Interpolating self-energy of the infinite-dimensional Hubbard model: Modifying the iterative perturbation theory

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We develop an analytical expression for the self-energy of the infinite-dimensional Hubbard model that is correct in a number of different limits. The approach represents a generalization of the iterative perturbation theory to arbitrary fillings. In the weak-coupling regime perturbation theory to second order in the interaction U is recovered. The theory is exact in the atomic limit. The high-energy behavior of the self-energy up to order $1/E^2$ and thereby the first four moments of the spectral density are reproduced correctly. Referring to a standard strong-coupling moment method, we analyze the limit $U\mapsto\infty$. Different modifications of the approach are discussed and tested by comparing with the results of an exact diagonalization study. [S0163-1829(97)02224-8]

I. INTRODUCTION

The theoretical understanding of correlated electron systems represents a central problem in condensed-matter physics. One of the simplest, but nontrivial models that describe interacting fermions on a lattice, is the Hubbard model.[1–3] It is currently studied intensively to gain insight into the fundamental mechanisms responsible for itinerant magnetism, metal-insulator (Mott) transitions, and high-temperature superconductivity. However, with the exception of the one-dimensional case,[4] an exact solution is not known, and, to our knowledge, a completely satisfactory understanding of its properties has not yet been achieved.

As was shown by Metzner and Vollhardt,[5] the Hubbard model is simplified considerably in the limit of high spatial dimensions d. However, it still remains a nontrivial model, the essential properties of which are comparable to those at low dimensions $d=2,3$. An exact solution of the $d=\infty$ Hubbard model or a reliable approximation for the entire range of the model parameters will thus provide a proper dynamical mean-field theory of the Hubbard model in any dimension.[6,7]

In the limit $d=\infty$ the Hubbard model can be mapped onto the single-impurity Anderson model (SIAM) supplemented by a self-consistency condition.[10,8,9] Thereby it becomes possible to make use of various methods that are available for impurity problems.

Using the mapping onto an effective impurity problem, essentially exact results for the infinite-dimensional Hubbard model can be obtained from quantum Monte Carlo (QMC) calculations[8,11,12] and exact diagonalization methods (ED).[13,14] However, these approaches, though exact, suffer from severe limitations. Within ED calculations one is restricted to a small number of orbitals, and thus a smooth density of states cannot be obtained. On the other hand, QMC yields its results for the discrete Matsubara energies or along the imaginary time axis. Therefore, it is difficult to access the low-temperature regime where statistical errors become important within the QMC method. Furthermore, to obtain dynamical quantities such as the density of states, the analytical continuation to the real axis becomes necessary, which cannot be performed reliably in all cases. For these reasons the application of approximate methods for the infinite-dimensional Hubbard model still remains necessary.

The development of approximate methods should be guided by exactly solvable limiting cases and other rigorous analytical results available. Such information imposes a number of strong necessary conditions on any approximation. Moreover, comparison with the numerically exact results of ED or QMC techniques allows for a judgment of the quality of the approximation a posteriori.

For the SIAM, weak-coupling approaches are known to yield reliable quantitative information.[15–18] As has been demonstrated by Yosida and Yamada,[15,16] perturbation theory in U is quite well behaved for the symmetric case when expanding around the Hartree-Fock solution.

Based on these findings, Georges and Kotliar[10] introduced a method called iterative perturbation theory (IPT) for the $d=\infty$ Hubbard model at half-filling ($n=1$). Within IPT the SIAM is solved by means of second-order perturbation theory around the Hartree-Fock solution (SOPT-HF) for arbitrary hybridization functions followed by the self-consistent mapping onto the Hubbard model. IPT leads to convincing results as has been proven by comparison with ED and QMC studies.[19–21] Furthermore, a direct treatment of zero temperature and real energies is possible. The method turns out to be superior to the direct application of SOPT-HF to the Hubbard model. The latter does not yield a metal-insulator transition, and Fermi-liquid behavior never breaks down.[22]

The success of IPT may be partly due to the fact that at $n=1$ the perturbational treatment accidentally reproduces the atomic limit. Away from half-filling this desirable property is lost, and (the naive extension of) IPT is known to give unphysical results.

In a recent paper[23] Kajueter and Kotliar proposed a modification of the IPT scheme introducing an interpolating self-energy for the SIAM (see also Refs. 24 and 25). The self-energy exactly reproduces the trivially solvable limiting cases of vanishing interaction, $U=0$, of the completely filled and the empty band (chemical potential $\mu\mapsto\pm\infty$), and the atomic limit. For small U it is exact up to order U^2. The low-energy behavior ($E\mapsto 0$) is fixed by imposing the Friedel sum rule[26] (equivalently, the Luttinger theorem[27,28]). At

half-filling the approach reduces to the usual IPT. Finally, the self-energy has the correct asymptotic form for high energies $E \mapsto \infty$: the first two coefficients within an expansion in $1/E$ are reproduced exactly. Results for the spectral density and the integrated spectral weight based on the approach have been compared with ED calculations, and a rather convincing agreement between both methods has been observed indeed.[23]

The correct high-energy behavior may be quite important, since this is closely connected with the moments of the spectral density.[29] The moments are defined by

$$M_{d\sigma}^{(m)} = \frac{1}{\hbar} \int_{-\infty}^{\infty} E^m A_{d\sigma}(E) dE, \tag{1}$$

where $A_{d\sigma}$ denotes the one-electron spectral density of the localized (d) state in the SIAM. The moments can be calculated from the Hamiltonian directly.[30] With increasing m, however, they include equal-time correlation functions of higher and higher order. This fact limits the number of moments that can be used in practice for the determination of the high-energy behavior of the self-energy.

In their recent approach, Kajueter and Kotliar could take into account exactly the moments up to $m=2$. The main purpose of this paper is to demonstrate that improvement is still possible. Modifying their approach, we will show that a self-energy function can be constructed that respects the $m=3$ moment additionally, while all other mentioned limiting cases are still recovered as before. Thereby, higher-order correlation functions enter the theory. As will be shown, these can be expressed without further approximations in terms of the one-electron spectral density and can thus be determined self-consistently. Our analysis stresses the importance of this $m=3$ moment, especially what concerns spontaneous magnetism.

The interpolating self-energy for the SIAM is exact in the case of small U and in the atomic limit; to see whether it can be considered as a reasonable interpolation between the weak- and the strong-coupling regime, we furthermore investigate (analytically) the limit $U \mapsto \infty$. Contact is made with a standard strong-coupling moment method [the spectral-density approach (SDA)].[31–34] The SDA, within the context of the Hubbard model, has proven its usefulness in several previous studies. Thereby, we can provide an additional independent justification for the interpolating self-energy.

The theory is evaluated numerically. Different versions of the approach are tested, which are all compatible with the mentioned limiting cases. Finally, we compare with the results of an exact diagonalization study from Ref. 23.

II. MAPPING ONTO SIAM

To begin with, we briefly recall the procedure by which the Hubbard model can be mapped onto the SIAM and introduce some basic notations.

The Hubbard model reads

$$H = \sum_{ij\sigma} (T_{ij} - \mu \delta_{ij}) c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}. \tag{2}$$

We consider a d-dimensional lattice with hopping between nearest neighbors. Provided that the hopping integrals are scaled appropriately, $T_{\langle ij \rangle} = t = t^*/(2\sqrt{d})$ ($t^* = \text{const}$), a nontrivial model is obtained in the limit $d \mapsto \infty$.[5] The (noninteracting) Bloch density of states for the $d=\infty$ simple cubic lattice is a Gaussian;[5] a semielliptic Bloch density of states is obtained for the Bethe lattice with infinite coordination number.[35]

The basic quantity to be calculated within the model is the one-electron Green function

$$G_{ij\sigma}(E) = \langle\langle c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\rangle_E. \tag{3}$$

Its diagonal elements can be written in the form

$$G_{\sigma}(E) \equiv G_{ii\sigma}(E) = \int_{-\infty}^{\infty} \frac{\hbar \rho^{(\mathrm{B})}(z)}{E - (z-\mu) - \Sigma_{\sigma}(E)} dz. \tag{4}$$

For $d \mapsto \infty$ the self-energy of the Hubbard model, $\Sigma_{\sigma}(E)$, becomes $\mathbf{k}$ independent or site-diagonal.[5,28,36]

The Anderson model for a single impurity (SIAM) is given by

$$H_{\mathrm{SIAM}} = \sum_{k\sigma} (\epsilon_k - \mu) c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{\sigma} (\epsilon_d - \mu) c_{d\sigma}^{\dagger} c_{d\sigma} + U n_{d\sigma} n_{d-\sigma} + \sum_{k\sigma} V_{kd} (c_{d\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} c_{d\sigma}). \tag{5}$$

In all practical calculations the hybridization strength between the conduction band and the localized d level, V_{kd}, enters via the the hybridization function which is defined by

$$\Delta(E) = \sum_k \frac{V_{kd}^2}{E - \epsilon_k}. \tag{6}$$

Let us also introduce the impurity Green function:

$$G_{d\sigma}(E) = \langle\langle c_{d\sigma}; c_{d\sigma}^{\dagger} \rangle\rangle_E. \tag{7}$$

From its equation of motion we immediately have

$$G_{d\sigma}(E) = \frac{\hbar}{E - (\epsilon_d - \mu) - \Delta(E+\mu) - \Sigma_{d\sigma}(E)}, \tag{8}$$

where $\Sigma_{d\sigma}(E)$ is the d-level self-energy.

While in the $d=\infty$ limit of the Hubbard model all spatial degrees of freedom are frozen, the local (temporal) fluctuations still constitute a nontrivial problem. This, however, is equivalent to the SIAM. The Hubbard model and the SIAM can be connected by the following self-consistency condition:[8–10]

$$\Delta_{\sigma}(E+\mu) = E - (\epsilon_d - \mu) - \Sigma_{\sigma}(E) - \hbar (G_{\sigma}(E))^{-1}. \tag{9}$$

Δ has to be interpreted as an effective hybridization function that provides a coupling of the d level to the external bath of conduction electrons that simulates all temporal degrees of freedom in the Hubbard model. In the case of a ferromagnetic phase, the hybridization function must be spin dependent. Provided that the condition (9) is fulfilled, the self-energy of the Hubbard model is identical with the d-level self-energy of the impurity problem, $\Sigma_{\sigma}(E) = \Sigma_{d\sigma}(E)$. This also implies the corresponding identity between the respective Green functions: $G_{\sigma}(E) = G_{d\sigma}(E)$.

If one is able to solve the SIAM for arbitrary hybridization functions $\Delta_{\sigma}(E)$, the following two-step procedure for

solving the $d=\infty$ Hubbard model is suggested:[8–10] Given a hybridization function, we calculate (by solving the SIAM) the self-energy $\Sigma_{d\sigma}(E)$ in the first step. In the second step, using Eqs. (4) and (9), a new hybridization function is generated. Both steps are iterated until self-consistency is achieved.

In the following we concentrate on the first step, which represents the actual problem. We intend to derive an analytical expression for the self-energy of the SIAM that respects various exactly solvable limiting cases and other rigorous facts available.

III. SPECTRAL MOMENTS

The overall shape of the one-electron spectral density,

$$A_{d\sigma}(E)=-\frac{1}{\pi}\mathrm{Im}G_{d\sigma}(E+i0), \tag{10}$$

is fixed by their low-order spectral moments to a large extent. The definition of the moments is given in Eq. (1). A completely equivalent but independent representation is easily derived using the Heisenberg equation of motion for the time-dependent operators in the definition of the spectral density. We obtain

$$M_{d\sigma}^{(m)}=\langle[\mathcal{L}^m c_{d\sigma},c_{d\sigma}^{\dagger}]_+\rangle, \tag{11}$$

where $\mathcal{L}\mathcal{O}=[\mathcal{O},H_{\mathrm{SIAM}}]_-$ denotes the commutator of an operator $\mathcal{O}$ with the Hamiltonian, and $[,]_+$ is the anticommutator. The straightforward calculation up to $m=3$ yields

$$\begin{aligned}
M_{d\sigma}^{(0)}&=1,\\
M_{d\sigma}^{(1)}&=\tilde{\epsilon}_d+U\langle n_{d-\sigma}\rangle,\\
M_{d\sigma}^{(2)}&=\tilde{\epsilon}_d^2+2\tilde{\epsilon}_d U\langle n_{d-\sigma}\rangle+U^2\langle n_{d-\sigma}\rangle+\sum_k V_{kd}^2,\\
M_{d\sigma}^{(3)}&=\tilde{\epsilon}_d^3+3\tilde{\epsilon}_d^2 U\langle n_{d-\sigma}\rangle+\tilde{\epsilon}_d U^2\langle n_{d-\sigma}\rangle(2+\langle n_{d-\sigma}\rangle)\\
&\quad+U^3\langle n_{d-\sigma}\rangle+\sum_k V_{kd}^2(\tilde{\epsilon}_k+2\tilde{\epsilon}_d+2U\langle n_{d-\sigma}\rangle)\\
&\quad+U^2\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle)\tilde{B}_{d-\sigma}.
\end{aligned} \tag{12}$$

Here we have defined $\tilde{\epsilon}_{d,k}=\epsilon_{d,k}-\mu$, $\tilde{B}_{d\sigma}=B_{d\sigma}-\mu$, and

$$\tilde{B}_{d\sigma}=\tilde{\epsilon}_d+\frac{1}{\langle n_{d\sigma}\rangle(1-\langle n_{d\sigma}\rangle)}\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}c_{d\sigma}(2n_{d-\sigma}-1)\rangle. \tag{13}$$

We notice that the $m=3$ moment includes higher-order correlation functions.

We can use these explicit results for the moments to fix the high-energy behavior of the self-energy. For this purpose we consider the following representation of the d Green function:

$$G_{d\sigma}(E)=\int_{-\infty}^{\infty}\frac{A_{d\sigma}(E')}{E-E'}dE'. \tag{14}$$

Expanding the denominator in powers of $1/E$, we get

$$G_{d\sigma}(E)=\sum_{m=0}^{\infty}\frac{\hbar}{E^{m+1}}M_{d\sigma}^{(m)}. \tag{15}$$

The coefficients in the $1/E$ expansion of the self-energy,

$$\Sigma_{d\sigma}(E)=\sum_{m=0}^{\infty}\frac{1}{E^m}C_{d\sigma}^{(m)}, \tag{16}$$

can be obtained by inserting Eqs. (15) and (16) and the analogous expansion to the hybridization function into Eq. (8):

$$\begin{aligned}
C_{d\sigma}^{(0)}&=U\langle n_{d-\sigma}\rangle,\\
C_{d\sigma}^{(1)}&=U^2\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle),\\
C_{d\sigma}^{(2)}&=U^2\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle)[\tilde{B}_{d-\sigma}+U(1-\langle n_{d-\sigma}\rangle)].
\end{aligned} \tag{17}$$

An approximate expression for the self-energy of the SIAM should be consistent with this rigorously derived high-energy behavior.

The Hartree-Fock approximation for the self-energy,

$$\Sigma_{d\sigma}^{(0)}(E)=U\langle n_{d-\sigma}\rangle, \tag{18}$$

only respects the zeroth-order coefficient in the high-energy expansion. The zeroth and the first coefficient are reproduced by the self-energy

$$\Sigma_{d\sigma}^{(1)}(E)=U\langle n_{d-\sigma}\rangle+\frac{U^2\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle)}{E+\mu-\epsilon_d-U(1-\langle n_{d-\sigma}\rangle)}, \tag{19}$$

which is obtained when applying the Hartree-Fock decoupling scheme not at the first but at the second level in the hierarchy of equations of motion for the Green function. This is analogous to the ''Hubbard-I'' approximation[1] within the context of the Hubbard model. The simplest form of a self-energy that implies the correct expansion coefficients up to order $1/E^2$ is given by

$$\Sigma_{d\sigma}^{(2)}(E)=U\langle n_{d-\sigma}\rangle+\frac{U^2\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle)}{E+\mu-B_{d-\sigma}-U(1-\langle n_{d-\sigma}\rangle)}. \tag{20}$$

The higher-order correlation functions included in $B_{d\sigma}$ have to be determined self-consistently as well as the mean occupation numbers $\langle n_{d\sigma}\rangle$. Both $\Sigma^{(1)}$ and $\Sigma^{(2)}$ are correct in the atomic limit. $B_{d\sigma}$ reduces to ϵ_d in this case, and $\Sigma^{(1)}$ just coincides with the self-energy of the atomic limit.

The self-energy (20) is the result found within the SDA.[31–34] Actually, the SDA is a standard strong-coupling approach to the Hubbard model. Its main idea is to start from a two-pole ansatz for the spectral density and to fix all parameters in the ansatz such that the moments (up to $m=3$) are correct. Recent investigations of the $d=2$ Hubbard model[37,38] point out that the results of the SDA are identical to those of the Roth approach[39] and the Mori-Zwanzig projection technique.[40,41] All methods yield a two-pole structure for the interacting Green function. Neglecting quasiparticle damping (for damping effects cf. Ref. 42), this two-pole

structure can be made plausible for the strong-coupling regime: an analysis of Harris and Lange[43] rigorously shows that additional structures merely have a spectral weight of the order $(t/U)^4$ or less. It is remarkable that such a simple form (20) of the self-energy is able to reproduce at least qualitatively the correct dispersion of the Hubbard bands. This has been proven for the $d=2$ case by comparisons[37,38] with QMC (Refs. 44 and 45) and with ED calculations[46] on small square Hubbard arrays. We thus believe that the step going from the Hubbard-I solution [Eq. (19)] to a solution [Eq. (20)] that respects the $m=3$ moment additionally is quite important, at least for $U\mapsto\infty$. It is even decisive if spontaneous magnetism is considered as it is known that Hubbard's original solution predicts magnetic order only under extreme circumstances.[1] Within the SDA the spin dependence of B_σ induces a spin-dependent shift of the bands that favors magnetism. Indeed, the results for the ferromagnetic and antiferromagnetic Hubbard models seem to be qualitatively correct.[47] On the other hand, the SDA completely fails to reproduce Fermi-liquid behavior for small U. At half-filling it predicts an insulator for each $U>0$ and thereby is not able to describe the Mott transition as well. Apart from the neglection of quasiparticle damping, however, the SDA yields plausible results for $U\mapsto\infty$.

The conclusion from the preceding discussion should be that it may be quite important to account for the $m=3$ moment, especially what concerns spontaneous magnetism. This will guide our search for an approximate self-energy in the case of the SIAM, which can be identified with the self-energy of the $d=\infty$ Hubbard model via the self-consistent mapping.

IV. MODIFICATION OF IPT

Our approach is a modification of the IPT.[10] Within the usual IPT the SIAM is solved by means of perturbation theory up to second order in the coupling U. The self-energy is given by

$$\Sigma_{d\sigma}^{(\mathrm{IPT})}(E)=U\langle n_{d-\sigma}\rangle+\Sigma_{d\sigma}^{(\mathrm{SOC})}(E). \tag{21}$$

The first-order term is the Hartree-Fock (HF) self-energy; the second-order contribution (SOC) reads

$$\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)=\frac{U^2}{\hbar^3}\int\int\int\frac{A_{d\sigma}^{(\mathrm{HF})}(x)A_{d-\sigma}^{(\mathrm{HF})}(y)A_{d-\sigma}^{(\mathrm{HF})}(z)}{E-x+y-z}\times[f(x)f(-y)f(z)+f(-x)f(y)f(-z)]\times dxdydz. \tag{22}$$

Here $f(x)=1/[\exp(\beta x)+1]$ is the Fermi function, and $\beta=1/k_BT$. The Hartree-Fock spectral density

$$A_{d\sigma}^{(\mathrm{HF})}(E)=-\frac{1}{\pi}\mathrm{Im}G_{d\sigma}^{(\mathrm{HF})}(E+i0) \tag{23}$$

is obtained from

$$G_{d\sigma}^{(\mathrm{HF})}(E)=\frac{\hbar}{E-(\epsilon_d-\tilde{\mu}_\sigma)-\Delta_\sigma(E+\mu)-U\langle n_{d-\sigma}\rangle}. \tag{24}$$

The parameter $\tilde{\mu}_\sigma$ has been introduced for later purposes. Within IPT we have $\tilde{\mu}_\sigma=\mu$.

Following Kajueter and Kotliar,[23] we consider an ansatz for the self-energy:

$$\Sigma_{d\sigma}(E)=U\langle n_{d-\sigma}\rangle+\frac{a_\sigma\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)}{1-b_\sigma\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)}. \tag{25}$$

a_σ, b_σ, and $\tilde{\mu}_\sigma$ are treated as free parameters, which will be fixed such that the approximation becomes exact in a number of limiting cases. It is assumed that Eq. (25) provides a reasonable interpolation between the different limits.

In Ref. 23 Kajueter and Kotliar determined the parameter a_σ to get the correct $m=2$ moment of the resulting spectral density and the parameter b_σ to get the correct result for the atomic limit. Here, in contrast a_σ and b_σ will be fitted to the $m=2$ and to the $m=3$ moments.

This can be performed straightforwardly: We start by expanding the denominator in Eq. (22) in powers of $1/E$ to obtain the high-energy behavior of $\Sigma_{d\sigma}^{(\mathrm{SOC})}$:

$$\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)=\sum_{m=1}^{\infty}\frac{1}{E^m}D_{d\sigma}^{(m)}, \tag{26}$$

where the coefficients are given by

$$D_{d\sigma}^{(1)}=U^2\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})$$

$$D_{d\sigma}^{(2)}=U^2\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})(B_{d-\sigma}^{(\mathrm{HF})}-\tilde{\mu}_\sigma+U\langle n_{d-\sigma}\rangle). \tag{27}$$

Here

$$\langle n_{d\sigma}\rangle^{(\mathrm{HF})}=\frac{1}{\hbar}\int_{-\infty}^{\infty}f(E)A_{d\sigma}^{(\mathrm{HF})}(E)dE \tag{28}$$

is a fictive (Hartree-Fock) particle number, and

$$B_{d\sigma}^{(\mathrm{HF})}=\epsilon_d+\frac{1}{\langle n_{d\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d\sigma}\rangle^{(\mathrm{HF})})}\sum_k V_{kd}\langle c_{k\sigma}^\dagger c_{d\sigma}\rangle^{(\mathrm{HF})}\times(2\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}-1) \tag{29}$$

is the Hartree-Fock value of the higher-order correlation functions defined in Eq. (13). Comparing with the exact coefficients given in Eq. (17), we notice that the IPT self-energy $\Sigma_{d\sigma}^{(\mathrm{IPT})}$ does not have the correct high-energy behavior away from half-filling.

From the equation of motion for the Green function $\langle\langle c_{d\sigma};c_{k\sigma}^\dagger\rangle\rangle^{(\mathrm{HF})}$ it can be seen that the hybridization-induced correlation functions in the definition of $B_{d\sigma}^{(\mathrm{HF})}$ can be expressed in terms of the localized HF Green function:

$$\sum_k V_{kd}\langle c_{k\sigma}^\dagger c_{d\sigma}\rangle^{(\mathrm{HF})}=-\frac{1}{\pi\hbar}\mathrm{Im}\int_{-\infty}^{\infty}f(E)\Delta_\sigma(E+i0+\mu)\times G_{d\sigma}^{(\mathrm{HF})}(E+i0)dE. \tag{30}$$

The high-energy behavior of the interpolating self-energy can be derived from the expansion (26) and from Eq. (25).

Comparing with the exact coefficients of the $1/E$ expansion in Eq. (17) again, we have to choose

$$a_\sigma=\frac{\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle)}{\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})} \tag{31}$$

and

$$b_\sigma=\frac{B_{d-\sigma}-\mu-B_{d-\sigma}^{(\mathrm{HF})}+\tilde{\mu}_\sigma+U(1-2\langle n_{d-\sigma}\rangle)}{U^2\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})} \tag{32}$$

to ensure the correct high-energy behavior of the self-energy $\Sigma_{d\sigma}$ and thereby the correct moments of the resulting spectral density up to $m=3$. The result (31) and (32) reduces to the approach of Ref. 23 if $B_{d\sigma}$ and $B_{d\sigma}^{(\mathrm{HF})}$ are replaced by ϵ_d.

It is easily verified that our approach is correct in the atomic limit. Setting $V_{kd}=0$, the Hartree-Fock spectral density (23) reduces to a δ function, which allows one to calculate the second-order contribution (22) and thus the self-energy (25) immediately. It turns out to coincide with the self-energy of the atomic limit (19).

Next, we have to check the weak-coupling limit: provided that the parameter $\tilde{\mu}_\sigma$ is chosen such that $\tilde{\mu}_\sigma\mapsto\mu_0\equiv\mu|_{U=0}$ for $U\mapsto 0$ (see below), we have $\langle n_{d\sigma}\rangle\mapsto\langle n_{d\sigma}\rangle$ for $U\mapsto 0$. Furthermore, since $B_{d\sigma}\mapsto B_{d\sigma}^{(\mathrm{HF})}$ as $U\mapsto 0$, we have $b_\sigma\sim 1/U$. Therefore, expanding the self-energy (25) in powers of U, we see that it is correct up to order U^2 indeed. In particular, this implies that all Fermi-liquid properties as described in Ref. 28 will be recovered for small U at least.

Finally, the parameter $\tilde{\mu}_\sigma$ has to be fixed. The most natural choice is the following:

$$\tilde{\mu}_\sigma=\mu. \tag{33}$$

Another possibility is due to an approach of Martin-Rodero *et al.*[24,25] where $\tilde{\mu}_\sigma$ is determined from the condition

$$\langle n_{d\sigma}\rangle^{(\mathrm{HF})}=\langle n_{d\sigma}\rangle. \tag{34}$$

In Ref. 23 Kajueter and Kotliar imposed the Friedel sum rule[26] as a condition to fix $\tilde{\mu}_\sigma$. Via the self-consistency condition (9) this is equivalent to the Luttinger theorem,[27] which in the case of the $d=\infty$ Hubbard model reads[28]

$$\mu=\mu_0+\Sigma_\sigma(0). \tag{35}$$

Let us briefly discuss the implications of the different choices. First we notice that in all cases we have $\tilde{\mu}_\sigma\mapsto\mu_0$ for $U\mapsto 0$ as it must be to ensure the correct weak-coupling behavior of the self-energy. Furthermore, the validity of the approach within all other limiting cases that have been considered is not affected by the condition chosen.

Inspecting the original derivation in Ref. 27, we recall that the validity of the Luttinger theorem depends on a number of presuppositions. For example, the theorem holds if perturbation theory applies. Obviously, for small U all conditions (33)–(35) yield a theory that is compatible with the Luttinger theorem up to order U^2 at least. Here, another supposition is more important, namely, $\mathrm{Im}\Sigma_\sigma(E)=0$ at $E=0$. In particular, this implies $T=0$.[50] Therefore, applying the third condition (35) does not allow one to consider finite temperatures. On the other hand, the conditions (33) and (34) do not suffer from this difficulty.

The second condition (34) implies (for a constant hybridization function Δ_σ) that $\tilde{\mu}_\sigma=\mu_0+U\langle n_{d-\sigma}\rangle$. This exactly compensates the energetic shift of the Hartree-Fock Green function (24) by $U\langle n_{d-\sigma}\rangle$. $G_{d\sigma}^{(\mathrm{HF})}$ thereby becomes independent of U, and $\Sigma_{d\sigma}^{(\mathrm{SOC})}$ reduces to the second-order contribution from a weak-coupling theory in which the *free* ($U=0$) instead of the HF d Green function is used in the calculation of the proper irreducible self-energy. This, however, must not be confused with the plain (or conventional) weak-coupling theory, where the free chemical potential μ_0 would have to be replaced by μ additionally and which artificially breaks particle-hole symmetry.[48] The second-order contribution within SOPT-HF is recovered only when using the first condition (33). Arguments in favor or against a particular weak-coupling approach have previously been developed by demanding the correct high-energy behavior (up to order $1/E$).[10,19] Such reasoning, however, is not meaningful in the present context since the correct high-energy behavior (up to order $1/E^2$) is reproduced in each case.

Let us mention that choosing $\tilde{\mu}_\sigma=\mu$ (first condition) introduces a slight complication: Because of the shift of $G_{d\sigma}^{(\mathrm{HF})}$ by the HF contribution $U\langle n_{d-\sigma}\rangle$, it may happen that $\langle n_{d\sigma}\rangle^{(\mathrm{HF})}=0$ (or $\langle n_{d\sigma}\rangle^{(\mathrm{HF})}=1$) for strong U and $T=0$, which means that the parameters a_σ and b_σ are no longer well defined. However, within the limit $\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}\mapsto 0$ (or $\mapsto 1$) we have

$$\frac{\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)}{\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})}$$

$$\mapsto\frac{U^2}{\hbar^3}\int\int\int\frac{A_{d\sigma}^{(\mathrm{HF})}(x)A_{d-\sigma}^{(\mathrm{HF})}(y)A_{d-\sigma}^{(\mathrm{HF})}(z)}{E-x+y-z}dxdydz. \tag{36}$$

Therefore, although a_σ and b_σ diverge, the interpolating self-energy remains finite.

So far it can be concluded that there are no differences between the three possibilities considered that are *crucial*. However, we notice that the third condition implies a restriction of the theory to zero temperature. We defer further discussion to Secs. VII and VIII.

V. SELF-CONSISTENT DETERMINATION OF HIGHER CORRELATION FUNCTIONS

The definition of the parameter b_σ involves the band filling $\langle n_{d\sigma}\rangle$ and the higher-order correlation functions included in $B_{d\sigma}$, which are still unknown. A satisfactory theory cannot be constructed unless it is possible to determine these correlation functions without further approximations. No problems are introduced for the band filling that may be expressed in terms of the spectral density:

$$\langle n_{d\sigma}\rangle=\frac{1}{\hbar}\int_{-\infty}^{\infty}f(E)A_{d\sigma}(E)dE. \tag{37}$$

In the following we demonstrate that also $B_{d\sigma}$ can be reduced to the spectral density or the Green function, respectively. According to its definition, $B_{d\sigma}$ partly consists of a sum of one-particle correlation functions. Applying the general spectral theorem[51] and exploiting the equation of motion for the Green function $\langle\langle c_{d\sigma};c_{k\sigma}^{\dagger}\rangle\rangle$, we have

$$\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}c_{d\sigma}\rangle = -\frac{1}{\pi\hbar}\mathrm{Im}\int_{-\infty+i0}^{\infty+i0} f(E) \times \Delta_{\sigma}(E+\mu)G_{d\sigma}(E)dE. \quad (38)$$

Now we are left with the higher-order correlation functions only. Using the commutator

$$[c_{d\sigma},H]_- = \tilde{\epsilon}_d c_{d\sigma} + U c_{d\sigma}n_{d-\sigma} + \sum_p V_{pd}c_{p\sigma}, \quad (39)$$

the remaining terms in $B_{d\sigma}$ can be written in the form

$$\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}c_{d\sigma}n_{d-\sigma}\rangle = -\frac{\tilde{\epsilon}_d}{U}\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}c_{d\sigma}\rangle - \frac{1}{U}\sum_{kp} V_{kd}V_{pd}\langle c_{k\sigma}^{\dagger}c_{p\sigma}\rangle + \frac{1}{U}\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}[c_{d\sigma},H]_-\rangle. \quad (40)$$

The first term on the right-hand side has just been treated above. Using the spectral theorem and the equation of motion, one gets for the second one:

$$\sum_{kp} V_{kd}V_{pd}\langle c_{k\sigma}^{\dagger}c_{p\sigma}\rangle = -\frac{1}{\pi\hbar}\mathrm{Im}\int_{-\infty+i0}^{\infty+i0} f(E)\Delta_{\sigma}(E+\mu) \times [\Delta_{\sigma}(E+\mu)G_{d\sigma}(E)+\hbar]dE. \quad (41)$$

Applying once more the general spectral theorem, performing a Fourier transformation to the time representation, and using the Heisenberg equation of motion, the third term can be written as

$$\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}[c_{d\sigma},H]_-\rangle = \sum_k V_{kd}\left(-\frac{1}{\pi\hbar}\right)\mathrm{Im}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(E)e^{iE(t-t')/\hbar}\left(i\hbar\frac{\partial}{\partial t}\right) \times \langle\langle c_{d\sigma}(t);c_{k\sigma}^{\dagger}(t')\rangle\rangle d(t-t')dE. \quad (42)$$

Integration by part and back transformation to energy representation finally yields

$$\sum_k V_{kd}\langle c_{k\sigma}^{\dagger}[c_{d\sigma},H]_-\rangle = -\frac{1}{\pi\hbar}\mathrm{Im}\int_{-\infty+i0}^{\infty+i0} f(E) \times E\Delta_{\sigma}(E+\mu)G_{d\sigma}(E)dE. \quad (43)$$

Combining all results, we obtain

$$\langle n_{d\sigma}\rangle(1-\langle n_{d\sigma}\rangle)\tilde{B}_{d\sigma} = \langle n_{d\sigma}\rangle(1-\langle n_{d\sigma}\rangle)\tilde{\epsilon}_d - \frac{1}{\pi\hbar}\mathrm{Im}\int_{-\infty+i0}^{\infty+i0} f(E)\Delta_{\sigma}(E+\mu) \times \left(\frac{2}{U}\Sigma_{d\sigma}(E)-1\right)G_{d\sigma}(E)dE, \quad (44)$$

where once more we exploited the equation of motion for $G_{d\sigma}$. This completes the theory since $\langle n_{\sigma}\rangle$ and $B_{d\sigma}$ can be determined self-consistently from the d Green function.

VI. STRONG-COUPLING LIMIT

So far we have shown that the appropriate choice of the parameters a_{σ} and b_{σ} in the ansatz (25) yields a self-energy that is exact in a number of limiting cases, namely, trivially for $U=0$, for $\langle n_{d\sigma}\rangle=0$ and $\langle n_{d\sigma}\rangle=1$ and furthermore in the atomic limit and for small U up to order U^2. The high-energy expansion yields the correct coefficients up to order $(1/E)^2$. Thereby the first moments of the spectral density up to $m=3$ are reproduced exactly, which is one additional moment compared with the approach of Kajueter and Kotliar.[23]

It is easily shown that the general particle-hole symmetry requires $B_{d\sigma}$ to be zero at half-filling in the paramagnetic phase (and for a symmetric Bloch density of states). Since in this case $B_{d\sigma}^{(\mathrm{HF})}=0$ and $\mu=\tilde{\mu}_{\sigma}=U/2$, it follows that $b_{\sigma}=0$. Consequently, the theory reduces to the conventional IPT for $\langle n_{d\sigma}\rangle=\langle n_{d-\sigma}\rangle=0.5$.

We now turn to the strong-coupling case $U\mapsto\infty$ in order to check whether the theory can be regarded as a reasonable interpolation between the weak- and the strong-coupling regime. In the following we exclusively focus on the SIAM; any approach that uses the self-consistent mapping of the Hubbard model onto the SIAM can only be as reliable as the approximation employed for the solution of the latter. Hence, for the present purposes the hybridization function Δ can be assumed to be independent of U.

Let us consider the first condition (33) for determining the fictive chemical potential, i.e., $\tilde{\mu}_{\sigma}=\mu$. As mentioned above, for small U all Fermi-liquid properties are recovered. For large U the spectral density $A_{d\sigma}$ is expected to consist roughly of two dominant features separated by U at about ϵ_d and ϵ_d+U. Assuming $\langle n_{d\sigma}\rangle=\langle n_{d-\sigma}\rangle<0.5$ for simplicity, the chemical potential will be located within the lower part: $\mu\sim\epsilon_d$. Looking at the HF Green function (24), we notice that $\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}=0$ for $T=0$ and for U larger than a certain critical value U_{c1}, and thus the relation (36) applies. In particular, at the Fermi edge $E=0$,

$$-\frac{1}{\pi}\mathrm{Im}\frac{\Sigma_{d\sigma}^{(\mathrm{SOC})}(i0)}{\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})} = \frac{U^2}{\hbar^3}\int\int A_{d\sigma}^{(\mathrm{HF})}(x)A_{d-\sigma}^{(\mathrm{HF})}(y)A_{d-\sigma}^{(\mathrm{HF})}(y-x)dxdy. \quad (45)$$

A simple analysis shows this twofold convolution integral to be nonzero for interactions U smaller than another critical value U_{c2} ($>U_{c1}$). Via Eq. (25) this implies a nonzero value of the imaginary part of the interpolating self-energy at

$E=0$. For $U>U_{c2}$ we have $\mathrm{Im}\Sigma_{d\sigma}(E)\equiv 0$ in the vicinity of $E=0$. Therefore, non-Fermi-liquid behavior is implied for all $U>U_{c1}$.

On the contrary, at $T=0$ the second condition (34) yields $\mathrm{Im}\Sigma_{d\sigma}(E)\sim E^2$ for $E\mapsto 0$ irrespective of the value for U.

Some more statements can be made if $U\mapsto\infty$. For this purpose we first determine the total weight and the center of gravity of the imaginary part of the second-order contribution $\Sigma_{d\sigma}^{(\mathrm{SOC})}$. Let us consider the integral

$$\int_{-\infty}^{\infty} E^m\left(-\frac{1}{\pi}\right)\mathrm{Im}\Sigma_{d\sigma}^{(\mathrm{SOC})}(E+i0)\,dE, \tag{46}$$

for $m=0,1$. Since $\Sigma_{d\sigma}^{(\mathrm{SOC})}$ is analytical in the upper half of the complex E plane, the contour along the real axis can be deformed into a contour C where each point of C has a distance from 0 that is larger than R and $R\mapsto\infty$. On the contour C one is allowed to replace $\Sigma_{d\sigma}^{(\mathrm{SOC})}$ by its asymptotic form (26). After that C can be redeformed into an integration along the real axis and the evaluation of the integral becomes trivial. The total weight and the center of gravity turn out to be $D_{d\sigma}^{(1)}$ and $D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}$, respectively, where $D_{d\sigma}^{(m)}$ are the coefficients from the expansion (26). Analogously, the total weight and the center of gravity of $-\mathrm{Im}\Sigma_{d\sigma}(E)/\pi$ are given in terms of its $1/E$ expansion coefficients as $C_{d\sigma}^{(1)}$ and $C_{d\sigma}^{(2)}/C_{d\sigma}^{(1)}$.

At energies with $|E-D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}|\mapsto\infty$, the imaginary part of the second-order contribution vanishes, and the real part approaches:

$$\mathrm{Re}\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)\mapsto\frac{D_{d\sigma}^{(1)}}{E-D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}}. \tag{47}$$

Now let us *assume* that there is a zero $E=E_\sigma^{(0)}$ of the denominator in Eq. (25),

$$1-b_\sigma\Sigma_{d\sigma}^{(\mathrm{SOC})}(E_\sigma^{(0)})=0, \tag{48}$$

at a sufficiently high energy; i.e., we assume that

$$|E_\sigma^{(0)}-D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}|\mapsto\infty \tag{49}$$

for $U\mapsto\infty$. This implies that the imaginary part of the interpolating self-energy

$$-\frac{1}{\pi}\mathrm{Im}\Sigma_{d\sigma}(E+i0)=\frac{a_\sigma}{\pi|b_\sigma|}\,\frac{-|b_\sigma|\mathrm{Im}\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)}{[1-b_\sigma\mathrm{Re}\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)]^2+[-|b_\sigma|\mathrm{Im}\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)]^2} \tag{50}$$

has a δ singularity at $E=E_\sigma^{(0)}$. Using Eq. (47) we can derive the asymptotic position

$$E_\sigma^{(0)}\mapsto B_{d-\sigma}-\mu+U(1-\langle n_{d-\sigma}\rangle) \tag{51}$$

and the asymptotic weight of the δ function:

$$-\frac{1}{\pi}\mathrm{Im}\Sigma_{d\sigma}(E+i0)\mapsto U^2\langle n_{d-\sigma}\rangle(1-\langle n_{d-\sigma}\rangle)\,\delta(E-E_\sigma^{(0)}). \tag{52}$$

The weight turns out to be equal to the *full* weight $C_{d\sigma}^{(1)}$ of $-\mathrm{Im}\Sigma_{d\sigma}(E)/\pi$. Subject to the assumption (49), Eq. (52) tells us that the weight of the δ peak at $E_\sigma^{(0)}$ will dominate $\mathrm{Im}\Sigma_{d\sigma}(E)$ eventually. The real part can be obtained from a Kramers-Kronig-type relation

$$\mathrm{Re}\Sigma_{d\sigma}(E)=U\langle n_{d-\sigma}\rangle-\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\Sigma_{d\sigma}(E'+i0)}{E-E'}dE'. \tag{53}$$

It turns out that it is given by $\Sigma_{d\sigma}^{(2)}(E)$, which is just the self-energy of the SDA [cf. Eq. (20)].

Equation (50) shows that the imaginary part of the interpolating self-energy is nonvanishing at $E=E_\sigma^{(0)}$ as well as at those energies E where $\mathrm{Im}\Sigma_{d\sigma}^{(\mathrm{SOC})}(E)\neq 0$, i.e., within a certain energy interval around $D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}$. We can thus consider $\Sigma_{d\sigma}(E)$ to consist of two additive parts. The dominating part of the self-energy has been identified as being equal to the self-energy of the SDA. The remaining part does not vanish as $U\mapsto\infty$ as can be seen when expanding the interpolating self-energy (25) in powers of $1/U$ directly. However, compared with the SDA part, its weight is smaller by a factor U^2. In fact, for strong U the remaining part can be neglected completely, provided that its energetic position, which is well approximated by the center of gravity $D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}$ of $\Sigma_{d\sigma}^{(\mathrm{SOC})}$, is well apart from ϵ_d and thereby insignificant with respect to the states that form the lower Hubbard band (again we assume that $\langle n_{d\sigma}\rangle=\langle n_{d-\sigma}\rangle<0.5$, for simplicity).

It can be concluded that for $U\mapsto\infty$ the interpolating self-energy $\Sigma_{d\sigma}(E)$ reduces to the SDA self-energy $\Sigma_{d\sigma}^{(2)}(E)$, if two conditions are fulfilled: the first is given by Eq. (49) and the second one reads

$$|D_{d\sigma}^{(2)}/D_{d\sigma}^{(1)}-\epsilon_d|\mapsto\infty \tag{54}$$

for $U\mapsto\infty$. Inserting Eq. (51) and the coefficients from Eq. (26) into (49), the first condition can be rewritten:

$$U^2\langle n_{d-\sigma}\rangle^{(\mathrm{HF})}(1-\langle n_{d-\sigma}\rangle^{(\mathrm{HF})})|b_\sigma|$$

$$\equiv|B_{d-\sigma}-\mu-B_{d-\sigma}^{(\mathrm{HF})}+\tilde{\mu}_\sigma+U(1-2\langle n_{d-\sigma}\rangle)|\mapsto\infty. \tag{55}$$

As $U\mapsto\infty$ the correlation functions $B_{d\sigma}$ and $B_{d\sigma}^{(\mathrm{HF})}$ stay finite. Restricting ourselves to the case $\langle n_{d\sigma}\rangle=\langle n_{d-\sigma}\rangle<0.5$, we have $\mu\mapsto$const. Thus we can write the two conditions in the form:

$$|\tilde{\mu}_\sigma+U(1-2\langle n_{d-\sigma}\rangle)|\mapsto\infty, \tag{56}$$

$$|\tilde{\mu}_\sigma - U\langle n_{d-\sigma}\rangle| \mapsto \infty. \tag{57}$$

In the following let us discuss the implications for the three choices that are considered for the determination of the parameter $\tilde{\mu}_\sigma$ according to Eqs. (33)–(35). We start with the case $\tilde{\mu}_\sigma = \mu$. Obviously, both conditions (56) and (57) are fulfilled. Therefore, the first choice yields the SDA self-energy in the limit $U \mapsto \infty$.

The second choice, $\langle n_{d\sigma}\rangle^{(\mathrm{HF})} = \langle n_{d\sigma}\rangle$, implies $\tilde{\mu}_\sigma \sim U\langle n_{d-\sigma}\rangle$. While this fulfills the first condition, it is at variance with the second one. As $U \mapsto \infty$ the overall energy dependence of the self-energy is given by the SDA; there are, however, non-negligible modifications for energies around $E = D^{(2)}_{d\sigma}/D^{(1)}_{d\sigma}$, i.e., within the lower Hubbard band. Compared with the SDA, the upper Hubbard band is completely unaffected, especially what concerns its spectral weight and its center of gravity. This implies that also the weight and the center of gravity of the lower Hubbard band agree with the predictions of the SDA, since the (zeroth and the) first moment of the total spectral density is reproduced exactly. In contrast to the SDA, however, the nonzero imaginary part of the self-energy leads to quasiparticle damping within the lower band. Via the Kramers-Kronig-type relation (53) the quasiparticle energies will be modified too.

The determination of $\tilde{\mu}_\sigma$ according to the Friedel sum rule (or equivalently the Luttinger theorem) is more implicit. Nevertheless, the following indirect argument can be given:

We take $T = 0$; furthermore we again restrict ourselves to the case $\langle n_{d\sigma}\rangle = \langle n_{d-\sigma}\rangle < 0.5$. Let us first mention that for the general proof[26] of the Friedel sum rule for the SIAM one has to resort to various identities that apply to Fermi liquids. In particular, one needs[26]

$$\mathrm{Im}\Sigma_{d\sigma}(E + i0) \sim E^2 \quad \text{for } E \mapsto 0. \tag{58}$$

Secondly, we show that the SDA is at variance with the sum rule.[52] For $\langle n_{d\sigma}\rangle < 0.5$ the pole of the SDA self-energy at $E = B_{d-\sigma} - \mu - U(1 - \langle n_{d-\sigma}\rangle) > 0$ lies outside the range of integration. Thus $\Sigma^{(2)}_{d\sigma}(E)$ is real and

$$\frac{\partial \Sigma^{(2)}_{d\sigma}(E)}{\partial E} = \frac{-U^2\langle n_{d-\sigma}\rangle(1 - \langle n_{d-\sigma}\rangle)}{[E + \mu - B_{d-\sigma} - U(1 - \langle n_{d-\sigma}\rangle)]^2} < 0 \tag{59}$$

for all energies $-\infty < E < 0$. Since $\mathrm{Im}G_{d\sigma}(E + i0) \leqslant 0$ for all E and $\mathrm{Im}G_{d\sigma}(E + i0) < 0$ for a certain energy range within $-\infty < E < 0$, it follows that

$$\mathrm{Im}\int_{-\infty + i0}^{i0} G_{d\sigma}(E)\frac{\partial \Sigma^{(2)}_{d\sigma}(E)}{\partial E} dE > 0, \tag{60}$$

which according to Ref. 26 implies that the Friedel sum rule is not obeyed.

Thirdly, since $\tilde{\mu}_\sigma$ is fixed by imposing the validity of the Friedel sum rule and since the SDA implies (60), we can conclude that the interpolating self-energy must be different from the SDA self-energy in all cases, especially for $U \mapsto \infty$. Consequently, one of the two conditions (56) or (57) must be violated. If it is assumed that the first one holds, it follows that $\langle n_{d-\sigma}\rangle^{(\mathrm{HF})} = 0$ for U larger than a certain critical value. Analogously to the above discussion of the case $\tilde{\mu}_\sigma = \mu$, this would imply $\mathrm{Im}\Sigma_{d\sigma}(0) \neq 0$, a consequence that is not compatible with the Friedel sum rule. Hence, we must have $\langle n_{d-\sigma}\rangle^{(\mathrm{HF})} \neq 0$ implying that for $U \mapsto \infty$ the second condition does not hold. Similar to the case $\langle n_{d\sigma}\rangle^{(\mathrm{HF})} = \langle n_{d\sigma}\rangle$, it can thus be concluded that apart from quasiparticle damping the overall shape of the spectral density follows the predictions of the SDA, in particular, what concerns the energetic positions and the spectral weights of both Hubbard bands.

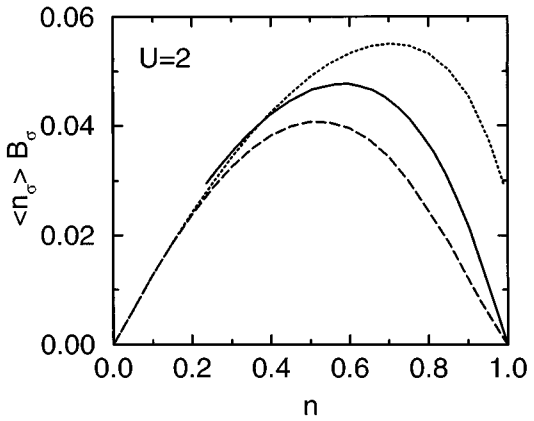

FIG. 1. ''Band shift'' $\langle n_\sigma\rangle B_\sigma$ as a function of filling $n = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle$ for $U = 2$ (energies are given in units of W; W: width of the semielliptic Bloch-density of states). Dotted line: calculation for $\tilde{\mu}_\sigma = \mu$ [first condition (33)]. Dashed line: calculation with $\tilde{\mu}_\sigma$ being determined by $\langle n_\sigma\rangle^{(\mathrm{HF})} = \langle n_\sigma\rangle$ [second condition (34)]. Solid line: $\mu = \mu_0 + \Sigma_\sigma(0)$ [third condition (35)].

Summing up, it has turned out that all three choices to determine $\tilde{\mu}_\sigma$ more or less make contact with a standard strong-coupling approach (SDA) for $U \mapsto \infty$. This fact provides additional justification for the interpolating self-energy since the SDA is known to yield rather satisfactory results, at least on the qualitative level. Therefore, we believe that the theory is able to yield reliable results well beyond the weak-coupling regime. Let us also mention that within this context it is important that the theory correctly accounts for the $m = 3$ moment. Otherwise, we would have ended up for $U \mapsto \infty$ with the ''Hubbard-I'' self-energy $\Sigma^{(1)}_{d\sigma}(E)$ only.

VII. RESULTS

We have evaluated the theory numerically. The procedure is described briefly in Ref. 23. The additional computational effort due to the inclusion of the higher-order correlation functions via $B_{d\sigma}$ is almost negligible, and thus the algorithm remains comparatively fast. The results being discussed in the following have been obtained for the Bethe lattice with infinite coordination number. The semielliptic Bloch density of states has a finite width W. All energies are given in units of W. Furthermore, we choose $\epsilon_d = 0$.

Within the SDA the correlation functions $B_{d\sigma}$ lead to an additional energetic shift of the lower and the upper Hubbard band. For strong U the effective shift of the lower $-\sigma$ Hubbard band is given by $\langle n_\sigma\rangle B_\sigma$.[53] Figure 1 shows the dependence of this ''band shift'' on the occupation number n for $U = 2$ as obtained from our modified IPT. Results for the three different conditions (33)–(35) are shown. In all cases

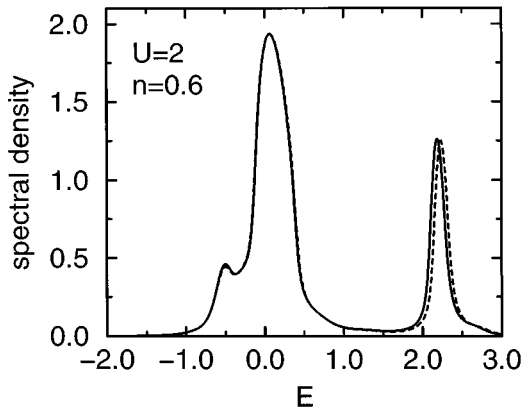

FIG. 2. Spectral density as a function of energy for $U=2$ and $n=0.6$. Calculations assuming $\mu=\mu_0+\Sigma_\sigma(0)$. Solid line: complete theory. Dashed line: $B_\sigma=0$.

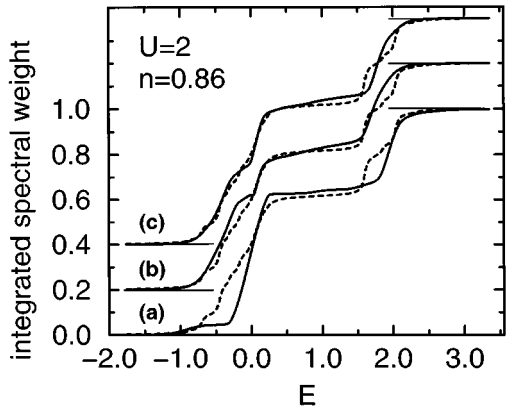

FIG. 3. Integrated spectral weight as a function of energy for $U=2$ and $n=0.86$. Solid lines: result for (a) $\tilde{\mu}_\sigma=\mu$. (b) $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$, (c) $\mu=\mu_0+\Sigma_\sigma(0)$. Dashed line [(a)–(c)]: exact diagonalization (8 sites), from Ref. 23, slightly smoothed. [The vertical scale applies to (a). The curves (b) and (c) have been shifted constantly.]

we find a nonzero but small band shift. Except for the case $\tilde{\mu}_\sigma=\mu$, the curves closely resemble the corresponding results of the SDA (Ref. 53) for a $d=3$ bcc lattice. This regards the absolute magnitude as well as the overall dependence on n. The calculation for $\tilde{\mu}_\sigma=\mu$ yields a nonzero value for B_σ as $n\mapsto 1$, while it results in $B_\sigma=0$ for $n=1$. Contrary, the second and the third condition predict a continuous dependence on n at half filling. Another difficulty is observed for the case $\mu=\mu_0+\Sigma_\sigma(0)$. Below $n=0.23$ a self-consistent solution could not be found. This also holds true (at a slightly different n) if we set $B_\sigma=0$.

The effect of B_σ on the spectral density can be seen in Fig. 2 where we compare the result for the complete theory with the result for $B_\sigma=0$ (the approach of Ref. 23). In both cases we have chosen the third condition (35) to determine $\tilde{\mu}_\sigma$. The occupation number has been fixed at $n=0.6$ where according to Fig. 1 the band shift is at its maximum. Qualitatively similar to the spectra expected for the SIAM, both curves clearly show up three features: the lower and the upper Hubbard band at $E\approx-0.5$ and $E\approx 2.2$ and a peak around $E=0$, which is reminiscent of the Kondo resonance being strongly broadened away from half filling. We notice that the difference between both spectra is rather small. While the low-energy features are completely unaffected, the upper Hubbard band slightly shifts to lower energies when taking into account the $m=3$ moment. This is contrary to the SDA, which predicts an energetic shift of the upper Hubbard band (with respect to the Fermi energy) to higher energies by an amount $(1-n)B_\sigma>0$. The effect can be traced back to the (implicit) U dependence of the hybridization function.

It has not yet been finally clarified what is the optimum choice to determine the fictive chemical potential $\tilde{\mu}_\sigma$. For this purpose we compare with results from the exact diagonalization method of Caffarel and Krauth.[13,14] We take the data from Kajueter and Kotliar[23] for 8 sites, $U=2$ and $n=0.86$. Because of the finite number of orbitals considered in the calculation, the resulting spectral density is not smooth. Rather than comparing the spectral densities directly, a comparison of the integrated spectral weight is more appropriate. This is shown in Fig. 3. There is close agreement between the ED result and the modified IPT calculation provided that condition (34) or (35) is used [curves (b) and (c)]. In both cases the residual discrepancies can be attributed to the finite system size in the ED calculation. Significant differences, however, are observed between the ED result and the calculation for $\tilde{\mu}_\sigma=\mu$ [curve (a)]. In particular, spectral weight is missing around $E=-0.5$.

Figure 4 shows the corresponding spectral densities. We notice that there are only minor differences between the results for $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$ and $\mu=\mu_0+\Sigma_\sigma(0)$. Apart from the lower and the upper Hubbard bands the spectra exhibit a sharp (Kondo) resonance at $E=0$. On the other hand, the spectral density that is calculated for $\tilde{\mu}_\sigma=\mu$ looks completely different. One can no longer distinguish unambiguously between the lower Hubbard band and the resonance. At $E=-0.6$ a minimum can be found. The corresponding nearly constant trend of the integrated weight in Fig. 3 at the same energy, however, is at variance with the ED result, which predicts a steep increase. Furthermore, the upper Hubbard band is significantly shifted to higher energies com-

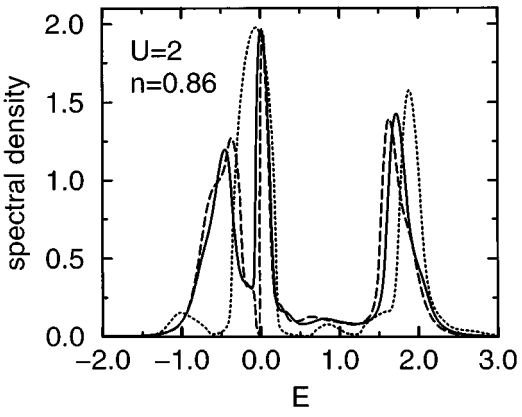

FIG. 4. Spectral density for $U=2$ and $n=0.86$. Dotted line: $\tilde{\mu}_\sigma=\mu$. Dashed line: $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$. Solid line: $\mu=\mu_0+\Sigma_\sigma(0)$.

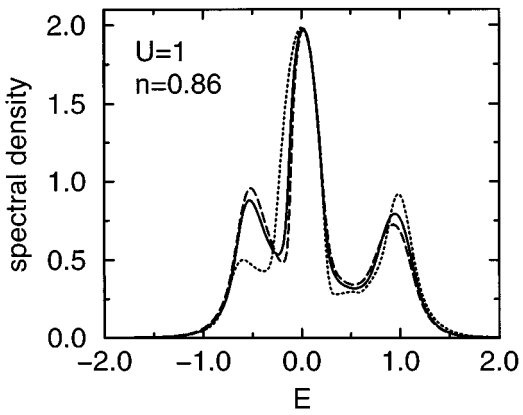

FIG. 5. The same as Fig. 4, but $U=1$.

pared with the results for the second and the third condition, which according to Fig. 3 reliably reproduce the peak position.

There is one unsatisfactory property of the modified IPT when using the second condition $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$, namely, the drop of the spectral density just below the Fermi edge $E=0$ as can be seen in Fig. 4. This behavior, however, is only found for very strong interaction. Figure 3 shows results for $U=1$, which still means strong correlation. Here we notice an almost perfect agreement between the results for the second and the third conditions. Although much closer agreement between all three versions is obtained generally if the interaction is reduced from $U=2$ to $U=1$, the result for $\tilde{\mu}_\sigma=\mu$ is still significantly different. Remarkably, all three curves in Fig. 5 almost coincide at $E=0$. According to Ref. 28 this indicates that Luttinger's theorem is fulfilled approximately when using the first (33) or second (34) condition.

VIII. CONCLUSIONS AND OUTLOOK

In this paper we have presented a modification of the recent approach of Kajueter and Kotliar.[23] Using the self-consistent mapping onto the SIAM, an approximate analytical expression for the self-energy of the infinite-dimensional Hubbard model could be constructed that reproduces a number of exactly solvable limits. The conceptual improvement consists in the consideration of an additional, the $m=3$, moment of the spectral density. It has been shown that the higher-order correlation functions that are included in the extra term B_σ can be expressed without further approximations by means of the spectral density. This allows for a self-consistent (numerical) solution. The additional computational effort needed is almost negligible. The Green function on the real axis at $T=0$ can be computed fast compared with QMC or ED techniques.

The theory contains a fictive chemical potential $\tilde{\mu}_\sigma$ that is considered to be a free parameter that can be fixed by a rather arbitrary condition without losing rigor in all limiting cases mentioned. In this paper we have taken into account three different possibilities to determine $\tilde{\mu}_\sigma$. The numerical results prove that the different choices may imply considerable differences between the shapes of the resulting spectral densities, especially for very strong interaction U. Thus further information was needed to get a conclusive theory. We have compared our results with the data of an ED study taken from Ref. 23. By the comparison the most simple choice $\tilde{\mu}_\sigma=\mu$ is excluded.

For both choices, $\mu=\mu_0+\Sigma_\sigma(0)$ and $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$, we encountered a minor difficulty: self-consistent solutions could not be found for fillings below $n=0.23$ (at $U=2$) when taking the first one; using the latter, we observed an implausible drop of the spectral density just below the Fermi edge which, however, is present in the case of very strong interaction only.

The condition $\mu=\mu_0+\Sigma_\sigma(0)$ represents the Luttinger theorem for the $d=\infty$ Hubbard model. Imposing the Luttinger theorem as a condition to fix $\tilde{\mu}_\sigma$ as has been suggested by Kajueter and Kotliar[23] implies a considerable restriction of the theory: in this form the theorem is only meaningful for a paramagnet at $T=0$.[50] This disadvantage is not present when using the condition $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$, which was introduced by Martin-Rodero *et al.* originally.[24,25] Finite temperatures and ferromagnetism or antiferromagnetism can be treated without difficulty. Furthermore, the condition is much easier to handle numerically. On the other hand, the difference found between the numerical results for the spectral density using either $\mu=\mu_0+\Sigma_\sigma(0)$ or $\langle n_\sigma\rangle^{(\mathrm{HF})}=\langle n_\sigma\rangle$ are rather small, and the agreement with the ED data is equally good.

The usefulness of the $m=3$ moment is apparent in the limit of strong correlations $U\mapsto\infty$. This limit of the approach has been investigated within the SIAM, i.e., for a fixed hybridization function $\Delta(E)$. The mean energetic positions and the weights of the upper and the lower Hubbard bands agree with the predictions of the SDA and with the exact results of Harris and Lange.[43] Here the $m=3$ moment turns out to be decisive. Otherwise, one would have ended up with the ''Hubbard-I'' solution only.

The results for the paramagnetic $d=\infty$ Hubbard model on the Bethe lattice at $T=0$ have shown the effect of B_σ on the spectral density to be rather small. Previous studies, however, strongly suggest that the $m=3$ moment is quite important in the context of spontaneous magnetism. This is obvious, for instance, when comparing the SDA (correct moments up to $m=3$) with the Hubbard-I solution (correct moments up to $m=2$). While the Hubbard-I solution yields magnetic order only under extreme circumstances, magnetism is favored within the SDA: the term B_σ opens the possibility for a spin-dependent band shift. Consistent with the results found here, the effect of B_σ in the paramagnetic phase is small within the SDA as well.[53] Comparing the Hubbard-III alloy-analogy solution with a recently developed modification[42] where again B_σ is included additionally also stresses the importance of the $m=3$ moment for spontaneous magnetism.

The application of the presented method to magnetic phases represents an interesting task for future studies. Let us mention that ferromagnetism in the $d=\infty$ Hubbard model for an fcc-type lattice has been found recently in a QMC calculation.[49] Particle-hole symmetry requires $B_\sigma=0$ at half filling (for a symmetric Bloch density of states) in the paramagnetic phase. In this case the usual IPT is recovered.

However, $B_\sigma \neq 0$ is possible for an antiferromagnet at half filling. Future work may thus check whether the approach can improve the IPT results for antiferromagnetic order at $n=1$ which are not completely satisfactory.[21]

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