density $\rho(\omega)$ as a function of the ratio $U/\Delta$ for the particle-hole symmetric case of $n = 1$. We compare our results with those obtained by Tan, Li, and Callaway using Lanczos numerical technique for finite-sized $3 \times 3$ (two-dimensional 2D) lattices. Our calculation reproduces all the essential features seen in their numerical work; a central "Kondo" peak at small and intermediate $U$ with some weight transferred to the Hubbard subbands, evolving smoothly into the split-band picture in the large-$U$ limit. The CPA results are obtained as the first truncation of our self-consistent scheme, and provide a good agreement with the numerical work in the large-$U$ limit, as expected. The paper is organized as follows. Section II deals with the actual calculation of the DOS, and Sec. III is devoted to a short discussion of our results.

II. CALCULATION OF THE sp DOS

We start with the single-band Hubbard model

$$H = t \sum_{\langle ij \rangle} [c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}] - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i\sigma} n_{i1-\sigma} n_{i\sigma},$$

where the sum goes over nearest neighbors, and $\sigma$ is the spin. Within the CPA, when we focus on a $\sigma$ spin, the $-\sigma$ spin configuration is assumed frozen. Here the $\sigma$ and $-\sigma$ spins are considered to comprise a binary alloy with concentrations $x = (1-n^{-\sigma})$ and $y = n^{-\sigma}$, and site energies $e_i^\sigma = -\mu$ and $e_i^\sigma = -\mu + U$. The latter represent the actual local potentials seen by a $\sigma$ spin at site $i$ when that site is either empty ($e_i^\sigma$) or occupied by a $-\sigma$ spin ($e_i^\sigma$). The unperturbed local propagator is given by [assuming a Lorentzian unperturbed DOS,
\[ \rho_0(\omega) = \frac{\Delta}{\pi \hbar} \left( \omega^2 + \Delta^2 \right)^{-1}, \]
\[ G_0^\dagger(\omega) = \int \rho_0(\epsilon) G_0(\epsilon, \omega) d\epsilon \]
\[ = [\omega + \mu + i\Delta]^{-1}. \]

Using Dyson's equation, the perturbed propagator is
\[ G_\sigma(\omega) = [\omega + \Sigma^\prime(\omega) + i\Delta]^{-1}, \]
where \( \Sigma^\prime(\omega) \) is the multiple-scattered self-energy calculated using Soven's equation
\[ \Sigma^\prime(\omega) = \epsilon^r - [\epsilon^r - \Sigma^\prime(\omega)][2\pi G^\sigma(\omega)][\epsilon^r - \Sigma^\prime(\omega)]. \]  (3)

With \( \epsilon^r = -\mu + U n^{d-\sigma} \) and \( G \) from Eq. (2), we get a closed analytic form for \( \Sigma \). (The imaginary part is finite \( \epsilon \) at the chemical potential, and so the CPA smears out the Fermi surface. This is a serious shortcoming.) Plugging this into Eq. (2) yields a result for the local \( G^\sigma(\omega) \) identical to that obtained from an exact treatment of the Falicov-Kimball model in infinite dimensions,
\[ G_\sigma^\dagger(\omega) = (2\pi)^{-1} \left[ \frac{1 - n^{d-\sigma}}{\omega + \mu + i\Delta} + \frac{n^{d-\sigma}}{\omega + \mu - U + i\Delta} \right]. \]  (4)

and identical results are obtained by consideration of the local propagator of a single \( d \) impurity \( \delta \) hybridized with a conduction electron sea. Effectively, one views the CPA as being identical to the replacement of the problem of interacting fermions to the problem of free fermions self-consistently embedded in an effective medium with a (complex) self-energy \( \Sigma(\omega) \). This is in the spirit of the earlier CPA-like approaches, and is due to the fact that multiple-scattering corrections introduce a finite lifetime for the single-particle excitations. Thus, within the CPA, the \( \sigma \) spin moves in a static, random potential provided by the \( -\sigma \) spins. The \( \sigma \) spin diagonal-site energy is given by \( [-\mu + \Sigma(\omega)] \) with the \( -\sigma \) spin held fixed. If we now allow the \( -\sigma \) spins to hop in this effective medium, the local properties of the \( -\sigma \) spin can be calculated by viewing this spin as being embedded in an effective medium with site-diagonal energy \( [-\mu + \Sigma(\omega)] \). The problem is clearly of an iterative nature; to proceed, we consider an auxiliary impurity model
\[ H_{eff} = \sum_{k\sigma} \epsilon_k + \Sigma(\omega) c_k^\dagger c_k + \frac{i}{2} \sum_{k\sigma} \left[ \epsilon + \Delta c_k^\dagger d_\sigma + H.c. \right] \]
\[ + \epsilon^d \sum_{\sigma} n_{\sigma d} + U \sum_{\sigma} n_{\sigma d} n_{\sigma d} \]. \]  (5)

To look at the local spectral density, we start with the equation of motion for the local \( G^{dd}(\omega) \). This leads to the mixed and higher-order Green's function \( G^{kk}(\omega) = \langle c_{k\sigma} d_{k\sigma}^\dagger \rangle \) and \( G^{dd}(\omega) = \langle n_{d-\sigma} d_{\sigma}^\dagger \rangle \) on the right-hand side; the equation of motion for \( \Gamma^{dd}(\omega) \) leads to a higher-order mixed \( \Gamma^{kk}(\omega) = \langle n_{d-\sigma} c_{k\sigma} d_{\sigma}^\dagger \rangle \). However, the equations of motion for these higher-order Green's functions close because of the property \( n_{\sigma d}^2 = n_{\sigma} \). The final set of equations reads
\[ \omega G^{dd}(\omega) = (2\pi)^{-1} + U \Gamma^{dd}(\omega) - \mu G^{dd}(\omega) + \Sigma t_k G^{kd}(\omega), \]
\[ \omega G^{kd}(\omega) = \left[ \epsilon_k + \Sigma(\omega) \right] G^{kd}(\omega) + t_k G^{dd}(\omega), \]
\[ \omega \Gamma^{kl}(\omega) = \left[ \epsilon_k + \Sigma(\omega) \right] \Gamma^{kl}(\omega) + t_k \Gamma^{dd}(\omega). \]  (6)

Solving for \( G^{dd}(\omega) \), we get
\[ 2\pi G^{dd}(\omega) = \frac{1 - n^{d-\sigma}}{\omega + \mu - U + i\Delta}, \]
where
\[ \Delta(\omega) = \sum_k \frac{t_k^2}{[\omega - \epsilon_k - \Sigma(\omega)]} = -i\pi\Delta^2 \rho(\omega), \]

neglecting the real part. This can easily be shown to be derived from the following self-energy:
\[ \Sigma^{d}(\omega) = Un^{d-\sigma} + \frac{U\gamma n^{d-\sigma}(1 - n^{d-\sigma})}{\omega + \mu - U(1 - n^{d-\sigma}) + i\pi\Delta^2 \rho(\omega)}. \]  (7)

Here, \( \rho(\omega) \) is the actual DOS of the full interacting system [cf. Eq. (1)] and the chemical potential \( \mu \) is determined from the constraint
\[ \int \rho^{d}_{\sigma}(\omega) d\omega = 0.5, \]
where
\[ -\pi\rho^{d}_{\sigma}(\omega) = \text{Im} \left( \frac{1}{[\omega + \mu - \Sigma^{d}_{\sigma}(\omega) + i\Delta]} \right). \]  (8)

It is clear from Eqs. (5)–(7) that our approach is exact in both the band and the atomic limit. In fact, the above equations allow us to devise a self-consistency scheme for the calculation of the local spectral density of the model. We study the half-filled \( (n = 1) \) case and consider only the paramagnetic solution \( n^{d-\sigma} = n^{d-\sigma} = 0.5 \). We choose the free DOS to be a Lorentzian of half-width \( \Delta \), \( \rho_{0}(\omega) = (\Delta/\pi)(\omega^{2} + \Delta^{2})^{-1} \), and plug it into Eqs. (5) and (6) to calculate the new \( \rho \) [cf. Eq. (7)] and calculate \( \mu \) from the constraint equation (7). This is resubstituted back into the set of Eqs. (5)–(7) and the process is iterated to convergence; i.e., until the successive values of \( \rho(\omega) \) differ by less than \( 10^{-7} \). The results of our calculation are shown in Figs. 1–3 for various values of \( U/\Delta \), where \( \Delta \) is the free bandwidth. It is seen that our calculation reproduces all the essential features of the finite-sized-lattice calculation of Tan, Li, and Callaway. In the case of small \( U \) \( (U = 0.25\Delta) \), we observe a sharp central "quasiparticle" peak, with some spectral weight transferred to the subbands. As \( U/\Delta \) is raised, there is a continuous transfer of spectral weight from the quasicoherent low-energy region to the incoherent high-energy electron and hole (Hubbard) subbands \( (U = 0.75\Delta) \) until at \( U = U_{c} \), the central peak disappears. This signals the onset of the Mott-Hubbard insulating phase, where the spectrum is totally incoherent. The above behavior is easily explained within our approach. The central Kondo peak arises due to the "impurity-conduction electron hybridization" within the impurity approach (corresponding to the hopping in the original Hubbard model), and it represents an impurity site occupied by either an
up- or a down-spin electron. The Hubbard subbands correspond, as usual, to an empty or a doubly occupied impurity. For the Lorentzian case, \( U_c = \infty \), but with a semieliptical DOS, we expect similar physics at and around \( U \sim \Delta \). It is worth remarking that the CPA is qualitatively correct in the split-band regime, but completely misses the low-energy structures seen at weak and intermediate \( U/\Delta \). Indeed, the CPA results can readily be obtained from our analysis as a first truncation of our iterative procedure, simply by setting \( \Sigma(\omega) = 0 \) in Eq. (5), and noticing that within the spirit of the single-impurity Anderson model,

\[
\Sigma_k = \left[ \frac{\epsilon_k}{i} \right] = -i \pi \Delta \rho(\mu) = -i \Delta
\]

for the Lorentzian case. This yields Eq. (4), which is precisely our earlier CPA result.\(^5\)

III. DISCUSSIONS

We are concerned with the particle-hole symmetric limit, i.e., \( \mu = U/2 \). In this regime, the local spectral density exhibits a three-peaked structure; a narrow Abrikosov-Suhl peak of width the Kondo temperature \( T_K = \Delta \exp[-\pi U/4\Delta] \),\(^7\) and two satellite peaks corresponding to the Hubbard subbands. The quasiparticle residue is of order \( T_K/\Delta \), and thus vanishes at the metal-insulator transition (MIT). The effective mass calculated from \( m^*/m = 1/Z \) thus diverges at the MIT. The imaginary part of the self-energy at \( \omega = \mu \) vanishes throughout the metallic phase (Fig. 4). Hence, our analysis preserves the Fermi surface, in contrast to earlier CPA-like theories.\(^8\) The intensity of the central Kondo peak is very small, in fact, it is less than 10% of the spectral weight associated with the total uncorrelated DOS. It is, however, sufficient to pin strongly the Fermi level for \( n = 1 \)
the neighborhood of unity. This metallic state is very similar to the local moment phase in the problem of a magnetic impurity in a nonmagnetic host metal.

In conclusion, we have presented a simple scheme to take into account the effects neglected in the CPA-like theories proposed earlier. Some work along these lines has been reported of late; however, these attempts are numerically cumbersome, and so hide the nature of the approximations that go into the calculations. Our analysis is sufficiently simple that the nature of the physical approximations is displayed transparently. Even though our analysis is strictly valid in the limit of infinite dimensionality, our calculation reproduces all the essential features seen in a numerical study of finite 2D lattices by Tan, Li, and Callaway. This suggests that our approach could be used to devise approximations to the 2D and 3D systems. We have considered only the paramagnetic solutions here. Study of magnetic order within this approach would require consideration of a two-particle Green's function. This is left for the future.

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\begin{thebibliography}{9}
\bibitem{4} Mukul S. Laad (unpublished).
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The earlier Hubbard approximations violate the Luttinger theorem; it has been an open question in the literature to reconcile Hubbard's decoupling approximations with Luttinger's theorem constraint. In the CPA, this constraint is violated in the metallic phase.

A. Georges and W. Krauth (unpublished). These authors use a different approach compared to ours, but find results similar to those obtained here.