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Coherent potential approximation and projection operators for interacting electrons

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A theory of the single-particle excitation spectrum is presented on the basis of the projection operator method combined with the many-body coherent-potential approximation (CPA). The theory describes the dynamics of the excitations by means of an energy-dependent Liouville operator accompanied by a coherent potential which is determined by the self-consistent CPA condition. It is shown that the present theory is essentially equivalent to the dynamical CPA and the dynamical mean-field theory. The Hubbard III approximation and the modified perturbation theory are rederived from the theory. A renormalized perturbation scheme for the Green function is developed on the basis of a general formula for the memory function. It interpolates between the weak- and strong-Coulomb interaction limits, and yields the metal-insulator transition for half-filled bands. Numerical calculations have been performed for the Gutzwiller-Hubbard model on a hypercubic lattice in infinite dimensions. The results show that the theory describes quantitatively the quasiparticle weight vs Coulomb interaction curve, yielding a reasonable critical Coulomb interaction for the metal-insulator transition. It produces the overall features of the excitation spectra and the momentum distributions for various Coulomb interaction strengths.

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I. INTRODUCTION

The single-particle excitation spectrum plays a central role in the description of interacting electrons in solids. It does not only describe the photoemission and inverse-photoemission spectra, but also determines the thermodynamics and the phase transitions of the system.[1] The excitations are usually described by means of a Green function, and enormous efforts have been made for the development of a corresponding theory. In the past decade, there has been considerable progress as regards the single-site theory of Green functions. In the physics of strongly correlated electron systems the dynamical mean-field theory (DMFT) plays an important role. It is based on work by Metzner and Vollhardt[2] who introduced a model suitable in infinite dimensions. Müller-Hartmann[3] showed that the self-energy does not depend on momentum in infinite dimensions, and introduced a self-consistent equation to determine the self-energy. In the subsequent development of DMFT a number of investigators participated.[4–8] One can determine the self-energy by solving self-consistently an impurity problem in an effective medium. The DMFT combined with various many-body techniques[9] to solve the impurity problem has been extensively applied to the metal-insulator transition and to heavy-fermion systems showing a large linear specific-heat coefficient at low temperatures.

The same theory can be traced back to the many-body coherent potential (CPA) by Hirooka and Shimizu.[10] They extended the CPA for the alloys problem[11–16] to the many-body case by using the temperature Green function. The coherent potential describing the local electron correlations was determined according to Shiba's suggestion[17] so that the Green function for an impurity with local Coulomb interactions embedded in the coherent potential agrees with that of the medium with the same coherent potential.

In the theory of itinerant magnetism, a single-site theory was developed on the basis of the functional integral method[18–21] to describe the localized vs itinerant behavior of magnetism.[22–29] It interpolates between the weak- and strong-Coulomb interaction limits. The theory transforms an interacting electron system into an independent electron system placed in a time-dependent random potential. The latter is treated by means of the CPA. Hubbard[23] and Hasegawa[24] established a theory called the single-site spin-fluctuation theory within the high-temperature approximation. Kakehashi[28] developed the dynamical CPA which fully takes into account the dynamical spin and charge fluctuations. The dynamical CPA describes on the same footing the many-body energy bands as well as the local moment behavior of magnetism.[29] The many-body CPA, the dynamical CPA, and the DMFT are equivalent to each other. This was suggested on various levels,[5,6,9] but a clear proof has been given only recently.[30] The CPA has been recognized to be a useful method to treat electron correlations in solids ranging from metals to insulators.

The theories mentioned above are based on the temperature Green function. The excitation spectrum is obtained by an analytic continuation of that function. It is more directly obtained from the retarded Green function by taking the imaginary part of its Laplace transform. The single-site approximation of the retarded Green function for a narrow-band model was proposed by Hubbard[31] in the early 1960s. He proposed an alloy-analogy approximation for strongly correlated electron systems and obtained the metal-insulator transition by solving the CPA equation.[13] The approximation did not lead to a Fermi-liquid state for weak-Coulomb interactions. The projection operator method[1,32–38] is one of the most advanced theories along this line. It is a technique to calculate the Laplace transform of the retarded Green function, which is expressed in terms of a Liouville operator. Choosing a suitable operator space generated by the Liouville operator, one can calculate the excitations of the system from molecules to solids on various levels of approximations. It enables us to perform first-principles calculations by making use of the wave operator method,[39] and also to compute the momentum dependent self-energy starting from a local description by using the incremental method.[40]

In spite of a wide range of applicability of the projection operator method, the method to treat efficiently excitations in solids by means of an effective medium has not yet been developed. In the present paper, we propose a combination of the projection operator method with the many-body CPA. This is essentially equivalent to the dynamical CPA and the DMFT. We develop an interpolation scheme for single-particle excitations between the weak- and strong-Coulomb interaction limits. This is a first step towards first-principles calculations based on the projection operator method in CPA.

The basic idea of the theory is to describe the retarded Green function by means of an energy-dependent Liouville operator of a Hamiltonian with a coherent potential. The coherent potential is determined self-consistently by using the concept of the CPA. The self-consistency of the CPA allows us to optimally include within the single-site approximation the effects of the chemical environment on the local, i.e., on-site electron correlations. This enables us to describe phase transitions caused by electron correlations as well as the correlated energy bands of the system.

In the following section, we briefly review the projection operator method starting from a narrow-band model Hamiltonian. Equations of motion are presented according to the Mori[32] and Zwanzig[33] method, which is used in the following sections. We present the many-body CPA to the projection operator method in Sec. III. The Liouville operator is approximated by an energy-dependent Liouville operator for an effective Hamiltonian with a coherent potential. The CPA equation determines the coherent potential and is presented in Sec. III A. It is shown that the self-consistent equation is essentially equivalent to those obtained in the original many-body CPA, the dynamical CPA, and the DMFT. After having established the CPA, we rederive in Sec. III B the self-consistent equation in the Hubbard III alloy-analogy approximation. Next we present in Sec. III C an interpolation formula for the memory function by using the relevant part of the operator space in the atomic limit and in the itinerant limit. We also derive the self-energy of the modified perturbation theory in the DMFT.[41]

In Sec. IV, we develop the renormalized perturbation theory (RPT) on the basis of the interpolation formula for the memory function. The zeroth- and the first-order approximations are examined in detail for half-filled bands in Secs. IV A and IV B, respectively. In Sec. IV C, we are adopting the decoupling approximation to the higher-order terms. We derive a closed form of the memory function and present a simplified theory by using a cutoff function. By means of a numerical calculation for a half-filled band, we demonstrate that the theory describes the overall features of the excitation spectra from the weak- to the strong-Coulomb interaction limit. Section V is devoted to a summary. Also remaining problems are discussed in that section.

II. PROJECTION OPERATOR METHOD

We adopt in the present paper a tight-binding model[42,43] with an intraatomic Coulomb interaction U,

$$H = H_0 + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

$$H_0 = \sum_{i,\sigma} (\epsilon_0 - \mu) n_{i\sigma} + \sum_{i,j,\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma}. \tag{2}$$

Here ϵ_0 and t_{ij} are the atomic level and the transfer integral between sites i and j, respectively. Furthermore, $a^{\dagger}_{i\sigma}$ ($a_{i\sigma}$) denotes the creation (annihilation) operator for an electron with spin σ on site i, and $n_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$ is the electron-density operator for spin σ on site i. For convenience, we have added the chemical potential μ to the Hamiltonian.

The single-particle excitations are described by the retarded Green functions defined by

$$G_{i\sigma j\sigma'}(t-t') = -i\theta(t-t')\langle [\hat{a}_{i\sigma}(t), \hat{a}^{\dagger}_{j\sigma'}(t')]_{+}\rangle. \tag{3}$$

Here $\theta(t)$ is the step function, $\hat{a}^{\dagger}_{i\sigma}(t)$ ($\hat{a}_{i\sigma}(t)$) is the creation (annihilation) operator in the Heisenberg representation, and $[\,,]_{+}$ denotes the anticommutator between the Fermion operators. The average $\langle\ \rangle$ is taken over the grand canonical ensemble.

By making use of a Laplace transform, the Fourier transform of the retarded Green function is expressed by an inner product in the operator space as[1]

$$G_{i\sigma j\sigma'}(z) = \left(a^{\dagger}_{i\sigma} \left| \frac{1}{z-L} a^{\dagger}_{j\sigma'} \right. \right). \tag{4}$$

Here $z = \omega + i\delta$ with δ being an infinitesimal positive number. The Liouville operator L is a superoperator acting on an operator A as $LA = [H, A]_{-}$ ($[\,,]_{-}$ is the commutator between the operators.) The inner product between the operators A and B is defined by $(A|B) = \langle [A^{+}, B]_{+}\rangle$.

A series of equations of motion for the retarded Green function is obtained by using the projection technique of Mori and Zwanzig.[32,33] The first-order equation for the Green function $G_{i\sigma j\sigma'}(z) = (\boldsymbol{G})_{i\sigma j\sigma'}(z)$ is given by

$$[z - \boldsymbol{L} - \boldsymbol{M}(z)]\boldsymbol{G}(z) = 1, \tag{5}$$

$$L_{i\sigma j\sigma'} = (a^{\dagger}_{i\sigma} | L a^{\dagger}_{j\sigma'}), \tag{6}$$

$$M_{i\sigma j\sigma'}(z) = \left(QLa^{\dagger}_{i\sigma} \left| \frac{1}{z - QLQ} QLa^{\dagger}_{j\sigma'} \right. \right), \tag{7}$$

where $Q = 1 - P$, and P is a projection operator defined by

$$P = \sum_{i\sigma} |a^{\dagger}_{i\sigma})(a^{\dagger}_{i\sigma}|. \tag{8}$$

The operator Q eliminates the operator subspace used in the definition of the Green function (4).

In the case of Hamiltonian (1), the frequency matrix $L_{i\sigma j\sigma'}$ and the memory function $M_{i\sigma j\sigma'}(z)$ are given by

$$L_{i\sigma j\sigma'} = (\boldsymbol{H}_0)_{i\sigma j\sigma'} + U\langle n_{i-\sigma}\rangle \delta_{ij}\delta_{\sigma\sigma'}, \tag{9}$$

$$(\boldsymbol{H}_0)_{i\sigma j\sigma'} = [(\epsilon_0 - \mu)\delta_{ij} + t_{ij}]\delta_{\sigma\sigma'}, \tag{10}$$

$$M_{i\sigma j\sigma'}(z)=U\left(A^{\dagger}_{i\sigma}\left|\frac{1}{z-\bar{L}}A^{\dagger}_{j\sigma'}\right.\right)U. \tag{11}$$

Here $\bar{L}=QLQ$ and $A^{\dagger}_{i\sigma}=a^{\dagger}_{i\sigma}\delta n_{i-\sigma}$, where $\delta n_{i\sigma}$ is defined by $n_{i\sigma}-\langle n_{i\sigma}\rangle$. The Green function (4) is then written as

$$G_{i\sigma j\sigma'}(z)=[\{z-\boldsymbol{H}_0-\boldsymbol{\Sigma}(z)\}^{-1}]_{i\sigma j\sigma'}, \tag{12}$$

$$\Sigma_{i\sigma j\sigma'}(z)=U\langle n_{i-\sigma}\rangle\delta_{ij}\delta_{\sigma\sigma'}+M_{i\sigma j\sigma'}(z). \tag{13}$$

Here $\Sigma_{i\sigma j\sigma'}(z)$ is the self-energy of the system.

When we neglect the memory function, we obtain the Green function in Hartree-Fock approximation. The effects of electron correlations are contained in the memory function $M_{i\sigma j\sigma'}(z)$. Within the Mori-Zwanzig method it is obtained from a second-order equation. Defining the reduced memory function

$$\bar{G}_{i\sigma j\sigma'}(z)=U^{-2}M_{i\sigma j\sigma'}(z)=\left(A^{\dagger}_{i\sigma}\left|\frac{1}{z-\bar{L}}A^{\dagger}_{j\sigma'}\right.\right), \tag{14}$$

we can express the equation for the memory function in the form

$$[z-\bar{\boldsymbol{L}}-\bar{\boldsymbol{M}}(z)]\bar{\boldsymbol{G}}(z)=\boldsymbol{\chi}, \tag{15}$$

$$\bar{L}_{i\sigma j\sigma'}=(A^{\dagger}_{i\sigma}|\bar{L}A^{\dagger}_{j\sigma'})\chi^{-1}_{j\sigma'}, \tag{16}$$

$$\bar{M}_{i\sigma j\sigma'}(z)=(\overline{QLA}^{\dagger}_{i\sigma}|(z-\overline{QLQ})^{-1}\overline{QLA}^{\dagger}_{j\sigma'})\chi^{-1}_{j\sigma'}. \tag{17}$$

$$\chi_{i\sigma j\sigma'}=\chi_{i\sigma}\delta_{ij}\delta_{\sigma\sigma'}=\langle n_{i-\sigma}\rangle(1-\langle n_{i-\sigma}\rangle)\delta_{ij}\delta_{\sigma\sigma'}. \tag{18}$$

Here $\bar{Q}=1-\bar{P}$ and

$$\bar{P}=\sum_{i\sigma}|A^{\dagger}_{i\sigma})\chi^{-1}_{i\sigma}(A^{\dagger}_{i\sigma}|. \tag{19}$$

In deriving the above equations we have assumed that there is no noncollinear spin arrangement, i.e., $\langle a^{\dagger}_{i\sigma}a_{i-\sigma}\rangle=0$. The projection operator $\bar{Q}$ in Eq. (17) eliminates the operator space $\{A^{\dagger}_{i\sigma}\}$ used in the second-order equation. In the same way, we can derive an equation of motion for $\bar{M}_{i\sigma j\sigma'}(z)$. The higher-order equations become more and more difficult in treatment.

III. COHERENT POTENTIAL APPROXIMATION COMBINED WITH THE PROJECTION OPERATOR METHOD

A. Many-body CPA within the projection method

In principle one can obtain the self-energy by solving a series of the equations of motion presented in the last section. These equations however produce higher-order memory functions and the evaluation of various L-matrix elements consisting of static averages is not trivial. A way to reduce the difficulty is to adopt a single-site approximation to the self-energy. We shall treat here the self-energy by using the coherent potential approximation.

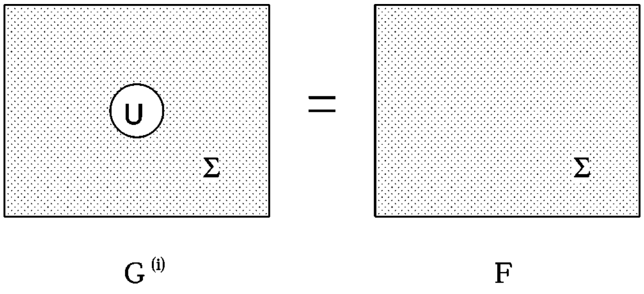

FIG. 1. Schematic picture showing the coherent potential approximation. The left-hand side shows an impurity with a Coulomb interaction U embedded in an effective medium with a coherent potential Σ. The right-hand side shows a uniform state of the effective medium. The left and the right are described by the impurity Green function $G^{(i)}$ and the coherent Green function F, respectively.

It should be noted that the same Green function (12) is obtained from an energy-dependent Liouville operator $L'(z)$ for an effective Hamiltonian $H'(z)$,

$$H'(z)=H_0+\sum_{i,j,\sigma,\sigma'}a^{\dagger}_{i\sigma}\Sigma_{i\sigma j\sigma'}(z)a_{j\sigma'}. \tag{20}$$

This suggests to describe the Green function in the single-site approximation by means of an energy-dependent effective Liouville operator $\tilde{L}(z)$ such that

$$\tilde{L}(z)A=[\tilde{H}(z),A]_{-}, \tag{21}$$

$$\tilde{H}(z)=H_0+\sum_{i\sigma}\Sigma_{\sigma}(z)a^{\dagger}_{i\sigma}a_{i\sigma}. \tag{22}$$

Here we have assumed that all the sites are equivalent so that the site-diagonal self-energy becomes independent on the sites. We call the self-energy $\Sigma_{\sigma}(z)$ the coherent potential.

The retarded Green function to the Liouville operator $\tilde{L}(z)$, which we shall call the coherent Green function, is obtained from the Dyson equation (12) as

$$F_{i\sigma j\sigma'}=[\{z-\tilde{\boldsymbol{H}}(z)\}^{-1}]_{i\sigma j\sigma}\delta_{\sigma\sigma'}, \tag{23}$$

$$[\tilde{\boldsymbol{H}}(z)]_{i\sigma j\sigma'}=[\{\epsilon_0-\mu+\Sigma_{\sigma}(z)\}\delta_{ij}+t_{ij}]\delta_{\sigma\sigma'}. \tag{24}$$

The coherent potential has to be determined from a self-consistent condition. Using Shiba's picture[17] of the coherent potential approximation (see Fig. 1), we consider the Liouville operator $L^{(i)}(z)$ of an impurity system which is obtained by replacing the coherent potential $\Sigma_{\sigma}(z)$ on the impurity site by the on-site Coulomb interaction $Un_{i\uparrow}n_{i\downarrow}$. Its Hamiltonian is given by

$$H^{(i)}(z)=\tilde{H}(z)-\sum_{\sigma}\Sigma_{\sigma}(z)a^{\dagger}_{i\sigma}a_{i\sigma}+Un_{i\uparrow}n_{i\downarrow}. \tag{25}$$

The impurity Green function to the Liouville operator is given by

$$G^{(i)}_{j\sigma k\sigma}(z)=\left(a^{\dagger}_{j\sigma}\middle|\frac{1}{z-L^{(i)}(z)}a^{\dagger}_{k\sigma}\right), \tag{26}$$

where $L^{(i)}(z)$ refers to $H^{(i)}(z)$, i.e., $L^{(i)}(z)A=[H^{(i)}(z),A]_{-}$.

The diagonal Green function is obtained from the Dyson equation (12) [and Eqs. (13) and (11)] by replacing the Liouville operator $\overline{L}$ by $L^{(i)}(z)$:

$$G^{(i)}_{i\sigma i\sigma}(z)=[F^{(i)}_{i\sigma i\sigma}(z)^{-1}-\Lambda^{(i)}_{i\sigma i\sigma}(z)]^{-1}. \tag{27}$$

Here $\Lambda^{(i)}_{i\sigma i\sigma}(z)$ is the self-energy to the impurity Hamiltonian (25). $F^{(i)}_{i\sigma i\sigma}(z)$ is a cavity Green function defined by

$$F^{(i)}_{i\sigma i\sigma}(z)=[\{z-\tilde{\boldsymbol{H}}^{(i)}(z)\}^{-1}]_{i\sigma i\sigma}, \tag{28}$$

$$[\tilde{\boldsymbol{H}}^{(i)}(z)]_{j\sigma k\sigma}=[\tilde{\boldsymbol{H}}(z)]_{j\sigma k\sigma}-\Sigma_{\sigma}(z)\,\delta_{ji}\delta_{ki}\ , \tag{29}$$

i.e., the self-energy at site i has been removed. $\tilde{\boldsymbol{H}}^{(i)}(z)$ denotes the Hamiltonian with vanishing electron interactions on the impurity site i in the effective medium (cavity effect).

The cavity Green function $F^{(i)}_{i\sigma i\sigma}(z)$ is expressed in terms of the coherent Green function according to the Dyson equation

$$F^{(i)}_{i\sigma i\sigma}(z)^{-1}=F_{i\sigma i\sigma}(z)^{-1}+\Sigma_{\sigma}(z). \tag{30}$$

Substituting Eq. (30) into Eq. (27), we obtain

$$G^{(i)}_{\sigma}(z)=[F_{\sigma}(z)^{-1}-\Lambda^{(i)}_{\sigma}(z)+\Sigma_{\sigma}(z)]^{-1}. \tag{31}$$

Here and in the following we omit the site indices in the Green functions and the self-energy for simplicity.

The diagonal coherent Green function $F_{\sigma}(z)$ $[=F_{i\sigma i\sigma}(z)]$ in Eq. (31) is given by

$$F_{\sigma}(z)=\int\frac{\rho(\epsilon)d\epsilon}{z-\epsilon_0+\mu-\Sigma_{\sigma}(z)-\epsilon}. \tag{32}$$

Here $\rho(\epsilon)$ is the density of states (DOS) per atom for the noninteracting system specified by t_{ij}. The self-energy $\Lambda^{(i)}_{\sigma}(z)$ $[=\Lambda^{(i)}_{i\sigma i\sigma}(z)]$ is expressed according to Eq. (13) as

$$\Lambda^{(i)}_{\sigma}(z)=U\langle n_{i-\sigma}\rangle+M^{(i)}_{\sigma}(z), \tag{33}$$

$$M^{(i)}_{\sigma}(z)=U^2(A^{\dagger}_{i\sigma}|[z-\overline{L}^{(i)}(z)]^{-1}A^{\dagger}_{i\sigma}), \tag{34}$$

with $\overline{L}^{(i)}(z)=QL^{(i)}(z)Q$.

The coherent potential in these equations is determined so that the impurity Green function in the effective medium is identical with the coherent Green function (see Fig. 1):

$$G^{(i)}_{\sigma}(z)=F_{\sigma}(z), \tag{35}$$

or equivalently

$$\Lambda^{(i)}_{\sigma}(z)=\Sigma_{\sigma}(z). \tag{36}$$

Equations (31) and (35) have the same form as obtained by analytic continuation of the temperature Green function in the many-body CPA.[10] The latter is equivalent to the dynamical CPA and the DMFT.[30] However, the projection method treats the dynamics and the static averages independently. Therefore the present theory is not exactly equivalent to the many-body CPA formulated in terms of the temperature Green function, since that theory treats both the dynamics and the thermal average on the same footing. But it should be essentially the same as the many-body CPA after a suitable single-site approximation has been made for the static averages in the self-energy (33).

The second point which should be mentioned at this stage is that the energy-dependent Liouville operator $L^{(i)}(z)$ is in general not Hermitian in the operator space because of the energy-dependent impurity Hamiltonian (25). The latter does not necessarily commute with Hamiltonian (1) which appears in the static averages contained in the memory function. This poses some restrictions on actual calculations of the memory function.

B. The Hubbard approximation

Electron correlations in the single-site approximation are described by the memory function $M^{(i)}(z)=U^2\overline{G}^{(i)}_{\sigma}(z)$. The reduced memory function $\overline{G}^{(i)}_{\sigma}(z)$ $[=\overline{G}^{(i)}_{i\sigma i\sigma}(z)]$ is obtained from the equation of motion (15) in which $\overline{L}$ has been replaced by $\overline{L^{(i)}}(z)$.

$$\sum_{k}\ [z\,\delta_{jk}-\overline{L}^{(i)}_{j\sigma k\sigma}(z)-\overline{M}^{(i)}_{j\sigma k\sigma}(z)]\overline{G}^{(i)}_{k\sigma l\sigma}(z)=\chi_{j\sigma}\delta_{jl}\,, \tag{37}$$

$$\overline{L}^{(i)}_{j\sigma k\sigma}(z)=[\tilde{L}_{Q}(z)]_{j\sigma k\sigma}+[-\Sigma_{\sigma}(z)+U(1-\langle n_{i-\sigma}\rangle)]\,\delta_{ji}\delta_{ki}\,, \tag{38}$$

$$[\tilde{L}_{Q}(z)]_{j\sigma k\sigma}=[\epsilon_0-\mu+\Sigma_{\sigma}(z)]\,\delta_{jk}+\sum_{l}\ t_{lk}(A^{\dagger}_{j\sigma}|B^{\dagger}_{kl\sigma})\chi^{-1}_{k\sigma}\,, \tag{39}$$

$$\overline{M}^{(i)}_{j\sigma k\sigma}(z)=\sum_{lm}\ t_{jl}t_{mk}\overline{\overline{G}}_{jl\sigma km\sigma}(z)\chi^{-1}_{k\sigma}\,, \tag{40}$$

$$\overline{\overline{G}}_{jl\sigma km\sigma}(z)=(\overline{Q}B^{\dagger}_{jl\sigma}|[z-\overline{QL^{(i)}}(z)\overline{Q}]^{-1}\overline{Q}B^{\dagger}_{km\sigma}). \tag{41}$$

Here $[\tilde{L}_{Q}(z)]_{j\sigma k\sigma}$ is the frequency matrix for the effective Hamiltonian $\tilde{H}(z)$. The new operators $\{B^{\dagger}_{jl\sigma}\}$ are defined by

$$B^{\dagger}_{jl\sigma}=a^{\dagger}_{l\sigma}\delta n_{j-\sigma}+a^{\dagger}_{j\sigma}\delta(a^{\dagger}_{l-\sigma}a_{j-\sigma})+a^{\dagger}_{j\sigma}\delta(a_{l-\sigma}a^{\dagger}_{j-\sigma}). \tag{42}$$

The self-energy of the Hubbard I approximation[43] is obtained by replacing in Eq. (37) $\overline{L}^{(i)}(z)$ with that in the atomic limit.[34] This corresponds to the neglect of the transfer integrals in the frequency matrix (38) and in the memory function (40). We obtain that $\overline{M}^{(i)}_{j\sigma k\sigma}(z)=0$ and

$$\begin{aligned}\overline{L}^{(i)}_{j\sigma k\sigma}(z)=[&\epsilon_0-\mu+\Sigma_{\sigma}(z)-\Sigma_{\sigma}(z)\,\delta_{ij}\\&+U(1-\langle n_{i-\sigma}\rangle)\,\delta_{ij}]\,\delta_{jk}\,.\end{aligned} \tag{43}$$

Substituting these values into Eq. (37), we obtain

$$\Lambda^{(i)}_{\sigma}(z)=U\langle n_{i-\sigma}\rangle+\frac{U^{2}\langle n_{i-\sigma}\rangle(1-\langle n_{i-\sigma}\rangle)}{z-\epsilon_{0}+\mu-U(1-\langle n_{i-\sigma}\rangle)}. \tag{44}$$

This is the self-energy in the Hubbard I approximation. Note that it is independent of the coherent potential Σ_{σ}. This means that the CPA condition (36) merely implies having the Hubbard I impurity self-energy on each site; the CPA equation does not improve the Hubbard I approximation.

The Hubbard I approximation is exact in the atomic limit. But in general one must also take into account the effects of electron hopping on the memory function. In this context, we note that $\tilde{L}_{Q}(z)$ in Eq. (39) is written by means of an effective Hamiltonian matrix with a shift $\Delta_{0\sigma}$ and a narrowing factor $r_{ij\sigma}$ as follows:

$$[\tilde{L}_{Q}(z)]_{j\sigma k\sigma}=[\epsilon_{0}-\mu+\Sigma_{\sigma}(z)+\Delta_{0\sigma}]\delta_{jk}+r_{jk\sigma}t_{jk}, \tag{45}$$

$$\Delta_{0\sigma}=\sum_{l} t_{lj}(A^{\dagger}_{j\sigma}|B^{\dagger}_{jl\sigma})\chi^{-1}_{j\sigma}, \tag{46}$$

$$r_{jk\sigma}=(A^{\dagger}_{j\sigma}|B^{\dagger}_{kj\sigma})\chi^{-1}_{k\sigma}, \tag{47}$$

where the relation

$$(A^{\dagger}_{j\sigma}|B^{\dagger}_{kl\sigma})=(A^{\dagger}_{j\sigma}|B^{\dagger}_{kj\sigma})\delta_{jl}+(A^{\dagger}_{j\sigma}|B^{\dagger}_{jl\sigma})\delta_{jk} \quad (l\neq k) \tag{48}$$

has been used.

Equation (45) is similar to the noninteracting part of the frequency matrix in the first order equation [see Eq. (24)]. For the half-filled band model with the nearest-neighbor transfer integral on the simple cubic lattice, we find that $r_{jk}=-3/8$ in the limit $U=0$ and $r_{jk}=0$ in the atomic limit. When we neglect $\overline{M}^{(i)}_{j\sigma k\sigma}(z)$ and assume that $r_{jk}\approx r_{\sigma}$, we can solve Eq. (37) explicitly, and obtain

$$\overline{G}^{(i)}_{\sigma}(z)=\frac{\langle n_{i-\sigma}\rangle(1-\langle n_{i-\sigma}\rangle)}{F'_{\sigma}(z)^{-1}+\Sigma_{\sigma}(z)-U(1-\langle n_{i-\sigma}\rangle)}, \tag{49}$$

$$F'_{\sigma}(z)=\int\frac{\rho(\epsilon)d\epsilon}{z-\epsilon_{0}+\mu-\Sigma_{\sigma}(z)-\Delta_{0\sigma}-|r_{\sigma}|\epsilon}. \tag{50}$$

Here we assumed a symmetric band with $\rho(\epsilon)=\rho(-\epsilon)$. Therefore the self-energy is given by

$$\Lambda^{(i)}_{\sigma}(z)=U\langle n_{i-\sigma}\rangle+\frac{U^{2}\langle n_{i-\sigma}\rangle(1-\langle n_{i-\sigma}\rangle)}{F'_{\sigma}(z)^{-1}+\Sigma_{\sigma}(z)-U(1-\langle n_{i-\sigma}\rangle)}. \tag{51}$$

When we neglect the shift $\Delta_{0\sigma}$ and the band narrowing factor r_{σ} (i.e., $\Delta_{0\sigma}\approx 0$ and $|r_{\sigma}|\approx 1$), we have $F'_{\sigma}(z)=F_{\sigma}(z)$. Substituting Eq. (51) into Eq. (31), we obtain for the impurity Green function

$$G^{(i)}_{\sigma}(z)=\frac{\langle n_{i-\sigma}\rangle}{F_{\sigma}(z)^{-1}-U+\Sigma_{\sigma}(z)}+\frac{1-\langle n_{i-\sigma}\rangle}{F_{\sigma}(z)^{-1}+\Sigma_{\sigma}(z)}. \tag{52}$$

The above expression is regarded as an averaged Green function when the effective potentials $\epsilon_{0}-\mu+U$ and $\epsilon_{0}-\mu$ are randomly distributed with concentrations $\langle n_{i-\sigma}\rangle$ and $1-\langle n_{i-\sigma}\rangle$, respectively.[13] The energy-dependent coherent potential $\Sigma_{\sigma}(z)$ is determined from the CPA condition (35).

Equations (35) and (52) are well known as Hubbard's self-consistent alloy-analogy approximation (Hubbard III scattering correction).[31] One of the problems of that approximation is that the system is not a Fermi liquid in the weak-Coulomb interaction region because of the static random potentials $\epsilon_{0}-\mu+U$ and $\epsilon_{0}-\mu$. However, it was the first theory which led to the metal-insulator transition in the half-filled band case.

C. Interpolation formula for the memory function

The equation of motion method presented in the last section is an approach starting from the atomic state because the operator space $\{A^{\dagger}_{i\sigma}\}$ used in the first-order equation describes exactly the atomic limit while the second-order equation introduces the effects of electron hopping. Therefore it is not simple to reproduce the Fermi-liquid state for weak-Coulomb interactions. We take here and in the following an alternative route which describes both the Fermi-liquid state and the atomic state.

For that purpose, we start from the reduced memory function $\overline{G}^{(i)}_{\sigma}(z)$ and divide the Liouville operator $\overline{L}^{(i)}(z)$ into a coherent part $\overline{L}_{0}(z)$ and an interaction part $\overline{L}^{(i)}_{I}(z)$, i.e.,

$$\overline{G}^{(i)}_{\sigma}(z)=(A^{\dagger}_{i\sigma}|[z-\overline{L}_{0}(z)-\overline{L}^{(i)}_{I}(z)]^{-1}A^{\dagger}_{i\sigma}). \tag{53}$$

Here $\overline{L}_{0}(z)=Q\tilde{L}(z)Q$ and $\overline{L}^{(i)}_{I}(z)=QL^{(i)}_{I}(z)Q$. $\tilde{L}(z)$ is given by Eq. (21) and $L^{(i)}_{I}(z)$ acts on a given operator A according to

$$L^{(i)}_{I}(z)A=\left[-\sum_{\sigma}\Sigma_{\sigma}(z)n_{i\sigma}+Un_{i\uparrow}n_{i\downarrow},A\right]_{-}. \tag{54}$$

Note that $|A^{\dagger}_{j\sigma})$ is an eigenstate of the Liouville operator $\overline{L}^{(i)}_{I}(z)$, i.e.,

$$\overline{L}^{(i)}_{I}(z)|A^{\dagger}_{j\sigma})=[-\Sigma_{\sigma}(z)+U(1-\langle n_{i-\sigma}\rangle)]\delta_{ij}|A^{\dagger}_{j\sigma}). \tag{55}$$

This implies that the operator space $|A^{\dagger}_{i\sigma})$ is sufficient to describe the exact atomic limit of the memory function (11), and therefore the self-energy (44).

The eigenstates of $\overline{L}_{0}(z)$, on the other hand, are given by $|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))$, i.e.,

$$\begin{aligned}&\overline{L}_{0}(z)|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\\&\quad=[\epsilon_{0}-\mu+\Sigma_{\sigma}(z)+\epsilon_{k}+\epsilon_{k'}-\epsilon_{k''}]|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma})).\end{aligned} \tag{56}$$

Here $a^{\dagger}_{k\sigma}$ ($a_{k\sigma}$) is the creation (annihilation) operator for an electron with momentum $\boldsymbol{k}$ and spin σ, and ϵ_{k} are the eigenvalues of the kinetic-energy term.

Since $A^{\dagger}_{i\sigma}$ is expanded in terms of $\{|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\}$ as

$$A^{\dagger}_{i\sigma}=\sum_{k,k',k''} a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma})\langle k|i\rangle\langle k'|i\rangle\langle i|k''\rangle, \quad (57)$$

$$\langle k|i\rangle=\langle i|k\rangle^{*}=\frac{1}{\sqrt{N}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}, \quad (58)$$

the memory function for $\overline{L}_0(z)$ is obtained as

$$(A^{\dagger}_{i\sigma}|[z-\overline{L}_0(z)]^{-1}A^{\dagger}_{i\sigma})=\sum_{k,k',k'',k_1,k'_1,k''_1}\frac{\langle i|k_1\rangle\langle i|k'_1\rangle\langle k''_1|i\rangle(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\langle k|i\rangle\langle k'|i\rangle\langle i|k''\rangle}{z-\epsilon_0+\mu-\Sigma_{\sigma}(z)-\epsilon_k-\epsilon_{k'}+\epsilon_{k''}}. \quad (59)$$

The Liouville operator $\overline{L}_0(z)$ becomes Hermitian in the weak-Coulomb interaction limit because $\widetilde{H}(z)$ commutes with H in that case. This means that in this limit $\{|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\}$ are orthogonal to each other:

$$\begin{aligned}(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\\ =\chi_{\sigma}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})\delta_{k_1k}\delta_{k'_1k'}\delta_{k''_1k''},\end{aligned} \quad (60)$$

$$\begin{aligned}\chi_{\sigma}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})=(1-\langle n_{k\sigma}\rangle_0)(1-\langle n_{k'-\sigma}\rangle_0)\langle n_{k''-\sigma}\rangle_0\\ +\langle n_{k\sigma}\rangle_0\langle n_{k'-\sigma}\rangle_0(1-\langle n_{k''-\sigma}\rangle_0).\end{aligned} \quad (61)$$

The subscript 0 stands for taking a thermal average in the Hartree-Fock approximation.

Inserting relation (60) into Eq. (59), we notice that in the weak-Coulomb interaction limit the memory function (59) reduces to the self-energy of the second-order perturbation theory.

$$\frac{\Sigma^{(2)}_{\sigma}(z)}{U^2}=\int\frac{d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')\chi_{\sigma}(\epsilon,\epsilon',\epsilon'')}{z-\epsilon_0+\mu-\Sigma_{\sigma}(z)-\epsilon_k-\epsilon_{k'}+\epsilon_{k''}}. \quad (62)$$

To describe both limits (44) and (62) explicitly, we separate $\overline{L}^{(i)}_I(z)$ into two parts by using the identity $\overline{P}+\overline{Q}=1$ as

$$\overline{L}^{(i)}_I(z)=\overline{P}\,\overline{L}^{(i)}_I(z)\overline{P}+\overline{L}^{(i)}_I(z)\overline{Q}. \quad (63)$$

The first term is the Liouville operator acting on the atomic subspace $\{A^{\dagger}_{i\sigma}\}$ while the second term acts on the space orthogonal to $\{A^{\dagger}_{i\sigma}\}$. Substituting Eq. (63) into Eq. (53), we expand $\overline{G}^{(i)}_{\sigma}(z)$ with respect to $\overline{P}\,\overline{L}^{(i)}_I(z)\overline{P}$. Using relation (55), we obtain the equation

$$\overline{G}^{(i)}_{\sigma}(z)=\frac{\overline{G}^{(i)}_{0\sigma}(z)}{1-\overline{L}^{(i)}_{I\sigma}(z)\overline{G}^{(i)}_{0\sigma}(z)}, \quad (64)$$

$$\overline{G}^{(i)}_{0\sigma}(z)=(A^{\dagger}_{i\sigma}|[z-\overline{L}_0(z)-\overline{L}^{(i)}_I(z)\overline{Q}]^{-1}A^{\dagger}_{i\sigma}), \quad (65)$$

$$\overline{L}^{(i)}_{I\sigma}(z)=\frac{-\Sigma_{\sigma}(z)+U(1-\langle n_{i-\sigma}\rangle)}{\langle n_{i-\sigma}\rangle(1-\langle n_{i-\sigma}\rangle)}. \quad (66)$$

The memory function $\overline{G}^{(i)}_{0\sigma}(z)$ contains the Liouville operator $\overline{L}_0(z)$ describing the weak-Coulomb scattering limit and the operator $\overline{L}^{(i)}_I(z)\overline{Q}$ which does not operate on the atomic state. It indicates that $\overline{G}^{(i)}_{0\sigma}(z)$ basically describes the excitations for weak interactions. The denominator in Eq. (64) shows that the memory function $\overline{G}^{(i)}_{\sigma}(z)$ is given by a renormalization of the memory function for the weak-coupling case via the atomic interactions described by $\overline{L}^{(i)}_{I\sigma}(z)$. Note that Eq. (64) is not an approximation.

The operator space $\{a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma})\}$ for weak-Coulomb interactions should be large enough to describe accurately the excitations between the strong- and weak-Coulomb interaction limits because it includes both the space $\{A^{\dagger}_{i\sigma}\}$ in the atomic limit and the space $\{B^{\dagger}_{jl\sigma}\}$ appearing in the second-order equation [see Eqs. (39) and (41)]. Therefore we may limit the space to $\{a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma})\}$. The memory function $\overline{G}^{(i)}_{0\sigma}(z)$ is then given by the matrix $\overline{\boldsymbol{G}}^{(i)}_0(z)$ as

$$\begin{aligned}\overline{G}^{(i)}_0(z)=\sum_{k,k',k'',k_1,k'_1,k''_1}\langle i|k_1\rangle\langle i|k'_1\rangle\langle k''_1|i\rangle\\ \times[\overline{\boldsymbol{G}}^{(i)}_0(z)]_{k_1k'_1k''_1\sigma kk'k''\sigma}\langle k|i\rangle\langle k'|i\rangle\langle i|k''\rangle,\end{aligned} \quad (67)$$

$$\overline{\boldsymbol{G}}^{(i)}_0(z)=\boldsymbol{\chi}_0[z-\overline{\boldsymbol{L}}_0-\boldsymbol{\chi}_0^{-1}\overline{\boldsymbol{L}}^{(i)}_{IQ}(z)]^{-1}. \quad (68)$$

Here $\boldsymbol{\chi}_0$ is the susceptibility matrix, $\overline{\boldsymbol{L}}_0$ is a diagonal matrix whose diagonal elements give the eigenvalues of $\overline{L}_0(z)$ [see Eq. (56)], and $\overline{\boldsymbol{L}}^{(i)}_{IQ}(z)$ is an interaction matrix of $\overline{L}^{(i)}_I(z)\overline{Q}$. Explicit expressions for the matrix elements are given in Appendix A.

D. Modified perturbation theory

Expression (64) for the memory function is quite general. For example, one can derive from it the self-energy in the modified perturbation theory of the dynamical mean-field theory. In this case we approximate $\overline{G}^{(i)}_{0\sigma}(z)$ by $A_{\sigma}\Sigma^{(2)}_{\sigma}(z)/U^2$ thereby using expression (62) for the weak-

Coulomb interaction limit. The self-energy $\Sigma_\sigma(z)$ in the denominator of $\Sigma_\sigma^{(2)}(z)$ is approximated by the Hartree-Fock one. We obtain then

$$\Lambda_\sigma^{(i)}(z)=U\langle n_{i-\sigma}\rangle+\frac{A_\sigma\Sigma_\sigma^{(2)}(z)}{1-B_\sigma\Sigma_\sigma^{(2)}(z)}, \tag{69}$$

$$B_\sigma=\frac{A_\sigma\overline{L}_{I\sigma}^{(i)}(z)}{U^2}. \tag{70}$$

The phenomenological parameter A_σ is determined so that the lowest moment of the exact memory function is reproduced. This yields

$$A_\sigma=\frac{\langle n_{i-\sigma}\rangle(1-\langle n_{i-\sigma}\rangle)}{\langle n_{i-\sigma}\rangle_0(1-\langle n_{i-\sigma}\rangle_0)}, \tag{71}$$

$$B_\sigma=\frac{U(1-2\langle n_{i-\sigma}\rangle)}{U^2\langle n_{i-\sigma}\rangle_0(1-\langle n_{i-\sigma}\rangle_0)}. \tag{72}$$

Here we have again adopted in B_σ the Hartree-Fock value for Σ_σ.

Equations (69), (71), and (72) are identical with the self-energy in the modified perturbation theory (MPT).[41] Actually the higher-order correction $\tilde{\Sigma}_\sigma=\Sigma_\sigma(z)-U\langle n_{i-\sigma}\rangle$, which was neglected before in the denominator of $\Sigma_\sigma^{(2)}(z)$ and in the numerator of $\overline{L}_{I\sigma}^{(i)}(z)$, is taken into account by replacing $\rho(\epsilon)$ in $\Sigma_\sigma^{(2)}(z)$ with the DOS $\tilde{\rho}^{(i)}(\epsilon)$ for the cavity Hamiltonian $\tilde{H}^{(i)}(z)=\Sigma_{jl\sigma}[\tilde{\boldsymbol{H}}^{(i)}(z)]_{j\sigma l\sigma}a_{j\sigma}^\dagger a_{l\sigma}$ so that the correct result of the second-order self-energy is obtained when $U\delta n_{i\uparrow}\delta n_{i\downarrow}$ is taken as the interaction. The effective chemical potential μ in the theory was determined so that the Friedel sum rule or the Luttinger theorem is satisfied. Note that the correct atomic limit is automatically contained in B_σ given by Eqs. (70) and (72). The MPT is known to be a useful theory describing the overall features of the metal-insulator transition. It does not, however, allow for a systematic improvement of the theory because of its phenomenological character.

IV. RENORMALIZED PERTURBATION THEORY

A. Zeroth approximation to the memory function

The simplest approximation to the memory function (64) is the neglect of the interaction $\overline{L}_I^{(i)}\overline{Q}$ in $\overline{G}_{0\sigma}^{(i)}(z)$. In this case, the reduced self-energy $\tilde{\Lambda}_\sigma^{(i)}(z)=\Lambda_\sigma^{(i)}(z)-U\langle n_{i-\sigma}\rangle$ is given by

$$\tilde{\Lambda}_\sigma^{(i)}(z)=\frac{U^2\overline{G}_{0\sigma}^{(i)}(z)}{1-\overline{L}_{I\sigma}^{(i)}(z)\overline{G}_{0\sigma}^{(i)}(z)}, \tag{73}$$

$$\overline{G}_{0\sigma}^{(i)}(z)=\int\frac{d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')X_\sigma^{(0)}(\epsilon,\epsilon',\epsilon'')}{z-\tilde{\epsilon}_\sigma-\tilde{\Sigma}_\sigma(z)-\epsilon-\epsilon'+\epsilon''}. \tag{74}$$

Here

$$\begin{aligned}X_\sigma^{(0)}&(\epsilon_k,\epsilon_{k'},\epsilon_{k''})\\&=N^3\sum_{k_1,k_1',k_1''}\langle i|k_1\rangle\langle i|k_1'\rangle\langle k_1''|i\rangle\\&\quad\times(a_{k_1\sigma}^\dagger\delta(a_{k_1'-\sigma}^\dagger a_{k_1''-\sigma})|a_{k\sigma}^\dagger\delta(a_{k'-\sigma}^\dagger a_{k''-\sigma}))\\&\quad\times\langle k|i\rangle\langle k'|i\rangle\langle i|k''\rangle,\end{aligned} \tag{75}$$

$$\tilde{\epsilon}_\sigma=\epsilon_0-\mu+U\langle n_{i-\sigma}\rangle, \tag{76}$$

$$\tilde{\Sigma}_\sigma(z)=\Sigma_\sigma(z)-U\langle n_{i-\sigma}\rangle. \tag{77}$$

Equation (73) reproduces the self-energy to the second-order perturbation theory in the weak-Coulomb interaction limit and yields the exact result in the atomic limit. The moments of the Green function are exact up to third order.

The approximate self-energy expression (73) is one of a Fermi liquid. In the following analysis, we assume a symmetric half-filled band so that $\tilde{\epsilon}_\sigma=0$. We omit the spin index for simplicity and consider the nonmagnetic ground state. Using the relations $\rho(-\epsilon)=\rho(\epsilon)$ and $X^{(0)}(-\epsilon,-\epsilon',-\epsilon'')=X^{(0)}(\epsilon,\epsilon',\epsilon'')$, we can verify the relation $\tilde{\Lambda}^{(i)}(\overline{z},\tilde{\Sigma}(\overline{z}))=-\tilde{\Lambda}^{(i)}(z^*,-\tilde{\Sigma}(\overline{z}))$. (Here $\overline{z}=-\omega+i\delta$, $z^*=\omega-i\delta$, and the dependence of the self-energy on $\tilde{\Sigma}(z)$ is explicitly shown for convenience.) Substituting the above relation into the CPA equation $\tilde{\Lambda}^{(i)}(\overline{z},\tilde{\Sigma}(\overline{z}))=\tilde{\Sigma}(\overline{z})$, we obtain $\tilde{\Lambda}^{(i)}(z^*,-\tilde{\Sigma}(\overline{z}))=-\tilde{\Sigma}(\overline{z})$. Comparing it with the CPA equation $\tilde{\Lambda}^{(i)}(z^*,\tilde{\Sigma}^*(z))=\tilde{\Sigma}^*(z)$, we arrive at the relation $\tilde{\Sigma}^*(z)=-\tilde{\Sigma}(\overline{z})$. This indicates that $\mathrm{Re}\tilde{\Sigma}(0^+)=0$. The CPA equation for $z=0^+$ is therefore given by

$$\begin{aligned}\tilde{\Lambda}^{(i)}(0^+)&=\frac{U^2M(0^+-i\mathrm{Im}\tilde{\Sigma}(0^+))}{1+4i\mathrm{Im}\tilde{\Sigma}(0^+)M(0^+-i\mathrm{Im}\tilde{\Sigma}(0^+))}\\&=i\mathrm{Im}\tilde{\Sigma}(0^+).\end{aligned} \tag{78}$$

Here

$$M(z)=\int\frac{d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')X^{(0)}(\epsilon,\epsilon',\epsilon'')}{z-\epsilon-\epsilon'+\epsilon''}. \tag{79}$$

Equation (78) shows that the Fermi-liquid condition $\mathrm{Im}\tilde{\Sigma}(0^+)=0$ is equivalent to $M(0^+)=0$. We obtain $\mathrm{Re}M(0^+)=0$ because of the relation $M(\overline{z})=-M(z)^*$. Therefore the condition reduces in the present case to

$$\begin{aligned}&-\frac{1}{\pi}\mathrm{Im}\,M(0^+)\\&\quad=\int d\epsilon d\epsilon'\ \rho(\epsilon)\ \rho(\epsilon')\ \rho(\epsilon+\epsilon')\ X^{(0)}(\epsilon,\epsilon',\epsilon+\epsilon')=0.\end{aligned} \tag{80}$$

One can expand the CPA equation $\tilde{\Lambda}^{(i)}(z)=\tilde{\Sigma}(z)$ with respect to $\tilde{\Sigma}(z)$ because the Fermi-liquid solution $\tilde{\Sigma}(z)$ is small near $|z|=0$. Solving the linearized CPA equation and expanding the solution of $\tilde{\Sigma}(z)$ with respect to z, we obtain near $z=0$,

$$\tilde{\Sigma}(z)=\frac{U^2\dfrac{\partial \mathrm{Re}M(0^+)}{\partial\omega}}{1+U^2\dfrac{\partial \mathrm{Re}M(0^+)}{\partial\omega}}\,\omega+O(\omega^2). \tag{81}$$

The quasiparticle weight Z (or the inverse effective mass m/m^*) defined by $1/[1-\partial \mathrm{Re}\Sigma(0^+)/\partial\omega]$ is therefore given by

$$Z=\frac{m}{m^*}=1+U^2\frac{\partial \mathrm{Re}M(0^+)}{\partial\omega}. \tag{82}$$

The critical Coulomb interaction $U_{c2}(m^*=\infty)$ for which the effective mass diverges is therefore determined by the condition

$$U=\frac{1}{\sqrt{-\dfrac{\partial \mathrm{Re}M(0^+)}{\partial\omega}}}. \tag{83}$$

Note that $M(z)$ depends generally on U via $X^{(0)}(\epsilon,\epsilon',\epsilon'')$. Therefore, Eq. (83) has to be solved self-consistently in general.

It should be noted that Eq. (78) also contains the solution $\mathrm{Im}\tilde{\Sigma}(0^+)=-\infty$ for an insulator leading to a vanishing DOS at the Fermi level. By applying the moment expansion

$$M(z)=\sum_{n=0}^{\infty}\frac{c_{2n}}{z^{2n+1}}, \tag{84}$$

we can verify that the CPA equation (78) has indeed a solution $\tilde{\Sigma}(0^+)=-\infty$. Near $z=0$, one can solve the CPA equation $\tilde{\Lambda}^{(i)}_{\sigma}(z)=\tilde{\Sigma}(z)$ by expanding it with respect to $1/x$ where $x=z-\Sigma(z)$. For small $|z|$, we obtain the solution as follows:

$$\tilde{\Sigma}(z)=\frac{U^2-16c_2}{4}\,\frac{1}{z}-\frac{32c_2}{U^2-16c_2}z+\cdots. \tag{85}$$

Thus, the critical Coulomb interaction $U_{c1}(\mathrm{gap})$ below which the insulator solution disappears is obtained from the condition

$$U=4\sqrt{c_2}, \tag{86}$$

$$c_2=\int d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')\times(\epsilon+\epsilon'-\epsilon'')^2X^{(0)}(\epsilon,\epsilon',\epsilon''). \tag{87}$$

To obtain the explicit form of the memory function we have to calculate the static expectation values in $X^{(0)}_{\sigma}(\epsilon,\epsilon',\epsilon'')$. We adopt here a simplified expression which also interpolates between the weak- and strong-Coulomb interaction limits:

$$\begin{aligned}&(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k_1'-\sigma}a_{k_1''-\sigma})|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\\&\quad\approx A_{\sigma}\chi_{\sigma}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})\,\delta_{k_1k}\delta_{k_1'k'}\,\delta_{k_1''k''}.\end{aligned} \tag{88}$$

Here $\chi_{\sigma}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})$ is the Hartree-Fock value of $X^{(0)}_{\sigma}(\epsilon,\epsilon',\epsilon'')$ given by Eq. (61), which satisfies condition (80). The renormalization factor A_{σ} defined by Eq. (71) is introduced so that the correct atomic limit is reproduced. A theory based on the correlated wave function will be published in a separate paper. Approximation (88) yields for $\overline{G}^{(i)}_{0\sigma}(z)$ the expression

$$\overline{G}^{(i)}_{0\sigma}(z)=A_{\sigma}\int\frac{d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')\chi_{\sigma}(\epsilon,\epsilon',\epsilon'')}{z-\tilde{\epsilon}_{\sigma}-\tilde{\Sigma}_{\sigma}(z)-\epsilon-\epsilon'+\epsilon''}. \tag{89}$$

For a half-filled band on a hypercubic lattice in infinite dimensions, $\tilde{\epsilon}_{\sigma}=0$, $A_{\sigma}=1$, and $\rho(\epsilon)=1/\sqrt{\pi}\exp(-\epsilon^2)$ in Eq. (89). Here the unit of energy has been chosen so that the second moment $\int d\epsilon\rho(\epsilon)\epsilon^2=1/2$. We find analytically that $U_{c1}(\mathrm{gap})=4\sqrt{3(1/4+1/\pi)/2}=3.693$ and numerically that $U_{c2}(m^*=\infty)=2.085$. This means that approximation (89) leads to a Fermi liquid for $U<U_{c2}$, a non-Fermi liquid for $U_{c2}<U<U_{c1}$, and an insulator with a gap for $U_{c1}<U$.

The results are similar to those obtained by Edwards and Hertz.[44,45] They improved the Hubbard III approximation so that the self-energy reproduces the result of second-order perturbation theory. Within the single-site approximation their theory yielded a Fermi liquid for $U<2$, a non-Fermi liquid for $2<U<2\sqrt{2}$, and an insulator for $2\sqrt{2}<U$ in unit of half the bandwidth of a semielliptical noninteracting DOS. More detailed calculations based on the Monte Carlo[46] and the numerical renormalization-group[47] (NRG) method, however, do not show any indication of a non-Fermi-liquid regime for intermediate Coulomb interaction strengths.

B. First-order approximation to the RPT

We consider here the first-order correction of $\tilde{\boldsymbol{L}}^{(i)}_{IQ}(z)=\boldsymbol{\chi}_0^{-1}\overline{\boldsymbol{L}}^{(i)}_{IQ}(z)$ to the memory function $\overline{G}^{(i)}_{0\sigma}(z)$. We expand Eq. (68) as

$$\overline{\boldsymbol{G}}^{(i)}_0(z)=\boldsymbol{\chi}_0[\boldsymbol{G}_0(z)+\boldsymbol{G}_0(z)\tilde{\boldsymbol{L}}^{(i)}_{IQ}(z)\boldsymbol{G}_0(z)]. \tag{90}$$

Here $\boldsymbol{G}_0(z)=[z-\boldsymbol{L}_0(z)]^{-1}$. Substituting Eq. (90) into Eq. (67), we obtain

$$\overline{G}_0^{(i)}(z)=\frac{1}{N^3}\sum_{k,k',k''}\frac{X_\sigma^{(0)}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})[1+\Delta_\sigma(z-\tilde{\tilde{\Sigma}}_\sigma(z),\tilde{\tilde{\Sigma}}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})]}{z-\tilde{\epsilon}_\sigma-\tilde{\tilde{\Sigma}}_\sigma(z)-\epsilon_k-\epsilon_{k'}+\epsilon_{k''}},\tag{91}$$

$$\Delta_\sigma(z-\tilde{\tilde{\Sigma}}_\sigma(z),\tilde{\tilde{\Sigma}}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})=N^3\sum_{k_1,k_1',k_1''}\frac{\langle i|k\rangle\langle i|k'\rangle\langle k''|i\rangle(\tilde{\boldsymbol{L}}_{IQ}^{(i)}(z))_{kk'k''\sigma k_1k_1'k_1''\sigma}\langle k_1|i\rangle\langle k_1'|i\rangle\langle i|k_1''\rangle}{z-\tilde{\epsilon}_\sigma-\tilde{\tilde{\Sigma}}_\sigma(z)-\epsilon_{k_1}-\epsilon_{k_1'}+\epsilon_{k_1''}}.\tag{92}$$

We call the first-order approximation mentioned above the RPT-1, while the zeroth-order approximation will be denoted by RPT-0.

One can make a phenomenological analysis of the low-energy properties starting from the ground state as follows. Assume again a half-filled symmetric band of a nonmagnetic state. The reduced self-energy is given by

$$\tilde{\Lambda}^{(i)}(z)=\frac{U^2M(z-\tilde{\tilde{\Sigma}}(z),\tilde{\tilde{\Sigma}}(z))}{1-\overline{L}_I^{(i)}(z)M(z-\tilde{\tilde{\Sigma}}(z),\tilde{\tilde{\Sigma}}(z))}.\tag{93}$$

Here

$$M(z,\tilde{\tilde{\Sigma}}(z))=\int\frac{d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')X(z,\tilde{\tilde{\Sigma}}(z),\epsilon,\epsilon',\epsilon'')}{z-\epsilon-\epsilon'+\epsilon''},\tag{94}$$

$$X(z,\tilde{\tilde{\Sigma}}(z),\epsilon,\epsilon',\epsilon'')=X^{(0)}(\epsilon,\epsilon',\epsilon'')[1+\Delta(z,\tilde{\tilde{\Sigma}}(z),\epsilon,\epsilon',\epsilon'')].\tag{95}$$

Note that $M(z,\tilde{\tilde{\Sigma}}(z))$ depends now on $\tilde{\tilde{\Sigma}}(z)$ via the matrix $\tilde{\boldsymbol{L}}_{IQ}^{(i)}(z)$.

Assuming the relations $\rho(-\epsilon)=\rho(\epsilon)$ and $X(-z,-\tilde{\tilde{\Sigma}}(z),-\epsilon,-\epsilon',-\epsilon'')=X(z,\tilde{\tilde{\Sigma}}(z),\epsilon,\epsilon,\epsilon'')$, we can now derive the Fermi-liquid condition by taking the same steps as before, i.e.,

$$\mathrm{Im}M(0^+,0)=0.\tag{96}$$

By expanding the self-energy $\tilde{\Lambda}^{(i)}(z)$ with respect to the small function $\tilde{\tilde{\Sigma}}(z)$ and using the above condition we can obtain for the CPA equation a linearized solution. By additionally expanding $\tilde{\tilde{\Sigma}}(z)$ for small values of z, we obtain near the Fermi energy

$$\tilde{\tilde{\Sigma}}(z)=\frac{U^2\dfrac{\partial\mathrm{Re}M(0^+,0)}{\partial\omega}\omega}{1+U^2\left(\dfrac{\partial\mathrm{Re}M(0^+,0)}{\partial\omega}-\mathrm{Re}\dfrac{\partial M(0^+,0)}{\partial\tilde{\tilde{\Sigma}}_\sigma}\right)}+O(\omega^2),\tag{97}$$

which is of Fermi-liquid type. Thus the quasiparticle weight is given by

$$Z=\frac{1+U^2\left(\dfrac{\partial\mathrm{Re}M(0^+,0)}{\partial\omega}-\mathrm{Re}\dfrac{\partial M(0^+,0)}{\partial\tilde{\tilde{\Sigma}}}\right)}{1-U^2\mathrm{Re}\dfrac{\partial M(0^+,0)}{\partial\tilde{\tilde{\Sigma}}}}.\tag{98}$$

The effective mass m^* diverges for $Z=0$ resulting in a critical Coulomb interaction $U_{c2}(m^*=\infty)$, which is obtained by solving the following equation.

$$U=\frac{1}{\sqrt{-\dfrac{\partial\mathrm{Re}M(0^+,0)}{\partial\omega}+\mathrm{Re}\dfrac{\partial M(0^+,0)}{\partial\tilde{\tilde{\Sigma}}}}}.\tag{99}$$

The insulator solution is obtained by expanding the CPA equation with respect to $1/x$. For small $|z|$, we find the form

$$\tilde{\tilde{\Sigma}}(z)=\frac{U^2-16(c_2+d_2^{(2)}+d_3^{(1)})}{4}\frac{1}{z}-\frac{32(c_2+d_2^{(2)}+3d_3^{(1)}/2)}{U^2-16(c_2+d_2^{(2)}+d_3^{(1)})}z+\cdots.\tag{100}$$

Therefore the critical value $U_{c1}(\mathrm{gap})$ at which the insulator solution disappears is obtained from the condition

$$U=4\sqrt{c_2+d_2^{(2)}+d_3^{(1)}}.\tag{101}$$

Here c_2 is given by Eq. (87), while $d_2^{(2)}$ and $d_3^{(1)}$ are new terms compared with Eq. (86) which are given by

$$d_2^{(2)}=\int d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')X^{(0)}(\epsilon,\epsilon',\epsilon'')\times[(\epsilon+\epsilon'-\epsilon'')\lambda_0^{(2)}(\epsilon,\epsilon',\epsilon'')+\lambda_1^{(2)}(\epsilon,\epsilon',\epsilon'')],\tag{102}$$

$$d_3^{(1)}=\int d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')X^{(0)}(\epsilon,\epsilon',\epsilon'')\times[(\epsilon+\epsilon'-\epsilon'')^2\lambda_0^{(1)}(\epsilon,\epsilon',\epsilon'')+(\epsilon+\epsilon'-\epsilon'')\lambda_1^{(1)}(\epsilon,\epsilon',\epsilon'')+\lambda_2^{(1)}(\epsilon,\epsilon',\epsilon'')].\tag{103}$$

$\lambda_n^{(1)}$ and $\lambda_n^{(2)}$ are the moments of the functions $\lambda_1(z,\epsilon,\epsilon',\epsilon'')$ and $\lambda_2(z,\epsilon,\epsilon',\epsilon'')$, which are defined by

$$\Delta(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')=-\tilde{\Sigma}(z)\lambda_1(z,\epsilon,\epsilon',\epsilon'')+\lambda_2(z,\epsilon,\epsilon',\epsilon''), \tag{104}$$

$$\lambda_1(z,\epsilon,\epsilon',\epsilon'')=\sum_{n=0}^{\infty}\frac{\lambda_n^{(1)}(\epsilon,\epsilon',\epsilon'')}{z^{n+1}}, \tag{105}$$

$$\lambda_2(z,\epsilon,\epsilon',\epsilon'')=\sum_{n=0}^{\infty}\frac{\lambda_n^{(2)}(\epsilon,\epsilon',\epsilon'')}{z^{n+1}}. \tag{106}$$

When the Hartree-Fock matrix elements (see Appendix A) are adopted, we find that $\partial \mathrm{Re} M(0^+,0)/\partial\omega=\partial\mathrm{Re}\Sigma^{(2)}(0^+)/\partial\omega=-0.230\,091$, $\partial\mathrm{Re}M(0^+,0)/\partial\tilde{\Sigma}=-0.157\,239$, $c_2=3(1/4+1/\pi)/2$, $d_2^{(2)}=0$, and $d_3^{(1)}=1/4$. Therefore we obtain $U_{c1}=4\sqrt{3/2\pi+5/8}=4.200$, $U_{c2}=3.705$, and

$$Z=\frac{1-\left(\dfrac{U}{U_{c2}}\right)^2}{1+\left(\dfrac{U}{U_2}\right)^2}. \tag{107}$$

Here $U_2=2.522$.

Figure 2 shows the dependence of Z on U in various approximations. It is remarkable that the first-order correction of $\tilde{\boldsymbol{L}}_{IQ}^{(i)}(z)$ significantly improves the result so that it is close to the one obtained by the NRG,[47] though $U_{c2}(=3.705)$ in the RPT-1 is somewhat smaller than that in the NRG ($=4.10$). Note that these findings were obtained by using Hartree-Fock matrix elements. The good agreement is presumably due to the fact that in a Fermi-liquid electrons near the Fermi surface are only weakly scattered by the Coulomb interactions.

C. Decoupling approximation to the higher-order terms

In the last section we showed that the first-order correction describes well the quasiparticle excitations near the Fermi level. We consider here an approximate treatment of the higher-order terms. For that purpose we expand Eq. (68) with respect to the interaction $\overline{\boldsymbol{L}}_{IQ}^{(i)}(z)$.

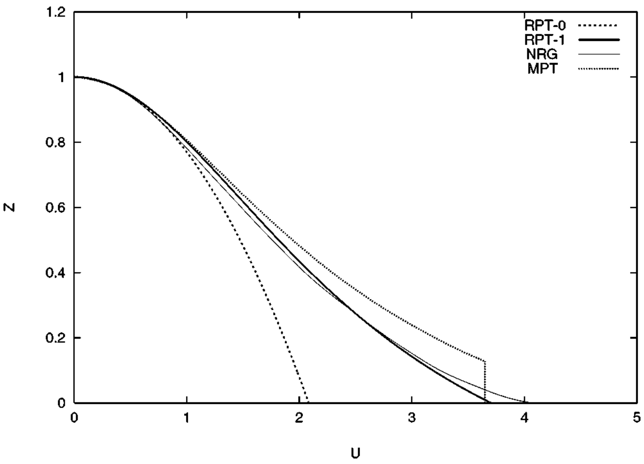

FIG. 2. Quasiparticle weight vs Coulomb interaction strength for the half-filled band case on a hypercubic lattice in infinite dimensions in various approximations. Dotted curve—zeroth approximation in the renormalized perturbation theory (RPT-0), solid curve—the first-order approximation (RPT-1) and decoupling approximation in the RPT, thin solid curve—numerical renormalization group theory (NRG) (Ref. 47), thin dotted curve—modified perturbation theory (MPT) (Ref. 48).

$$\overline{\boldsymbol{G}}_0^{(i)}(z)=\boldsymbol{\chi}_0\boldsymbol{G}_0+\boldsymbol{\chi}_0\boldsymbol{G}_0\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0+\boldsymbol{\chi}_0\boldsymbol{G}_0\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0+\cdots. \tag{108}$$

We decouple the higher-order terms by inserting the following projector between $\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0$'s:

$$(P_i)_{k_1k_1'k_1''\sigma kk'k''\sigma}=\langle k_1|i\rangle\langle k_1'|i\rangle\langle i|k_1''\rangle\langle i|k\rangle\langle i|k'\rangle\langle k''|i\rangle. \tag{109}$$

The approximate memory function $\overline{G}_{0\sigma}^{(i)}(z)$ is then obtained as

$$\overline{G}_{0\sigma}^{(i)}(z)=\frac{1}{N^3}\sum_{k,k',k''}\frac{X_\sigma^{(0)}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})}{z-\tilde{\epsilon}_\sigma-\tilde{\Sigma}_\sigma(z)-\epsilon_k-\epsilon_{k'}+\epsilon_{k''}} \times\left[1+\frac{\Delta_\sigma(z-\tilde{\Sigma}_\sigma(z),\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})}{1-(\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0)_{ii}}\right], \tag{110}$$

$$(\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0)_{ii}=\sum_{k,k',k'',k_1,k_1',k_1''}\frac{\langle i|k_1\rangle\langle i|k_1'\rangle\langle k_1''|i\rangle[\tilde{\boldsymbol{L}}_{IQ}^{(i)}(z)]_{k_1k_1'k_1''\sigma kk'k''\sigma}\langle k|i\rangle\langle k'|i\rangle\langle i|k''\rangle}{z-\tilde{\epsilon}_\sigma-\tilde{\Sigma}_\sigma(z)-\epsilon_k-\epsilon_{k'}+\epsilon_{k''}}. \tag{111}$$

Here $X_\sigma^{(0)}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})$ and $\Delta_\sigma(z-\tilde{\Sigma}_\sigma(z),\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})$ are given by Eqs. (75) and (92), respectively.

It should be noted that the reduced self-energy has the same form as Eq. (93) with the memory function $M(z,\tilde{\Sigma}_\sigma(z))$ given by Eq. (94), provided that the function $X_\sigma(z,\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})$ is defined by

$$X_\sigma(z,\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''}) = X_\sigma^{(0)}(\epsilon_k,\epsilon_{k'},\epsilon_{k''})\left[1+\frac{\Delta_\sigma(z,\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})}{1-R_\sigma(z,\tilde{\Sigma}_\sigma(z))}\right]. \tag{112}$$

Here $R_\sigma(z,\tilde{\Sigma}_\sigma(z))$ is defined by $(\tilde{\boldsymbol{L}}_{IQ}^{(i)}\boldsymbol{G}_0)_{ii}$ with $z-\tilde{\Sigma}_\sigma(z)$ in the denominator being replaced by z. This results in

$$R_\sigma(z,\tilde{\Sigma}_\sigma(z)) = \int d\epsilon d\epsilon' d\epsilon'' \rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')\Delta_\sigma(z,\tilde{\Sigma}_\sigma(z),\epsilon,\epsilon',\epsilon''). \tag{113}$$

Therefore the critical behavior of the low-energy excitations of a half-filled band are the same as those in first-order perturbation theory (for details see Appendix B), i.e., the Fermi-liquid condition for the half-filled band is given by Eq. (96), the quasiparticle weight is expressed by Eq. (98), and the critical Coulomb interaction $U_{c2}(m^*=\infty)$ is obtained by solving Eq. (99). Furthermore, we can prove that the insulator solution of the self-energy near the Fermi level is expressed by Eq. (100) because there is no effect of $R(z,\tilde{\Sigma}(z))$ on the low-energy excitations. Therefore we have the same equation (101) and the same critical Coulomb interaction $U_{c1}(\text{gap})$ as before.

For the Hartree-Fock matrix elements (see Appendix A), we obtain the same critical Coulomb interactions $U_{c1}(\text{gap}) = 4.200$ and $U_{c2}(m^*=\infty) = 3.705$ as before. The quasiparticle weight vs U curve is identical with that of the first-order approximation, i.e., the one described by Eq. (107) (see Fig. 2).

When we use Hartree-Fock matrix elements for $\boldsymbol{\chi}_0$ and $\tilde{\boldsymbol{L}}_{IQ}^{(i)}$, there is a discrepancy in the atomic region between the Hartree-Fock form $\Delta_\sigma(z,\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})$ and the exact one. In fact, in the atomic limit we obtain $\Delta_\sigma(z,\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''})=0$, irrespective of the values of $\{\epsilon_k,\epsilon_{k'},\epsilon_{k''}\}$, because

$$\sum_{k_1,k_1',k_1''} (\tilde{\boldsymbol{L}}_{IQ}^{(i)})_{kk'k''\sigma k_1 k_1' k_1''\sigma}\langle k_1|i\rangle\langle k_1'|i\rangle\langle i|k_1''\rangle = 0, \tag{114}$$

while the Hartree-Fock value does not vanish in that case, i.e., $\Delta_\sigma^{(HF)}(z,\tilde{\Sigma}_\sigma(z),\epsilon_k,\epsilon_{k'},\epsilon_{k''}) \neq 0$.

A conventional way to remove the inconsistency is to introduce a cutoff parameter q, which vanishes in the atomic region, when we adopt $\Delta_\sigma^{(HF)}$. We have then

$$G^{(i)}(z) = [F(z)^{-1} - \tilde{\Lambda}^{(i)}(z) + \tilde{\Sigma}(z)]^{-1}, \tag{115}$$

$$\tilde{\Lambda}^{(i)}(z) = \frac{U^2 M(z-\tilde{\Sigma}(z),\tilde{\Sigma}(z),q)}{1-\overline{L_I^{(i)}}(z)M(z-\tilde{\Sigma}(z),\tilde{\Sigma}(z),q)}, \tag{116}$$

$$M(z,\tilde{\Sigma}(z),q) = \int \frac{d\epsilon d\epsilon' d\epsilon'' \rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')\chi(\epsilon,\epsilon',\epsilon'')}{z-\epsilon-\epsilon'+\epsilon''} \times \left[1+\frac{q\Delta^{(HF)}(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')}{1-qR(z,\tilde{\Sigma}(z))}\right], \tag{117}$$

$$\begin{aligned}\Delta^{(HF)}(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'') = {} & -\tilde{\Sigma}(z)[\hat{F}(z-\epsilon'+\epsilon'')+\hat{F}(z-\epsilon \\ & +\epsilon'')+\hat{F}(-z+\epsilon+\epsilon')] \\ & +UK(z,\epsilon',\epsilon'') \\ & -\overline{L_I^{(i)}}(z)U^{-2}\Sigma^{(2)}(z).\end{aligned} \tag{118}$$

Here $R(z,\tilde{\Sigma}(z))$ is given by Eqs. (113) and (118). The functions $\hat{F}(z)$ and $K(z,\epsilon',\epsilon'')$ are defined by

$$\hat{F}(z) = \int \frac{\rho(\epsilon)d\epsilon}{z-\epsilon}, \tag{119}$$

$$K(z,\epsilon',\epsilon'') = \int \frac{d\omega d\omega'' \rho(\omega)\rho(\omega'')[f(\tilde{\epsilon}+\omega)-f(\tilde{\epsilon}+\omega'')]}{z-\omega-\epsilon'+\omega''} + \int \frac{d\omega d\omega' \rho(\omega)\rho(\omega')[1-f(\tilde{\epsilon}+\omega')-f(\tilde{\epsilon}+\omega)]}{z-\omega-\omega'+\epsilon''}. \tag{120}$$

As usual $f(\omega)$ is the Fermi distribution function defined by $f(\omega)=1/[\exp(\beta\omega)+1]$ and β denotes the inverse temperature.

We shall use the limiting values $q=1$ in the Fermi-liquid region and $q=0$ in the atomic region $[U>U_{c2}(m^*=\infty)]$ at the ground state. The CPA equation (35) and the impurity Green function (115) determine the coherent potential $\tilde{\Sigma}(z)$ self-consistently in the presence of the cutoff.

The self-energy with the cutoff q leads to the critical Coulomb interactions $U_{c1}(\text{gap}) = 4\sqrt{3(1/4+1/\pi)} = 3.693$ and $U_{c2}(m^*=\infty) = 3.705$ for the hypercubic lattice, which should be compared with $U_{c1}(\text{gap}) = 3.25$ and $U_{c2}(m^*=\infty) = 4.10$ in the NRG,[47] respectively. The metal-insulator phase transition occurs at $U_c = U_{c2}(m^*=\infty)$, below which the quasiparticle weight is given by Eq. (107) (see Fig. 2). In the present theory, the transition is of first order, though recent numerical calculations[47] suggest a second-order transition.

The single-particle excitation spectra calculated from the self-energy (116) are shown in Fig. 3. With increasing values of U, the width of the quasiparticle peak decreases and the upper and lower Hubbard bands develop. In the present

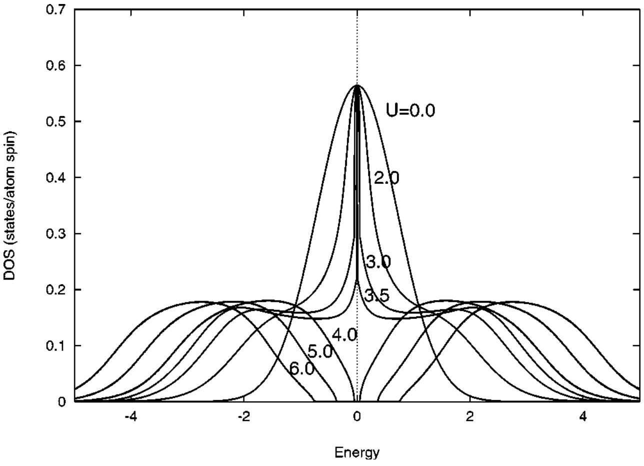

FIG. 3. Single-particle excitation spectra for various Coulomb interactions U. The half-filled band model on the hypercubic lattice in infinite dimensions is considered. The energy unit is chosen so that the second moment of the noninteracting density of states becomes 1/2.

theory a well-defined pseudogap region does not exist before U reaches $U_{c2}(m^{*}=\infty)$ because the Hubbard subbands do not well develop. This is due to the use of the Hartree-Fock matrix elements of $\boldsymbol{\chi}_0$ and $\tilde{\boldsymbol{L}}_{IQ}^{(i)}$ which neglect effects of electron correlations on the static averages.

As shown in Fig. 4, the momentum distribution has a jump at the Fermi energy indicating a Fermi-liquid state. The jump monotonically decreases with increasing values of U, and vanishes at $U=U_{c2}(m^{*}=\infty)$. Above $U_{c2}(m^{*}=\infty)$ there is no discontinuity, and the curves flatten with further increase of U. This behavior is similar to the one obtained by the MPT[48] and differs to the one of the Gutzwiller approximation.[42]

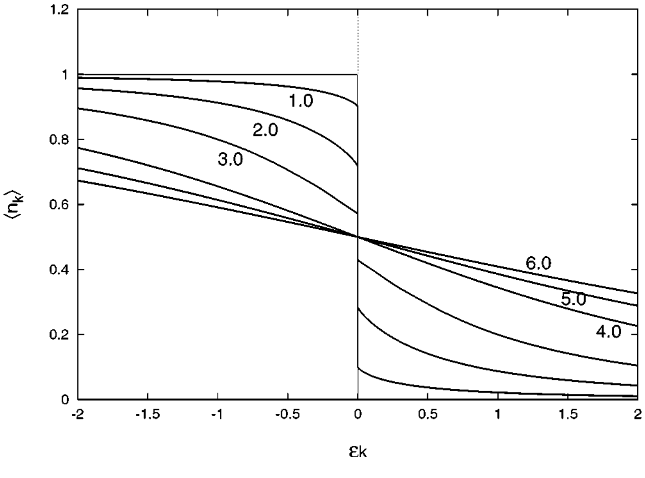

FIG. 4. Momentum distributions as a function of the energy ϵ_k for various Coulomb interaction strengths $U=1.0$, 2.0, 3.0, 4.0, 5.0, 6.0. The curve for the noninteracting electrons is shown by the thin line. A half-filled band model on the hypercubic lattice in infinite dimensions is considered.

V. SUMMARY AND DISCUSSION

We have presented a theory for the single-particle excitation spectrum in solids which combines the projection operator method with the many-body CPA. The theory starts from the energy-dependent Liouville operator describing the dynamics of local excitations in a coherent potential $\Sigma_{\sigma}(z)$. The latter is determined so that the retarded Green function of an impurity with a Coulomb interaction embedded in the medium $\Sigma_{\sigma}(z)$ is consistent with the coherent Green function of the medium.

We have shown that the present theory is essentially equivalent to single-site theories based on the temperature Green function, which are known, i.e., the many-body CPA, the dynamical CPA, and the DMFT. The present approach has the merit that the spectrum is directly obtained from the imaginary part of the Green function without using any numerical analytic continuation or artificial line broadening. Both are often required in the numerical approaches based on the temperature Green function. We rederived the Hubbard III approximation within the present formalism from the second-order equation of motion. We presented an interpolation formula for the memory function between the weak- and strong-coupling limits. On the basis of this formula, we derived the self-energy of the modified perturbation theory in the DMFT without making phenomenological assumptions concerning the self-energy.

Based on an interpolation formula for the memory function we have developed a renormalized perturbation theory which analytically interpolates between the weak- and strong-Coulomb interaction limits. When the Coulomb interactions are weak, an expansion of the memory function $\overline{G_{0\sigma}^{(i)}}(z)$ in terms of the interaction Liouvillian $\overline{L_I^{(i)}}(z)\overline{Q}$ leads to a good description of the quasiparticles near the Fermi level even when we limit ourselves to the first-order term and use Hartree-Fock matrix elements in the calculations. Higher-order corrections can be treated by a decoupling approximation. When strong interactions are considered the use of Hartree-Fock matrix elements in static averages must be corrected by the introduction of a cutoff parameter. With its help, we can describe the overall features of the single-particle excitation spectra from the weak- to the strong- Coulomb interaction limit. The theory yields the reasonable critical Coulomb interactions $U_{c1}(\text{gap})=3.694$ and $U_{c2}(m^{*}=\infty)=3.705$. Moreover, an analytic expression for the quasiparticle weight provides us with a simple and quantitative description of the effective mass.

We are convinced that the present theory can be applied to many problems because of its simplicity, in particular, to more complex systems which are not easily accessible by means of other numerical techniques such as the Monte Carlo and the NRG methods. Furthermore, the theory is compatible with the first-principles cumulant wave operator method which has been applied for ground-state electronic-structure calculations.[39] Thus it is possible to construct a first-principles theory of excitations by combining the latter with the present theory. These advantages are promising as regards a further development of the theory of excitations towards quantitative calculations.

The basic assumption of the present theory is the single-site approximation to the self-energy, i.e., the momentum independence of the self-energy. One of the merits of the projection operator method is that there is a technique available, i.e., the incremental method[40] to overcome that limitation. It allows us to include systematically pair-site, triple-site correlations, and higher-order cluster correlations, starting from the single-site approximation. The present method is in competition with the dynamical cluster approximation.[49] The latter includes short-ranged dynamical correlations in addition to the local dynamics of the DMFT. The incremental method combined with the CPA and its application to various problems are left for future investigations.

APPENDIX A: MATRIX ELEMENTS FOR THE MEMORY FUNCTION

We present here the expressions of various matrix elements which appear in the memory function (67) and (68):

$$\overline{\boldsymbol{G}}_0^{(i)}(z)=\boldsymbol{\chi}_0[z-\overline{\boldsymbol{L}}_0-\boldsymbol{\chi}_0^{-1}\overline{\boldsymbol{L}}_{IQ}^{(i)}(z)]^{-1}, \tag{A1}$$

$$\begin{aligned}(\boldsymbol{\chi}_0)_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma})),\end{aligned} \tag{A2}$$

$$\begin{aligned}(\overline{\boldsymbol{L}}_0)_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =[\tilde{\epsilon}_\sigma+\tilde{\Sigma}_\sigma(z)+\epsilon_k+\epsilon_{k'}-\epsilon_{k''}]\delta_{k_1k}\delta_{k'_1k'}\delta_{k''_1k''},\end{aligned} \tag{A3}$$

$$\begin{aligned}(\overline{\boldsymbol{L}}_{IQ}^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =(\overline{\boldsymbol{L}}_I^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}-\overline{L}_{I\sigma}^{(i)}(z)(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|A^{\dagger}_{i\sigma})\\ \times(A^{\dagger}_{i\sigma}|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma})),\end{aligned} \tag{A4}$$

$$\begin{aligned}(\overline{\boldsymbol{L}}_I^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =-\tilde{\Sigma}_\sigma(z)(\boldsymbol{\chi}_1^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}-\tilde{\Sigma}_{-\sigma}(z)(\boldsymbol{\chi}_2^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ +\tilde{\Sigma}_{-\sigma}(z)(\boldsymbol{\chi}_3^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}+U(\hat{\boldsymbol{L}}_U^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma},\end{aligned} \tag{A5}$$

$$\begin{aligned}(\boldsymbol{\chi}_1^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{i\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\langle i|k\rangle,\end{aligned} \tag{A6}$$

$$\begin{aligned}(\boldsymbol{\chi}_2^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}=(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{i-\sigma}a_{k''-\sigma}))\\ \times\langle i|k'\rangle,\end{aligned} \tag{A7}$$

$$\begin{aligned}(\boldsymbol{\chi}_3^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}=(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{i-\sigma}))\\ \times\langle k''|i\rangle,\end{aligned} \tag{A8}$$

$$\begin{aligned}(\hat{\boldsymbol{L}}_U^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{i\sigma}\delta n_{i-\sigma}\delta(a^{\dagger}_{k'-\sigma}a_{k''-\sigma}))\langle i|k\rangle\\ +(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}a^{\dagger}_{i-\sigma}\delta n_{i\sigma}a_{k''-\sigma})\langle i|k'\rangle\\ -(a^{\dagger}_{k_1\sigma}\delta(a^{\dagger}_{k'_1-\sigma}a_{k''_1-\sigma})|a^{\dagger}_{k\sigma}a^{\dagger}_{k'-\sigma}a_{i-\sigma}\delta n_{i\sigma})\langle k''|i\rangle.\end{aligned} \tag{A9}$$

Here $\tilde{\epsilon}_\sigma=\epsilon_0-\mu+U\langle n_{i-\sigma}\rangle$ and $\tilde{\Sigma}_\sigma(z)=\Sigma_\sigma(z)-U\langle n_{i-\sigma}\rangle$. $\overline{L}_{I\sigma}^{(i)}(z)$ is defined by Eq. (66).

In Hartree-Fock approximation, the matrix elements simplify to

$$(\boldsymbol{\chi}_0)_{k_1k'_1k''_1\sigma kk'k''\sigma}=\chi_\sigma(\epsilon_k,\epsilon_{k'},\epsilon_{k''})\delta_{kk_1}\delta_{k'k'_1}\delta_{kk'_1}, \tag{A10}$$

$$\begin{aligned}\chi_\sigma(\epsilon_k,\epsilon_{k'},\epsilon_{k''})=(1-\langle n_{k\sigma}\rangle_0)(1-\langle n_{k'-\sigma}\rangle_0)\langle n_{k''-\sigma}\rangle_0\\ +\langle n_{k\sigma}\rangle_0\langle n_{k'-\sigma}\rangle_0(1-\langle n_{k''-\sigma}\rangle_0),\end{aligned} \tag{A11}$$

$$\begin{aligned}(\boldsymbol{\chi}_0^{-1}\overline{\boldsymbol{L}}_{IQ}^{(i)})_{k_1k'_1k''_1\sigma kk'k''\sigma}\\ =-\tilde{\Sigma}_\sigma(z)\langle i|k\rangle\langle k_1|i\rangle\delta_{k'_1k'}\delta_{k''_1k''}-\tilde{\Sigma}_{-\sigma}(z)\langle i|k'\rangle\\ \times\langle k'_1|i\rangle\delta_{k_1k}\delta_{k''_1k''}+\tilde{\Sigma}_{-\sigma}(z)\langle k''|i\rangle\langle i|k''_1\rangle\delta_{k_1k}\delta_{k'_1k'}\\ +U\langle i|k\rangle\langle k_1|i\rangle\langle i|k''_1\rangle\langle k''|i\rangle(\langle n_{k\sigma}\rangle_0-\langle n_{k''-\sigma}\rangle_0)\delta_{k'_1k'}\\ +U\langle i|k\rangle\langle k_1|i\rangle\langle k'_1|i\rangle\langle i|k'\rangle(1-\langle n_{k'-\sigma}\rangle_0\\ -\langle n_{k\sigma}\rangle_0)\delta_{k''_1k''}-\overline{L}_{I\sigma}^{(i)}(z)\chi_\sigma(\epsilon_k,\epsilon_{k'},\epsilon_{k''})\langle k_1|i\rangle\\ \times\langle k'_1|i\rangle\langle i|k''_1\rangle\langle i|k\rangle\langle i|k'\rangle\langle k''|i\rangle.\end{aligned} \tag{A12}$$

The above expressions were used to calculate the critical Coulomb interactions in Sec. IV and to obtain the self-energy (116).

APPENDIX B: ANALYTIC PROPERTY OF THE SELF-ENERGY FOR LOW-ENERGY EXCITATIONS

We analyze in this Appendix the reduced self-energy at the ground state presented in Sec. IV C. For the half-filled band it has the following form:

$$\tilde{\Lambda}^{(i)}(z)=\frac{U^2M(z-\tilde{\Sigma}(z),\tilde{\Sigma}(z))}{1-\overline{L}_I^{(i)}(z)M(z-\tilde{\Sigma}(z),\tilde{\Sigma}(z))}, \tag{B1}$$

$$\begin{aligned}M(z,\tilde{\Sigma}(z))\\ =\int\frac{d\epsilon d\epsilon' d\epsilon''\rho(\epsilon)\rho(\epsilon')\rho(\epsilon'')X(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')}{z-\epsilon-\epsilon'+\epsilon''}.\end{aligned} \tag{B2}$$

Here $\overline{L_I^{(i)}}(z) = -4\tilde{\Sigma}(z)$ [see Eq. (66)], and $X(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')$ is given by Eq. (112).

We assume in the following a symmetric band implying that $\rho(-\epsilon)=\rho(\epsilon)$ and $X(-z,-\tilde{\Sigma}(z),-\epsilon,-\epsilon',-\epsilon'') = X(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')$. By using the symmetry relations, we verify the relation $\tilde{\Lambda}^{(i)}(\bar{z},\tilde{\Sigma}(\bar{z})) = -\tilde{\Lambda}^{(i)}(z^*,-\tilde{\Sigma}(\bar{z}))$ for $\bar{z} = -\omega + i\delta$. Therefore the CPA equation (36) for $\bar{z}$ is written as

$$\tilde{\Lambda}^{(i)}(z^*,-\tilde{\Sigma}(\bar{z})) = -\tilde{\Sigma}(\bar{z}). \tag{B3}$$

This demonstrates that $\tilde{\Sigma}(z)^* = -\tilde{\Sigma}(\bar{z})$. Therefore $\mathrm{Re}\tilde{\Sigma}(0^+)=0$. The CPA equation at $z=0^+$ is then expressed as

$$\begin{aligned}\tilde{\Lambda}_{\sigma}^{(i)}(0^+) &= \frac{U^2 M(0^+ - i\mathrm{Im}\tilde{\Sigma}(0^+), i\mathrm{Im}\tilde{\Sigma}(0^+))}{1 + 4i\mathrm{Im}\tilde{\Sigma}(0^+) M(0^+ - i\mathrm{Im}\tilde{\Sigma}(0^+), i\mathrm{Im}\tilde{\Sigma}(0^+))}\\ &= i\mathrm{Im}\tilde{\Sigma}(0^+). \end{aligned} \tag{B4}$$

Thus the condition for a Fermi liquid, i.e., $\mathrm{Im}\tilde{\Sigma}(0^+)=0$ is given by $M(0^+,0)=0$. Here $\mathrm{Re}M(0^+,0)=0$ because $M(\bar{z},0) = -M(z,0)^*$ is verified by using the symmetry properties of $\rho(\epsilon)$ and $X(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')$. Therefore, the Fermi-liquid condition requires

$$\mathrm{Im}M(0^+,0)=0. \tag{B5}$$

In the first-order approximation, this is the same as Eq. (96).

With the above condition, we can expand the self-energy $\tilde{\Lambda}^{(i)}(z)$ with respect to the coherent potential $\tilde{\Sigma}(z)$. Solving the linearized CPA equation, we obtain

$$\tilde{\Sigma}(z) = \frac{U^2 M(z,0)}{1 + U^2\left(4M(z,0)^2 + \dfrac{\partial M(z,0)}{\partial z} - \dfrac{\partial M(z,0)}{\partial \tilde{\Sigma}}\right)}. \tag{B6}$$

Note that $\tilde{\Sigma}(0^+)=0$ because $M(0^+,0)=0$. For small $|z|$, we can expand the functions in Eq. (B6) as

$$M(z,0) = \frac{\partial \mathrm{Re}M(0^+,0)}{\partial \omega}\omega + \cdots, \tag{B7}$$

$$\frac{\partial M(z,0)}{\partial z} = \frac{\partial \mathrm{Re}M(0^+,0)}{\partial \omega} + i\frac{\partial^2 \mathrm{Im}M(0^+,0)}{\partial \omega^2}\omega + \cdots, \tag{B8}$$

$$\frac{\partial M(z,0)}{\partial \tilde{\Sigma}} = \mathrm{Re}\frac{\partial M(0^+,0)}{\partial \tilde{\Sigma}} + i\mathrm{Im}\frac{\partial^2 M(0^+,0)}{\partial \omega \partial \tilde{\Sigma}}\omega + \cdots. \tag{B9}$$

Here we used the fact that $\mathrm{Re}M(z,0)$ [$\mathrm{Im}M(z,0)$] is an odd (even) function, and also that Re $\partial M(z,0)/\partial \tilde{\Sigma}$ [Im $\partial M(z,0)/\partial \tilde{\Sigma}$] is an even (odd) function. This is verified by using the symmetry properties of $\rho(\epsilon)$ and $X(z,\tilde{\Sigma}(z),\epsilon,\epsilon',\epsilon'')$.

Substituting Eqs. (B7)–(B9) into Eq. (B6), we obtain for the Fermi-liquid self-energy near $z=0$

$$\tilde{\Sigma}(z) = (1 - Z^{-1})\omega + O(\omega^2), \tag{B10}$$

$$Z = \frac{1 - \left(\dfrac{U}{U_{c2}}\right)^2}{1 + \left(\dfrac{U}{U_2}\right)^2}. \tag{B11}$$

Here the quasiparticle weight has the same form as in Eq. (98) which applied to the first-order approximation. The critical values U_{c2} and U_2 are defined by

$$U_{c2}^2 = \frac{1}{-\dfrac{\partial \mathrm{Re}M(0^+,0)}{\partial \omega} + \mathrm{Re}\dfrac{\partial M(0^+,0)}{\partial \tilde{\Sigma}}}, \tag{B12}$$

$$U_2^2 = -\frac{1}{\mathrm{Re}\dfrac{\partial M(0^+,0)}{\partial \tilde{\Sigma}}}. \tag{B13}$$

Note that the right-hand sides depend also on U. U_{c2} is identical with the right-hand side of Eq. (99) when the first-order approximation is used.

Equation (B4) describes also an insulator solution $\mathrm{Im}\tilde{\Sigma}(0^+) = -\infty$. Note that $M(z,\tilde{\Sigma})$ has the following form [see Eq. (112)].

$$M(z,\tilde{\Sigma}) = M_0(z) + \frac{-\tilde{\Sigma}(z)M_1(z) + M_2(z)}{1 + \tilde{\Sigma}(z)R_1(z) - R_2(z)}. \tag{B14}$$

Here $M_0(z), M_1(z), M_2(z)$, and $R_1(z), R_2(z)$ are functions which do not contain the self-energy $\tilde{\Sigma}(z)$. For large values of $|z|$, we can expand these functions as $M_0(z) = \sum_{n=0}^{\infty} c_{2n}/z^{2n+1}$, $M_1(z) = \sum_{n=0}^{\infty} d_{2n+1}^{(1)}/z^{2n+2}$, $M_2(z) = \sum_{n=0}^{\infty} d_{2n}^{(2)}/z^{2n+1}$, $R_1(z) = \sum_{n=0}^{\infty} r_{2n}^{(1)}/z^{2n+1}$, and $R_2(z) = \sum_{n=0}^{\infty} r_{2n+1}^{(2)}/z^{2n+2}$, thereby using the symmetry relations. From the moment analysis, we can show that $c_0 = 1/4$, $d_1^{(1)} = 0$, $d_0^{(2)} = 0$, and $r_0^{(1)} = 0$ exactly. Substituting these coefficients into Eq. (B14), we obtain the moment expansion of $M(z,\tilde{\Sigma})$ as follows.

$$M(z,\tilde{\Sigma}) = \frac{c_0}{z} + \frac{c_2 + d_2^{(2)}}{z^2} - \tilde{\Sigma}(z)\frac{d_3^{(1)}}{z^4} + \cdots. \tag{B15}$$

Using the above expansion for $x=z-\tilde{\tilde{\Sigma}}(z)$ in the CPA equation $\tilde{\Lambda}^{(i)}(z)=\tilde{\tilde{\Sigma}}(z)$, we obtain a self-consistent equation for large values of $|x|$ in the form

$$zx+U^2c_0-z^2-\frac{c_2+d_2^{(2)}+d_3^{(1)}}{c_0}+\frac{z(2c_2+2d_2^{(2)}+3d_3^{(1)})}{c_0x}+\cdots=0. \tag{B16}$$

Solving the quadratic equation for x, and expanding the solution with respect to z, we obtain an insulator solution near $z=0$ as

$$\tilde{\tilde{\Sigma}}(z)=\frac{U^2-U_1^2}{4}\frac{1}{z}-\frac{2U_1^2+16d_3^{(1)}}{U^2-U_1^2}z+\cdots. \tag{B17}$$

Here

$$U_1^2=16(c_2+d_2^{(2)}+d_3^{(1)}). \tag{B18}$$

Equations (B17) and (B18) are identical with Eqs. (100) and (101) within the first-order approximation. Within the decoupling approximation the formation of a gap is determined by the first-order expansion because U_1 does not contain any moments as regards $R_1(z)$ and $R_2(z)$.

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