Three-body scattering theory of correlated hole and electron states

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We describe a theoretical scheme for the determination of quasiparticle spectra starting from the energy band structure of a metal and treating the on-site Hubbard repulsion beyond the mean-field theory. The method relies upon an expansion of the many-body states in terms of uncorrelated states with a different number of electron-hole pairs. By truncating the expansion to include configurations with one or two pairs one can achieve approximate expressions of the electron and hole self-energies. The interparticle scattering matrices appearing in such expressions are conveniently calculated using the Fadeev approach. Calculations performed for a constant density of states allow us to illustrate the role of three-body correlations in the metal-insulator transitions.

I. INTRODUCTION

It is well known that the valence electron behavior of narrow band systems, such as the elements of the d electron series and their compounds, cannot be understood using the single-particle eigenvalues derived by density functional theory within the local density (LDA) or local spin density (LSD) approximation. The discrepancy between band theoretical results and experiments is evidenced by the occurrence of satellites and band narrowing effects in photoemission and inverse photoemission valence band spectra,[1-10] by the presence of large conductivity gaps in materials for which band structure theory predicts a metallic behavior,[11-13] by the observation in magnetic materials of spin patterns, considerably more complex that those calculated,[14] etc. Both LDA and LSD rely on the assumption that the exchange and correlation effects are locally the same as in the uniform electron gas with the corresponding density. This approximation fails to reproduce the electronic behavior in the case of sufficiently localized electron states, i.e., when the Coulomb energy involved in d charge fluctuations is much larger than or comparable to the single-particle bandwidth.[15,16]

To overcome these difficulties, the Hubbard model Hamiltonian has often been used to modify single-particle spectra.[1,11,17-27] The implicit assumption is that among the various many-body terms, which are responsible of the correlation effects, the Coulomb repulsion U between electrons of opposite spins sitting on the same atom is the one which is worst treated by the local density approximations. The LDA or LSD are believed to account for the correlation effects by some sort of mean-field approximation, which corresponds to assume that each orbital is occupied by an average number of valence electrons, i.e., to neglect d local valence charge fluctuations. In a perturbation expansion in powers of U, such a theory would correspond to the first order term, which seems to indicate that standard local density approximations should be strictly appropriate for low U values, i.e., when any change in the occupancy of d levels of a given atom is locally screened by the mobile sp valence electrons. When the on-site screening of the effective Coulomb interaction is not efficient the correlation effects are to be explicitly evaluated.

Among the properties which require an accurate treatment of the correlation, the quasiparticle spectra are of great importance not only because they allow us to test the adequacy of the theoretical treatment by direct comparison with the experimental spectra, but also because they provide a direct insight into the self-energy behavior. Density functional theory is primarily devised for the calculation of ground state properties and it is not meant for excited states. Even in cases where a mean-field theory is adequate to describe the ground state, such as tetrahedrally bonded semiconductors, the excited states may be poorly described by the Kohn-Sham eigenvalues and a self-energy calculations is needed to reproduce the lowest excitations.[28] It is expected that in narrow band systems, where the ground state properties are sometimes poorly described by the single particle theory, the self-energy effects can be even more important.

In developing a theoretical treatment that improves upon the LDA or LSD description of correlation effects by including the on-site Coulomb correlation beyond the mean-field approximation, one is faced with two problems. First one has to derive approximate solutions for the model Hamiltonian since exact analytical results are not available for two and three dimensions, even for simplified band structure models. Second one has to incorporate the strong electron correlation into an *a priori* electronic structure calculation for real solids, without losing the information provided by band structure theory. While most of the studies on the Hubbard Hamiltonian are based on a simplified description of the single-particle states, the actual systems have often a complex band structure, with several orbitals contributing to the Bloch states. This limits severely the possibility of extending the results derived for simple models to the description of real systems. One way of dealing with this problem that has become very fashionable in the past few years consists in deriving a simplified one- or few-band model Hamiltonian from the LDA band structure and then solving the model problem by some approximate approach or by using advanced numerical tools.[29,30] This method has

proved to be useful to derive effective Hamiltonians for the CuO_2 sheets in high-T_c superconductors.

An alternative approach is to develop a theory where the full complexity of the band structure is kept in the kinetic term and the correlation term is treated by some approximate scheme which allows to express the ground state energy and the quasiparticle spectra in terms of the single particle orbitals and/or density of states.[17,18,22-24,26,31] This type of theory has been applied often to the study of photoemission and Auger spectra of d band systems.[1,19,21-24,32-34]

The present paper follows after this line of research. We describe a method that allows us to calculate correlation effects in solids within the framework of the Hubbard model Hamiltonian and has a rather wide range of validity. It consists of a configuration-interaction expansion of the many-body states of the interacting system, where the various configurations taken into account at a given number of particle differ for the number and the kind of electron-hole couples. This method relies upon the Fadeev theory[35-37] of the many-body scattering matrix. The interactions between configurations with the same number of electron-hole couples are represented by a set of two-body scattering t matrices, which can be calculated exactly. The Fadeev theory is used to determine the total scattering matrix and therefore the resolvent giving the energy of the many-body system. For the sake of simplicity the presentation will be restricted to the case of a one-band Hamiltonian. However, the theory with certain additional approximations has been extended to deal with the many-band case and to describe correlation effects in complex solids,[38] much in the same way as in previous work based on the t-matrix approach.[31] Since we intend to apply the theory to the description of valence band spectra provided by photoemission, inverse photoemission, Auger electron spectroscopy, and others, the emphasis in the presentation is mainly on the determination of the self-energy and the quasiparticle properties.

It will be shown that some of the approaches commonly used in the application of the Hubbard Hamiltonian to real solids, such as the t-matrix theory[17,19,23,21] or the second order perturbation theory,[18,21,22,26,37] can be obtained as different approximations to the present theory. The present approach has two main advantages: first it is not limited to particular band fillings; second it can be applied for any value of the on-site repulsion term U. Both features are a considerable improvement with respect to the previous methods since the t-matrix theory applies in the low density limit only and the various form of perturbative approaches can be adopted in the small U or high U limit. It should be noted in this respect that the most interesting physical systems, such as, for example, the high T_c superconductors or some transition metal oxides, have a significant hole density and U values comparable with the single particle bandwith, so that the above mentioned approaches are not appropriate.

The plan of the paper is the following. We present in Sec. II the configuration expansion, which is the basis of our approach. In Sec. III we illustrate the form of this expansion when many-particle states with at most two

electron-hole couples are taken into account. Explicit expressions for the self-energy within the above approximation are presented in Sec. IV. The Fadeev approach to the interconfigurations scattering is illustrated in Sec. V, where the basic equations to be solved for the self-energy determination are given when configurations with only one electron-hole pair are considered. Numerical results are displayed in Sec. VI.

II. BASIC DEFINITIONS

The Hubbard Hamiltonian in momentum space is given by

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} \hat{a}^+_{\mathbf{k}\sigma} \hat{a}_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{p}} \hat{a}^+_{\mathbf{k}+\mathbf{p},\uparrow} \hat{a}_{\mathbf{k}\uparrow} \hat{a}^+_{\mathbf{k}'-\mathbf{p},\downarrow} \hat{a}_{\mathbf{k}'\downarrow},$$

(2.1)

where $\epsilon_{\mathbf{k}\sigma}$ are the single-particle energies, U is the on-site Coulomb repulsion, and N is the number of sites. In the following we will consider a solid with N_e electrons, the ratio $n \equiv N_e/2N$ giving the band filling; the system will be supposed paramagnetic, the extension to the ferromagnetic case requiring only minor modifications.

The first term of (2.1), hereafter indicated as $\hat{H}_0$, is commonly referred to as the kinetic term; the second one will be indicated as $\hat{H}'$ and referred to as the interaction or correlation term. $\hat{H}_0$ can be regarded as a single particle Hamiltonian obtained by a self-consistent average of all the electron-electron interactions except the intra-atomic Coulomb repulsion. It does not correspond to the Hamiltonian that is currently adopted in band structure calculations by density functional theory, since in those calculations the on-site repulsive interaction is included in the self-consistent field.

In photoemission one determines the binding energy of a valence electron with lattice wave vector $\mathbf{k}$ and spin projection σ defined by

$$\omega = E(N_e - 1, \mathbf{k}\sigma) - E_G,$$

(2.2)

where E_G is the energy of the ground state of the N_e-particle system and $E(N_e - 1, \mathbf{k}\sigma)$ is the energy of the system after the removal of an electron with momentum and spin $\mathbf{k}\sigma$. One can obtain the distribution of the binding energies by evaluating the spectral function associated with the resolvent operator of the $(N_e - 1)$-particle Hamiltonian

$$\hat{G}^{(-)}(z) = \frac{\hbar}{z - \hat{H}_{N_e-1}}, \quad z = -\omega + E_G + i\delta.$$

(2.3)

In the same way the inverse photoemission experiments allow us to determine the energy of an electron added to the system given by

$$\omega = E(N_e + 1, \mathbf{k}\sigma) - E_G,$$

(2.4)

which is related to the resolvent operator

$$\hat{G}^+(z) = \frac{\hbar}{z - \hat{H}_{N_e+1}}, \quad z = \omega + E_G + i\delta.$$

(2.5)

The key quantity describing the spectroscopical results is the spectral function for hole and electron states

$$A(\mathbf{k}\sigma, \omega) = \begin{cases} -\frac{1}{\pi}\mathrm{Im}G^{(-)}(\mathbf{k}\sigma, \omega) & \text{if } \omega \leq \mu \\ +\frac{1}{\pi}\mathrm{Im}G^{(+)}(\mathbf{k}\sigma, \omega) & \text{if } \omega \geq \mu, \end{cases} \quad (2.6)$$

where μ is the chemical potential and

$$G^{(\pm)}(\mathbf{k}\sigma, \omega)$$

$$= \langle \Phi^{(\pm)}(\mathbf{k}\sigma)|\hat{G}^{(\pm)}(\pm\omega + E_G + i\delta)|\Phi^{(\pm)}(\mathbf{k}\sigma)\rangle \quad (2.7)$$

is the one particle Green function. For $\omega \geq \mu$, $A(\mathbf{k}\sigma, \omega)$ describes the angle resolved inverse photoemission spectrum and for $\omega \leq \mu$ the photoemission results.

One can express the spectral function in terms of the electron-hole self-energy by using the equation

$$G^{(\pm)}(\mathbf{k}\sigma, \omega) = \frac{\hbar}{\pm\omega \mp \epsilon_{\mathbf{k}\sigma} \mp \Sigma^{(\pm)}(\mathbf{k}\sigma, \omega)}. \quad (2.8)$$

The real part of $\Sigma^{(\pm)}$ gives the modification of the single-particle energy $\epsilon_{\mathbf{k}\sigma}$ due to correlation, while the imaginary part allows to express the density of the electron-hole quasiparticle states.

The states that appear in (2.7) are eigenstates of the noninteracting Hamiltonian $\hat{H}_0$ after the addition or the removal of an electron with momentum $\mathbf{k}$ and spin projection σ,

$$|\Phi^+(\mathbf{k}\sigma)\rangle = \hat{a}^+_{\mathbf{k}\sigma}|\Phi^0_G\rangle, \quad (2.9)$$

$$|\Phi^{(-)}(\mathbf{k}\sigma)\rangle = \hat{a}_{\mathbf{k}\sigma}|\Phi^0_G\rangle. \quad (2.10)$$

They correspond to energies

$$E_{\mathbf{k}\sigma} = E_0 \pm \epsilon_{\mathbf{k}\sigma}. \quad (2.11)$$

Here $|\Phi^0_G\rangle$ is the ground state of the noninteracting N_e-particle system of energy $E_0 = \sum_{\mathbf{k}\sigma} f(\epsilon_{\mathbf{k}\sigma})\epsilon_{\mathbf{k}\sigma}$, where $f(\epsilon_{\mathbf{k}\sigma})$ is the Fermi factor and $\epsilon_{\mathbf{k}\sigma}$ are the single-particle eigenvalues.

The presence of the Coulomb repulsion term $\hat{H}'$ causes a coupling between $|\Phi^0_G\rangle$ and the excited states of the noninteracting N_e-particle system, which differ from $|\Phi^0_G\rangle$ for the presence of electron-hole couples. They can be written according the following notation:

$$|\Phi^0_{m\{k\}}\rangle = \hat{a}^+_{\mathbf{k}_1\sigma_1}\hat{a}^+_{\mathbf{k}_2\sigma_2}\cdots\hat{a}^+_{\mathbf{k}_m\sigma_m}$$
$$\times\hat{a}_{\mathbf{k}_{m+1}\sigma_{m+1}}\cdots\hat{a}_{\mathbf{k}_{2m}\sigma_{2m}}|\Phi^0_G\rangle$$
$$= |\mathbf{k}_1\sigma_1, \mathbf{k}_2\sigma_2\cdots\mathbf{k}_m\sigma_m, \mathbf{k}_{m+1}\sigma_{m+1}\cdots\mathbf{k}_{2m}\sigma_{2m}\rangle$$
$$(2.12)$$

with

$$\mathbf{k}_1 + \mathbf{k}_2 + \cdots + \mathbf{k}_m - \mathbf{k}_{m+1} - \mathbf{k}_{m+2}\cdots - \mathbf{k}_{2m} = 0$$
$$(2.13)$$

and

$$\sigma_1 + \sigma_2 + \cdots + \sigma_m - \sigma_{m+1} - \sigma_{m+2} + \cdots - \sigma_{2m} = 0.$$
$$(2.14)$$

m indicates the number of electron-hole couples and $\{k\}$

the set of wave vectors and spin that characterize the single-particle states where electron or holes are created. Also notice that the case $m = 1$ does not give a state distinct from $|\Phi^0_G\rangle$, due to conditions (2.13) and (2.14).

The set of the *noninteracting* states $|\Phi^0_{m\{k\}}\rangle$ with $m=1,2,\ldots$ is a complete set

$$\sum_{m\{k\}} |\Phi^0_{m\{k\}}\rangle\langle\Phi^0_{m\{k\}}| = 1 \quad (2.15)$$

that can be used to represent states of the *interacting* N_e-particle system having total momentum and spin equal to zero.

Similarly the states of the N_e-1 interacting system can be expressed as linear combinations of $|\Phi^{(-)}(\mathbf{p}\eta)\rangle$ and of the states of the noninteracting system which differ from $|\Phi^{(-)}(\mathbf{p}\eta)\rangle$ for the presence of electron-hole couples such as

$$|\Phi^{(-)}_{m\{k\}}(\mathbf{p}\eta)\rangle = \hat{a}^+_{\mathbf{k}_1\sigma_1}\hat{a}^+_{\mathbf{k}_2\sigma_2}\cdots\hat{a}^+_{\mathbf{k}_m\sigma_m}$$
$$\times\hat{a}_{\mathbf{k}_{m+1}\sigma_{m+1}}\cdots\hat{a}_{\mathbf{k}_{2m}\sigma_{2m}}$$
$$\times\hat{a}_{\mathbf{k}_{2m+1}\sigma_{2m+1}}|\Phi^0_G\rangle \quad (2.16)$$

with total lattice wave vector $-\mathbf{p}$ and spin $-\eta$. The same is true for the addition af an electron, where we can define states for $|\Phi^+_{m\{k\}}(\mathbf{p}\eta)\rangle$ with total lattice wave vector $\mathbf{p}$ and spin η. The states $|\Phi^{(\pm)}(\mathbf{p}\eta)\rangle$ and $|\Phi^{(\pm)}_{m\{k\}}(\mathbf{p}\eta)\rangle$, with $m=1,2,\ldots$, constitute then a complete set which allows us to represent the states of the interacting $(N_e \pm 1)$-particle system with defined lattice wave vector $\pm\mathbf{p}$ and spin projection $\pm\eta$.

The expansion of the many-body states in terms of the above given basis sets provides a configuration-interaction theory of the correlation effects in the N_e- and $(N_e \pm 1)$-electron systems. If one truncates these expansions to some fixed value $m_{\max}$ of the electron-hole couples number, one obtains an approximate form of the Hamiltonian, which we call effective Hamiltonian $\hat{H}_{N_e\pm1}$.

III. FORM OF THE EFFECTIVE HAMILTONIAN

In order to illustrate the method and to clarify its relation with previous approaches, we present the theory for the case $m_{\max} = 2$. Let us start with the N_e-particle case. The states that constitute the basis set in the approximation $m_{\max} = 2$ are $|\Phi^0_G\rangle$ and $|\Phi^0_{2\{k\}}\rangle$, where

$$|\Phi^0_{2\{k\}}\rangle = |\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow, \mathbf{k}_4 \downarrow\rangle$$
$$= \hat{a}^+_{\mathbf{k}_1\uparrow}\hat{a}^+_{\mathbf{k}_2\downarrow}\hat{a}_{\mathbf{k}_3\uparrow}\hat{a}_{\mathbf{k}_4\downarrow}|\Phi^0_G\rangle \quad (3.1)$$

is a configuration with total momentum and spin projection equal to zero and energy equal to

$$E(\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow, \mathbf{k}_4 \downarrow) = E_0 + \epsilon_{\mathbf{k}_1\uparrow} + \epsilon_{\mathbf{k}_2\downarrow} - \epsilon_{\mathbf{k}_3\uparrow} - \epsilon_{\mathbf{k}_4\downarrow}.$$
$$(3.2)$$

As also shown in Fig. 1(c) it presents two holes of momentum $-k_3, -k_4$ and two electrons of momentum k_1, k_2; in this sense it can be called a four-particle state.
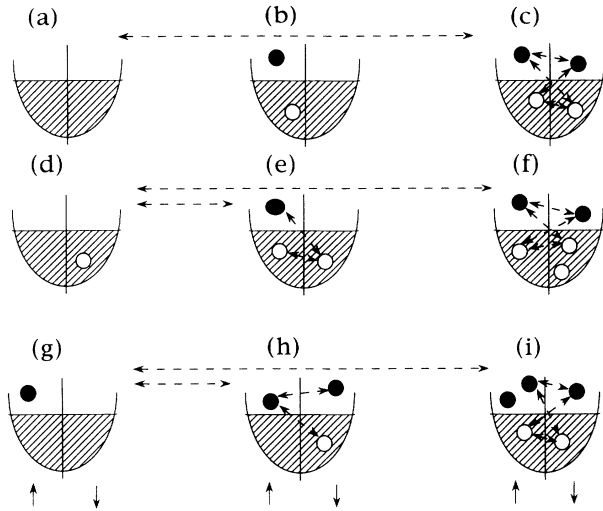
FIG. 1. Schematic representation of the basis states in the configuration expansion for the (a)–(c) N_e, (d)–(f) $N_e - 1$, and (g)–(i) $N_e + 1$ systems. Solid circles show electrons, open circles holes, and the hatched area the filled density of states. Dashed lines represent the interactions V_i, V, V', and V''.

In general the Hamiltonian for the N_e-particle system can be written as

$$\hat{H}_{N_e} = \langle \Phi_G^0 | \hat{H} | \Phi_G^0 \rangle | \Phi_G^0 \rangle \langle \Phi_G^0 |$$
$$+ \sum_{n\{k\}} \sum_{m\{k'\}} \langle \Phi_{n\{k\}}^0 | \hat{H} | \Phi_{m\{k'\}}^0 \rangle | \Phi_{n\{k\}}^0 \rangle \langle \Phi_{m\{k'\}}^0 |.$$
$$(3.3)$$

If we restrict our expansion to states with $m \leq 2$ we get the approximate Hamiltonian

$$\hat{H}_{N_e} \simeq \hat{H}_0^D + \hat{H}_4 + \hat{V}', \tag{3.4}$$

where $\hat{H}_0^D$ gives the ground state contribution and $\hat{H}_4$ those of the four-particle configurations, and $\hat{V}'$ is the interaction between the unperturbed ground state and four-particles configurations. More explicitly

$$\hat{H}_0^D = W_0 |\Phi_G^0 \rangle \langle \Phi_G^0 |, \tag{3.5}$$

$$\hat{V}' = -\frac{U}{N} \sum_{k_1 k_2 k_3 k_4} |\Phi_G^0 \rangle \langle k_4 \downarrow k_3 \uparrow k_2 \downarrow k_1 \uparrow | + \text{H.c.}, \tag{3.6}$$

$$\hat{H}_4 = \hat{H}_4^D + \hat{V}_4, \tag{3.7}$$

where

$$\hat{H}_4^D = \sum_{k_1 k_2 k_3 k_4} [W_0 + \epsilon_{k_1 \uparrow} + \epsilon_{k_2 \downarrow} - \epsilon_{k_3 \uparrow} - \epsilon_{k_4 \downarrow}]$$
$$\times | k_1 \uparrow, k_2 \downarrow, k_3 \uparrow, k_4 \downarrow \rangle \langle k_4 \downarrow, k_3 \uparrow, k_2 \downarrow, k_1 \uparrow |$$
$$(3.8)$$

with

$$W_0 = E_0 + \frac{U}{N} N_{e\uparrow} N_{e\downarrow} \tag{3.9}$$

and $N_{e\uparrow}$ ($N_{e\downarrow}$) the number of the spin up (down) electrons. Notice that the term $\hat{H}_0^D$ represents the Hamiltonian with the correlation term treated in mean-field approximation.

$\hat{V}_4$ consists of four contributions

$$\hat{V}_4 = \hat{V}_{41} + \hat{V}_{42} + \hat{V}_{43} + \hat{V}_{44} \tag{3.10}$$

corresponding to different scattering processes: (a) electron-electron scattering

$$\hat{V}_{41} = \frac{U}{N} \sum_{k_1 k_2 k_3 k_4} \sum_p |k_1 + p \uparrow, k_2 - p \downarrow, k_3 \uparrow, k_4 \downarrow \rangle$$
$$\times \langle k_4 \downarrow, k_3 \uparrow, k_2 \downarrow, k_1 \uparrow | + \text{H.c.}, \tag{3.11}$$

(b) the scattering of an electron with spin down and a hole with spin up

$$\hat{V}_{42} = -\frac{U}{N} \sum_{k_1 k_2 k_3 k_4} \sum_p |k_1 \uparrow, k_2 - p \downarrow, k_3 - p, \uparrow k_4 \downarrow \rangle$$
$$\times \langle k_4 \downarrow, k_3 \uparrow, k_2 \downarrow, k_1 \uparrow | + \text{H.c.}, \tag{3.12}$$

(c) the scattering of an electron with spin up and a hole with spin down

$$\hat{V}_{43} = -\frac{U}{N} \sum_{k_1 k_2 k_3 k_4} \sum_p |k_1 + p \uparrow, k_2 \downarrow, k_3 \uparrow, k_4 + p \downarrow \rangle$$
$$\times \langle k_4 \downarrow, k_3 \uparrow, k_2 \downarrow, k_1 \uparrow | + \text{H.c.} \tag{3.13}$$

and (d) hole-hole scattering

$$\hat{V}_{44} = \frac{U}{N} \sum_{k_1 k_2 k_3 k_4} \sum_p |k_1 \uparrow, k_2 \downarrow, k_3 - p \uparrow, k_4 + p \downarrow \rangle$$
$$\times \langle k_4 \downarrow, k_3 \uparrow, k_2 \downarrow, k_1 \uparrow | + \text{H.c.} \tag{3.14}$$

Let us consider now the case of $N_e - 1$ interacting particles where an electron of momentum and spin equal, say, to $k_0 \downarrow$ has been removed. The basis set is formed by state $|\Phi^{(-)}(k_0, \downarrow)\rangle$, which we will denote also as $|k_0 \downarrow\rangle$, with energy

$$E_{k_0 \downarrow} = E_0 - \epsilon_{k_0 \downarrow}; \tag{3.15}$$

by the states

$$|\Phi_{1\{k\}}^{(-)}(k_0 \downarrow)\rangle = |k_1 \uparrow, k_2 \downarrow, k_3 \uparrow\rangle = \hat{a}_{k_1 \uparrow}^+ \hat{a}_{k_2 \downarrow} \hat{a}_{k_3 \uparrow} |\Phi_G^0\rangle$$
$$(3.16)$$

with $k_1 - k_2 - k_3 = -k_0$ and energy

$$E(k_1 \uparrow, k_2 \downarrow, k_3 \uparrow) = E_0 + \epsilon_{k_1 \uparrow} - \epsilon_{k_2 \downarrow} - \epsilon_{k_3 \uparrow}; \tag{3.17}$$

and finally by states such as $|\Phi_{2\{k\}}^{(-)}(k_0 \downarrow)\rangle$, which we can write as

$$|k_1 \uparrow, k_2 \downarrow, k_3 \uparrow, k_4 \downarrow, k_0 \downarrow\rangle = \hat{a}_{k_1 \uparrow}^+ \hat{a}_{k_2 \downarrow}^+ \hat{a}_{k_3 \uparrow} \hat{a}_{k_4 \downarrow} \hat{a}_{k_0 \downarrow} |\Phi_G^0\rangle$$
$$(3.18)$$

with total momentum equal to $-k_0$, spin $\uparrow$ and energy

$E(\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow, \mathbf{k}_4 \downarrow, \mathbf{k}_0 \downarrow)$

$$= E_0 + \epsilon_{\mathbf{k}_1\uparrow} + \epsilon_{\mathbf{k}_2\downarrow} - \epsilon_{\mathbf{k}_3\uparrow} - \epsilon_{\mathbf{k}_4\downarrow} - \epsilon_{\mathbf{k}_0\downarrow}. \quad (3.19)$$

A pictorial representation of these states is shown in Figs. 1(d)–1(f). The basis set for the $(N_e - 1)$ particle case corresponds then to configurations with one hole (one-particle states), two holes plus one electron (three-particles states), and three holes plus two electrons (five-particle states)

The effective Hamiltonian appropriate for the $(N_e - 1)$-particle system in this approximation has the form

$$\hat{H}_{N_e-1} \simeq \hat{H}_1^D + \hat{H}_3 + \hat{H}_5 + \hat{V} + \hat{V}''. \quad (3.20)$$

The first term gives the energy of the one-hole configuration, the second describes the contributions of the three-particle configurations, and the third describes the contributions of the five-particle contributions. $\hat{V}$ and $\hat{V}''$ are the interactions between one-hole, three-particle and one-hole, five-particle configurations, respectively. More explicitly,

$$\hat{H}_1^D = W_1 |\mathbf{k}_0 \downarrow\rangle\langle\mathbf{k}_0 \downarrow |, \quad (3.21)$$

$$\hat{H}_3 = \hat{H}_3^D + \hat{V}_3, \quad (3.22)$$

$$\hat{H}_5 = \hat{H}_5^D + \hat{V}_5, \quad (3.23)$$

where

$$\hat{H}_3^D = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} \left[W_0 - \frac{U}{N}N_{e\uparrow} + \epsilon_{\mathbf{k}_1\uparrow} - \epsilon_{\mathbf{k}_2\downarrow} - \epsilon_{\mathbf{k}_3\uparrow} \right]$$
$$\times |\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow\rangle\langle\mathbf{k}_3 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_1 \uparrow |, \quad (3.24)$$

$$\hat{H}_5^D = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} [W_1 + \epsilon_{\mathbf{k}_1\uparrow} + \epsilon_{\mathbf{k}_2\downarrow} - \epsilon_{\mathbf{k}_3\uparrow} - \epsilon_{\mathbf{k}_4\downarrow}]$$
$$\times |\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow, \mathbf{k}_4 \downarrow, \mathbf{k}_0 \downarrow\rangle$$
$$\times \langle\mathbf{k}_0 \downarrow, \mathbf{k}_4 \downarrow, \mathbf{k}_3 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_1 \uparrow |. \quad (3.25)$$

Notice that

$$W_1 = E_0 - \epsilon_{\mathbf{k}_0\downarrow} + \frac{U}{N}N_{e\uparrow}(N_{e\downarrow} - 1) \quad (3.26)$$

represents the $(N_e - 1)$-particle energy with the Coulomb repulsion treated by mean-field approximation.

The term $\hat{V}_3$ describes the hole-hole and electron-hole scattering in the $m = 1$ configurations, respectively. It is given by

$$\hat{V}_3 = \hat{V}_{33} + \hat{V}_{31} \quad (3.27)$$

and

$$\hat{V}_{31} = \frac{U}{N}\sum_{\mathbf{p}}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} |\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow\rangle$$
$$\times \langle\mathbf{k}_3 \uparrow, \mathbf{k}_2 + \mathbf{p} \downarrow, \mathbf{k}_1 + \mathbf{p} \uparrow | + \text{H.c.}, \quad (3.28)$$

$$\hat{V}_{33} = -\frac{U}{N}\sum_{\mathbf{p}}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} |\mathbf{k}_1 \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_3 \uparrow\rangle$$
$$\times \langle\mathbf{k}_{3-\mathbf{p}} \uparrow, \mathbf{k}_2 + \mathbf{p} \downarrow, \mathbf{k}_1 \uparrow | + \text{H.c.} \quad (3.29)$$

The scattering processes that take place between two-electron three-hole configurations are represented by $\hat{V}_5$, which is made by the sum of the contributions from the different two-body interactions. The processes to be considered are the same occurring in $\hat{V}_4$, the only difference being that they take place in the presence of the spectator hole with momentum and spin $\mathbf{k}_0 \downarrow$. For this reason we do not give their expressions.

The term V gives the interaction between the one-hole configuration and the configurations with one electron-hole couple

$$\hat{V} = -\frac{U}{N}\sum_{\mathbf{k}_3}\sum_{\mathbf{p}} |\mathbf{k}_3 + \mathbf{p} \uparrow, \mathbf{k}_0 + \mathbf{p} \downarrow, \mathbf{k}_3 \uparrow\rangle\langle\mathbf{k}_0 \downarrow | + \text{H.c.}. \quad (3.30)$$

The interaction between the one-hole and the two-electron three-hole configurations is given by $\hat{V}''$ whose expression is

$$\hat{V}'' = -\frac{U}{N}\sum_{\mathbf{k}_1\mathbf{k}_2}\sum_{\mathbf{p}} |\mathbf{k}_0 \downarrow\rangle\langle\mathbf{k}_0 \downarrow, \mathbf{k}_2 - \mathbf{p} \downarrow, \mathbf{k}_1 + \mathbf{p} \uparrow, \mathbf{k}_2 \downarrow, \mathbf{k}_1 \uparrow | + \text{H.c.} \quad (3.31)$$

Equations (3.20)–(3.31) and their trivial extension to the case of $N_e + 1$ particles represent the form of the effective Hamiltonian.

IV. MATRIX ELEMENTS OF THE RESOLVENT AND SELF-ENERGY

To keep the notation as simple as possible we shall denote with $|s\rangle$ the single hole state $|\Phi_{0\{k\}}^{(-)}(\mathbf{k}_0 \downarrow)\rangle$, with $|t\rangle$ the two-hole one-electron states $|\Phi_{1\{k\}}^{(-)}(\mathbf{k}_0 \downarrow)\rangle$ and $|v\rangle$ the set of three-hole two-electron states $|\Phi_{2\{k\}}^{(-)}(\mathbf{k}_0 \downarrow)\rangle$. Adopting this shorthand notation, the basic equation (2.7) defining the hole Green function becomes

$$G^{(-)}(\mathbf{k}_0 \downarrow, \omega) = \langle s|\hat{G}^{(-)}(z)|s\rangle , \quad z = -\omega + E_G + i\delta. \quad (4.1)$$

The matrix elements of the resolvent $\hat{G}^{(-)}(z)$ of the effective Hamiltonian can be determined considering the following relations:

$$\hat{G}^{(-)}(z) = \hat{F}_3(z) + \hat{F}_3(z)[\hat{H}_1^\Delta + \hat{V} + \hat{V}'' + \hat{H}_5]\hat{G}^{(-)}(z)$$
$$+ \hat{F}_5(z) + \hat{F}_5(z)(\hat{H}_1^\Delta + \hat{V} + \hat{V}'' + \hat{H}_3)\hat{G}^{(-)}(z), \quad (4.2)$$

where

$$\hat{F}_3(z) = \frac{1}{z - \hat{H}_3}, \quad (4.3)$$

$$\hat{F}_5(z) = \frac{1}{z - \hat{H}_5} \quad (4.4)$$

are the resolvents for the three- and five-particle Hamiltonians, respectively.

Using the previous equations one can easily derive the following expression for the Green function:

$$G_{ss}(z) = \frac{1}{z - W_1 - \sum_{tt'} F_{3tt'} V_{t's} V_{st} - \sum_{vv'} F_{5vv'} V''_{v's} V''_{sv}},$$

$$\tag{4.5}$$

with the notation $G_{ij} \equiv \langle i|G^{(-)}|j\rangle$, $F_{3tt'} \equiv \langle t|\hat{F}_3|t'\rangle$, etc. This equation allows us to express the effective Hamiltonian resolvent in terms of the resolvents of the three- and five-particle Hamiltonians. From Eq. (2.8) we notice that the determination of the excitation energies of the $N_e - 1$ interacting particles as poles of the Green function can be reduced to the calculation of self-energy which in turn can be expressed, according to our theory, in terms of the matrix elements of $\hat{F}_3$ and $\hat{F}_5$ and of the ground state energy. Indeed by comparing Eq. (2.8) with Eq. (4.5) one obtains, for the hole self-energy,[39]

$$\Sigma^{(-)}(\omega) = E_G - W_0 + \frac{U}{N}N_{e\uparrow} - \sum_{tt'} V_{st} F_{3tt'} V_{t's}$$
$$- \sum_{vv'} V''_{sv} F_{5vv'} V''_{v's}. \tag{4.6}$$

The ground state energy E_G, calculated consistently with the configurations chosen to describe the $N_e - 1$ system, turns out to be given by

$$E_G = W_0 + \sum_{ff'} V'_{0f} F_{4ff'} V'_{f'0}, \tag{4.7}$$

where

$$\hat{F}_4(z) = \frac{1}{z - \hat{H}_4}, \tag{4.8}$$

and, for simplicity, $|0\rangle$ is the noninteracting ground state and $|f\rangle$ is the two-hole two-electron states $|\Phi^0_{2\{k\}}\rangle$.

The electron self-energy can be derived from the effective Hamiltonian for the $N_e + 1$ particles by following the same procedure. The result for an electron added in the state $\mathbf{k}_0 \downarrow$ is given by

$$\Sigma^{(+)}(\omega) = -E_G + W_0 + \frac{U}{N}N_{e\uparrow} + \sum_{tt'} V_{st} F_{3tt'} V_{t's}$$
$$+ \sum_{vv'} V''_{sv} F_{5vv'} V''_{v's}, \tag{4.9}$$

where $\hat{F}_3$ and $\hat{F}_5$ represent the resolvents for the two-electron one-hole and three-electron and two-hole configurations, respectively.

V. FADEEV EQUATIONS FOR THE INTERCONFIGURATIONS SCATTERING

The determination of the resolvent $\hat{F}_i$ defined in the preceding section is by no means trivial. To deal with the problem it has been proposed[35,36] to adopt the Fadeev approach to the scattering matrix from a potential that is the sum of different interactions. In this section we illustrate the basic equations of the method.

According to the definitions (4.3), (4.4), and (4.8), the resolvents $\hat{F}_i$ refer to Hamiltonians which can be separated in diagonal ($\hat{H}_i^D$) and off-diagonal ($\hat{V}_i$) terms [see Eqs. (3.7), (3.22), and (3.23)], which in turn can be treated as unperturbed and perturbation terms, respectively. We can then write $\hat{F}_i$ as

$$\hat{F}_i = \hat{F}_i^D + \hat{F}_i^D \hat{V}_i \hat{F}_i \tag{5.1}$$

or

$$\hat{F}_i = \hat{F}_i^D + \hat{F}_i^D \hat{J}_i \hat{F}_i^D, \tag{5.2}$$

having defined $\hat{J}_i$ as the scattering operator

$$\hat{J}_i = \hat{V}_i + \hat{V}_i \hat{F}_i^D \hat{J}_i \tag{5.3}$$

and $\hat{F}_i^D$ the "free" resolvent

$$\hat{F}_i^D = \frac{1}{z - \hat{H}_i^D}. \tag{5.4}$$

Expression (5.2) can be used without any further development to get a first comparison with previous work. In fact in Appendix B we show that the results of second order perturbation theory[18,26] are regained in the present context including configurations up to $m = 2$ and approximating the full resolvents $\hat{F}_4$, $\hat{F}_3$, and $\hat{F}_5$ with the free resolvents $\hat{F}_4^D$, $\hat{F}_3^D$, and $\hat{F}_5^D$.

Our goal, however, is to obtain an expression of self-energy valid for any interaction regime; for this reason we need an expression for the full resolvent $\hat{F}_i$. From now on we will show how to get it, reducing, however, the number of configurations to $m_{\max} = 1$, in order to make the problem more tractable. In this case the ground state energy of the N_e-particle system is $E_G = W_0$ while the electron-hole self-energy is given by

$$\Sigma^{(\pm)}(\omega) = \frac{U}{N}N_{e\uparrow} \pm \sum_{tt'} V_{st} F_{3tt'} V_{t's}. \tag{5.5}$$

In the $N_e - 1$ case the only resolvent to be calculated is $\hat{F}_3$

$$\hat{F}_3 = \hat{F}_3^D + \hat{F}_3^D \hat{J}_3 \hat{F}_3^D \tag{5.6}$$

with

$$\hat{J}_3 = \hat{V}_3 + \hat{V}_3 \hat{F}_3^D \hat{J}_3 = (\hat{V}_{33} + \hat{V}_{31}) + (\hat{V}_{33} + \hat{V}_{31})\hat{F}_3^D \hat{J}_3. \tag{5.7}$$

We can define the partial scattering operators $\hat{J}_{33}$ and $\hat{J}_{31}$

$$\hat{J}_3 = \hat{J}_{33} + \hat{J}_{31} \tag{5.8}$$

with

$$\hat{J}_{33} = \hat{V}_{33} + \hat{V}_{33}\hat{F}_3^D \hat{J}_3, \tag{5.9}$$

$$\hat{J}_{31} = \hat{V}_{31} + \hat{V}_{31}\hat{F}_3^D \hat{J}_3. \tag{5.10}$$

By introducing in (5.9) and (5.10) the scattering matrices for each single potential term defined as

$$\hat{T}_{31} = \hat{V}_{31} + \hat{V}_{31}\hat{F}_3^D \hat{T}_{31}, \tag{5.11}$$

$$\hat{T}_{33} = \hat{V}_{33} + \hat{V}_{33}\hat{F}_3^D \hat{T}_{33}, \tag{5.12}$$

we get, after some manipulation,

$$\hat{J}_{33} = \hat{T}_{33} + \hat{T}_{33}\hat{F}_3^D \hat{J}_{31}, \tag{5.13}$$

$$\hat{J}_{31} = \hat{T}_{31} + \hat{T}_{31}\hat{F}_3^D \hat{J}_{33}, \tag{5.14}$$

which are the Fadeev equations to be solved in order to get $\hat{J}_3$ from (5.8), $\hat{F}_3$ from (5.6), and finally $\Sigma^{(-)}$ from (5.5).

The derivation of the integral equation to be solved for the self-energy determination is given in Appendix A. We can summarize the main results as follows: For a given density of band states $n(\epsilon)$ and a given U (i) calculate

$$g_1(\omega) = \int_{-\infty}^{E_f} d\epsilon' \int_{E_f}^{\infty} d\epsilon \frac{n(\epsilon)n(\epsilon')}{\omega - \epsilon' + \epsilon - i\delta}, \tag{5.15}$$

$$g_2(\omega) = \int_{-\infty}^{E_f} d\epsilon' \frac{n(\epsilon')}{\omega - \epsilon' - i\delta}, \tag{5.16}$$

$$g_3(\omega) = \int_{-\infty}^{E_f} d\epsilon' \int_{-\infty}^{E_f} d\epsilon \frac{n(\epsilon)n(\epsilon)}{\omega - \epsilon' - \epsilon - i\delta}, \tag{5.17}$$

$$T_{31}(\omega) = \frac{-U}{1 - Ug_1(\omega)}, \tag{5.18}$$

$$T_{33}(\omega) = \frac{U}{1 + Ug_3(\omega)}, \tag{5.19}$$

$$K(\omega, \epsilon, \epsilon') = \int_{-\infty}^{E_f} d\epsilon'' \, n(\epsilon'') \, g_2(\omega + \epsilon'' - \epsilon)T_{31}(\omega + \epsilon'')$$
$$\times g_2(\omega + \epsilon'' - \epsilon')T_{33}(\omega - \epsilon''), \tag{5.20}$$

$$B(\omega, \epsilon) = \int_{-\infty}^{E_f} d\epsilon' \, n(\epsilon') \, g_2(\omega + \epsilon' - \epsilon)T_{31}(\omega + \epsilon')$$
$$\times \left(g_1(\omega - \epsilon') + \int_{E_f}^{\infty} d\epsilon'' \, n(\epsilon'') \, g_2(\omega + \epsilon' - \epsilon'') \right.$$
$$\left. \times g_3(\omega - \epsilon'')T_{33}(\omega - \epsilon'') \right); \tag{5.21}$$

(ii) solve the integral equation

$$A(\omega, \epsilon) = B(\omega, \epsilon) + \int_{E_f}^{\infty} d\epsilon' \, n(\epsilon') \, K(\omega, \epsilon, \epsilon')A(\omega, \epsilon'); \tag{5.22}$$

(iii) calculate

$$\Sigma^{(-)}(\omega) = U\frac{N - N_{e\uparrow}}{N} - \int_{E_f}^{\infty} d\epsilon \, n(\epsilon) \, T_{33}(\omega - \epsilon)$$
$$\times [1 + UA(\omega - \epsilon)]; \tag{5.23}$$

(iv) and get the hole quasiparticle spectrum

$$D^{(-)}(\omega) = -\frac{1}{\pi}\text{Im} \int_{-\infty}^{E_f} d\epsilon \, n(\epsilon) \, \frac{1}{\omega - \epsilon - \Sigma^{(-)}(\omega)},$$
$$\omega \leq \mu. \tag{5.24}$$

In order to get the self-energy for the N_e+1 system the same procedure must be followed, but changing the integrations over empty states into integrations over filled states and vice versa. The electron self-energy and quasiparticle spectrum are calculated as

$$\Sigma^{(+)}(\omega) = -\frac{U}{N}N_{e\uparrow} + \int_{-\infty}^{E_f} d\epsilon \, n(\epsilon) \, T_{33}(\omega - \epsilon)$$
$$\times [1 + UA(\omega - \epsilon)], \tag{5.25}$$

$$D^{(+)}(\omega) = +\frac{1}{\pi}\text{Im} \int_{E_f}^{\infty} d\epsilon \, n(\epsilon) \, \frac{1}{\omega - \epsilon - \Sigma^{+}(\omega)}, \quad \omega \geq \mu. \tag{5.26}$$

Since the present theory has been developed for $m_{\max} = 1$, the ground state energy of the N_e-particle system is the noninteracting one. As a consequence the chemical potential μ, whose value is essential in order to define the density of quasiparticle states for holes and electrons, coincides with the single-particle Fermi level E_f.

VI. NUMERICAL CALCULATIONS AND RESULTS

The system under consideration is characterized by the density of single-particle band states $n(\epsilon)$ and by the parameter U describing the on-site correlation. These quantities enter the definition of self-energy according to the theory outlined in Sec. V.

The solution of the integral equation (5.22) is the only computationally demanding step of the procedure. By taking advantage of the kernel being degenerate, one can transform the integral equation in a system of algebraic equations whose solution can be approached by standard numerical algorithms. In the definitions (5.15)–(5.17) a value of $\delta = 10^{-5}$–10^{-6} has been used. It is useful to define some quantities such as the bottom E_1 and the top of the band E_2; the band amplitude is $W = E_2 - E_1$, and $W_1 = E_f - E_1$, and $W_2 = E_2 - E_f$ are the occupied and the empty portion of the band, respectively. We can make the identifications $\frac{W_1}{W} = \frac{N_{e\uparrow}}{N}$ and $\frac{W_2}{W} = \frac{N - N_{e\uparrow}}{N}$, defining the band occupancy as $n = \frac{W_1}{W}$. We have chosen $W = 2.5$ eV.

The results we are going to discuss concern self-energies and spectral function for a system described by a constant single-particle density of states; we are interested in various regimes characterized by different band fillings and different values of the parameter U. Upon increasing U we expect two main effects: first and most important, the system must exhibit the Mott-Hubbard transition from a metallic situation to an insulating one; second, for sufficiently large U the t matrices exhibit real poles corresponding to bound states of hole-hole or electron-hole couples.

We start by considering the case of a half filled band ($n = 0.5$). Figure 2 shows the results of the present theory for hole and electron states in the case of $\frac{U}{W} = 0.5$. We notice in particular the nonzero value of the real part of self-energy at the Fermi level and the symmetric behavior of the two self-energies

$$\Sigma_r^{(-)}(\omega) = -\Sigma_r^{+}(2E_f - \omega), \tag{6.1}$$

which is an obvious consequence of the symmetry of our model system. Here and in the following $\Sigma_r^{(\pm)}$ and
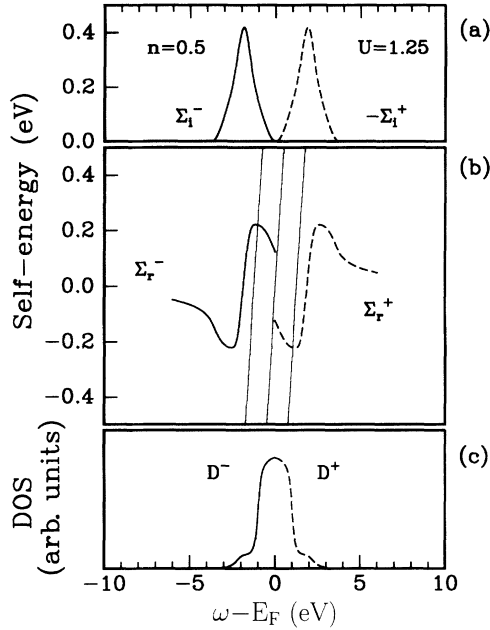
FIG. 2. Self-energy and density of quasiparticle states for hole (continuous line) and electron (dashed line) states calculated for $\frac{U}{W} = 0.5$ and for a constant density of states at half occupation. (a) The imaginary part $\Sigma_i^{(-)}$ and $-\Sigma_i^{(+)}$ of self-energy, (b) the real part $\Sigma_r^{(\pm)}$, and (c) the density of quasiparticle states. Energies are referred to E_f. The band amplitude is $W = 2.5$. The three straight lines correspond to $\omega - E_1$, $\omega - E_f$, and $\omega - E_2$.

$\Sigma_i^{(\pm)}$ indicate the real and the imaginary part of the self-energy, respectively.

As we expect, the self-energy correction is small in this case and the density of quasiparticle states is similar to the density of single-particle states, except for the presence of a satellite structure both in the filled and the empty part of the spectrum. The quasiparticle spectrum we get is not qualitatively different from the results of perturbative approaches: the system in particular maintains its metallic character. The system is still metallic for $\frac{U}{W} = 1$ (see Fig. 3), even if now the self-energy corrections are much larger, giving rise to satellite structures of stronger spectral weight at the two sides of the main structure.

By increasing U we expect the Mott-Hubbard transition to occur. Figures 4 and 5 show the quasiparticle spectra obtained for $\frac{U}{W} = 2$ and $\frac{U}{W} = 3$, respectively: the system is now an insulator with a finite gap between hole and electron quasiparticle states. It is interesting to proceed to a graphic identification of the quasiparticle states. According to (5.24) and (5.26) quasiparticle states correspond to the zeros of $\omega - E - \Sigma^{\pm}(\omega)$. It is therefore useful to look at the interceptions of the lines $\omega - E$ ($E_1 \leq E \leq E_f$ and $E_f \leq E \leq E_2$ for holes and electrons, respectively) and the curve representing the real part of $\Sigma^{\pm}(\omega)$. In Figs. 4 and 5 the lines $\omega - E_1$, $\omega - E_f$, and $\omega - E_2$ are reported. Each of these lines intercepts twice the curve Σ_r^{-}: one interception occurs in a region where the imaginary part of the self-energy is very small, giv-
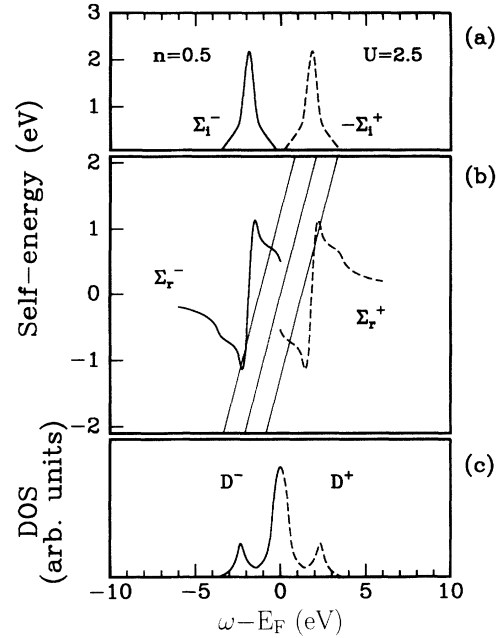

FIG. 3. Same as Fig. 2 with $\frac{U}{W} = 1$.

ing rise to a bound state; the other interception occurs in a region where the imaginary part of the self-energy has a maximum. In this energy region we find therefore a complex pole of the Green function, which is a state of finite lifetime or satellite.

We want to stress that the finite jump in the $\Sigma_r^{(\pm)}$ at E_f is essential in order to get the metal insulator transition. Due to the symmetry requirement (6.1), the absence of a jump on passing from $\Sigma_r^{(-)}$ to $\Sigma_r^{(+)}$ would correspond to $\Sigma_r^{(\pm)}(E_f) = 0$ and therefore to real poles in the spectral
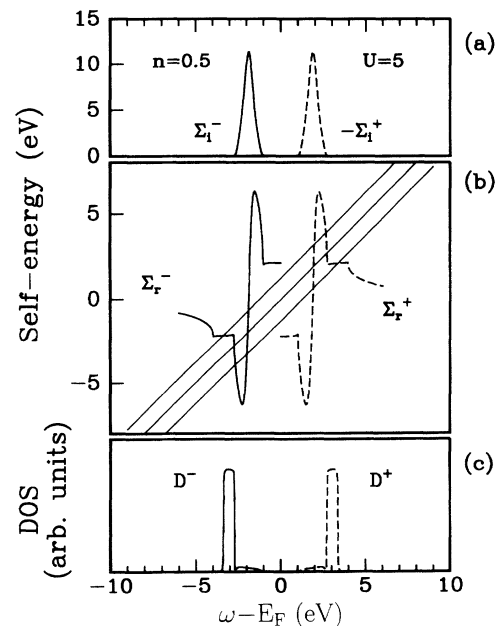

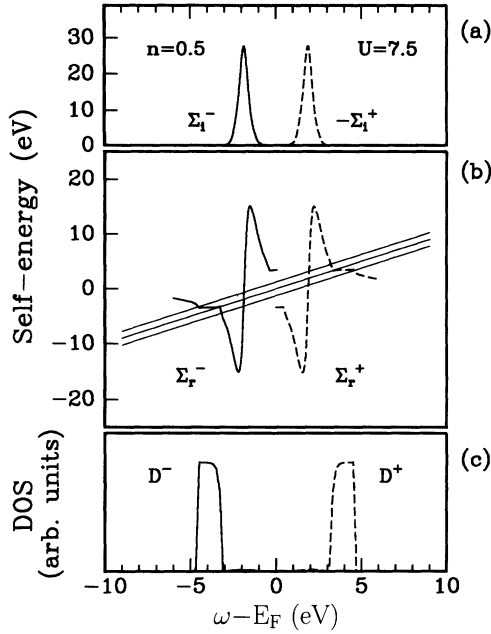FIG. 4. Same as Fig. 2 with $\frac{U}{W} = 2$.

FIG. 5.   Same as Fig. 2 with $\frac{U}{W} = 3$.

function around E_f, both in the hole and the electron part of the spectrum, giving rise to a metallic behavior.

Another point that should be noticed is that, unlike what is found in Figs. 2 and 3 for low U values, the real and the imaginary part of the self-energies reported in Figs. 4 and 5 do not seem to be related by the usual Kramers-Kronig relations. An analysis of the behavior of the scattering matrices T_{31} and T_{33}, which for the present model system have particularly simple expressions, would show in fact that for $\frac{U}{W} > \frac{W}{W_1}\frac{1}{2\ln 2}$ the scattering matrices exhibit poles on the real axis and therefore their real and imaginary parts are not linked by the Kramers-Kronig relations in the usual form, since the singularities on the real axis have to be explicitly included in the dispersion relations.[40] For $\frac{U}{W}$ larger than the above mentioned value the same is true of the real and the imaginary part of the self-energy.

We go on increasing U. It is well known that for very large $\frac{U}{W}$, i.e., in the so-called atomic limit, the Hubbard Hamiltonian can be solved exactly.[41] It has already been shown[35] that the present theory with $n_{max} = 1$ reproduces correctly the atomic limit. Indeed one can easily show that for $\frac{U}{W} \to \infty$ the expressions (5.23) and (5.25) of the self-energy become

$$\Sigma^{(\pm)}(\omega) = \frac{W_1}{W}\frac{W_2}{W}\frac{U^2}{\omega - \epsilon + U\left(1 - \frac{W_1}{W}\right)}, \qquad (6.2)$$

giving rise, in the case of a half filled band, to the one-particle Green function

$$G^{(\pm)}(\omega) = \frac{1}{2}\frac{1}{\omega - \epsilon \pm \frac{U}{2}}, \qquad (6.3)$$

where ϵ is the center of gravity of the density of band states. The hole and electron spectra consist then of a single peak at $\omega = \epsilon - \frac{U}{2}$ and $\omega = \epsilon + \frac{U}{2}$, respectively, and the system exhibits a Mott-Hubbard gap equal to U.

Figure 6 shows the results of the present theory for the case of a large but finite value of $\frac{U}{W}$, that is, $\frac{U}{W} = 8$. We can identify the value of the chemical potentials $\mu^{\pm}$

$$\mu^- = E_f + \Sigma_r^{(-)}(\mu^-), \qquad (6.4)$$

$$\mu^+ = E_f + \Sigma_r^{(+)}(\mu^+) \qquad (6.5)$$

by looking at the interception of the line $\omega - E_f$ with the curve representing $\Sigma_r^{(\pm)}(\omega)$. For $\frac{U}{W} = 8$ at half filling we find $\mu^{(\pm)} \simeq \pm\frac{U}{2}$ and an energy separation between the spectral functions for hole and electron states of about U.

We have also considered the same model density of states with a band occupation of $n = 0.8$. Figures 7–10 display the results of the present theory at different U. We expect the result for very large U to reproduce again the atomic limit. This is just the case for $\frac{U}{W} = 8$, where the quasiparticle density of states presents a gap of the order of U. The metallic character is obtained for $\frac{U}{W} \leq 1$.

The graphic identification of quasiparticle energies as interceptions between the curve $\Sigma_r^{(\pm)}(\omega)$ and the straight lines reported in Figs. 4, 5, 8, and 9 allows us to identify a regime for the metal-insulator transition. In fact it appears that if the condition

$$\Sigma_r^{(-)}(E_f) > W_1 \qquad (6.6)$$

or

$$|\Sigma_r^+(E_f)| > W_2 \qquad (6.7)$$

is satisfied, no quasiparticle state can exist at E_f in either the hole or the electron part of the spectrum and the system turns out to be an insulator. This behavior is found here for $\frac{U}{W} > 1$.
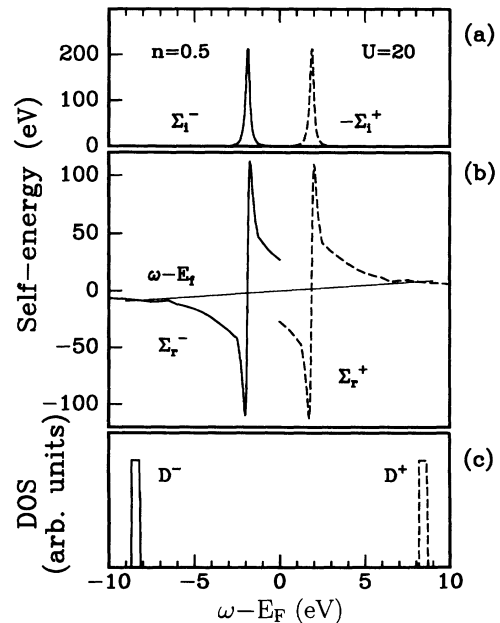

FIG. 6.   Same as Fig. 2 with $\frac{U}{W} = 8$. The straight line corresponding to $\omega - E_f$ is reported.
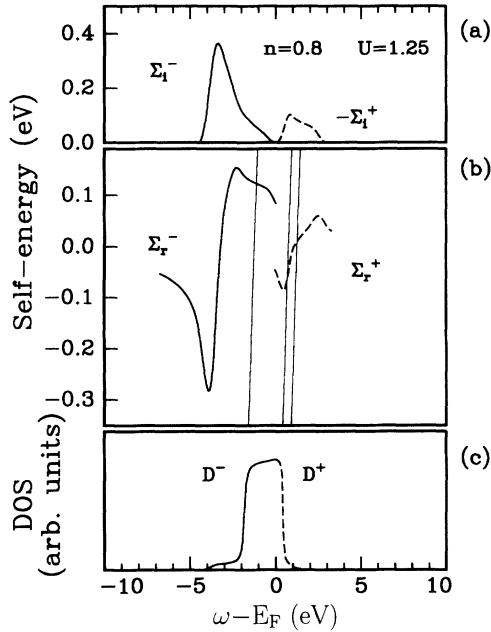
FIG. 7. Self-energy and density of quasiparticle states for hole (continuous line) and electron (dashed line) states calculated with $\frac{U}{W} = 0.5$ for a constant density of states and occupation $n = 0.8$. (a) The imaginary part $\Sigma_i^{(-)}$ and $-\Sigma_i^{(+)}$ of self-energy, (b) the real part $\Sigma_r^{(\pm)}$, and (c) the density of quasiparticle states. The band amplitude is $W = 2.5$. Energies are referred to E_f. The three straight lines correspond to $\omega - E_1$, $\omega - E_f$, and $\omega - E_2$.

It is interesting to compare the results of the present theory with the outcomes of the t-matrix approach.[19,31] Figure 11 shows such a comparison in terms of hole states calculated according to the two methods for an occupation $n = 0.8$. It turns out that for values of $\frac{U}{W} < 1$ the
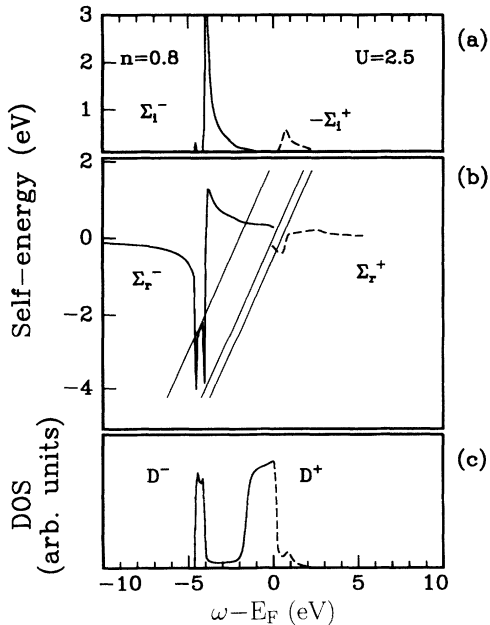

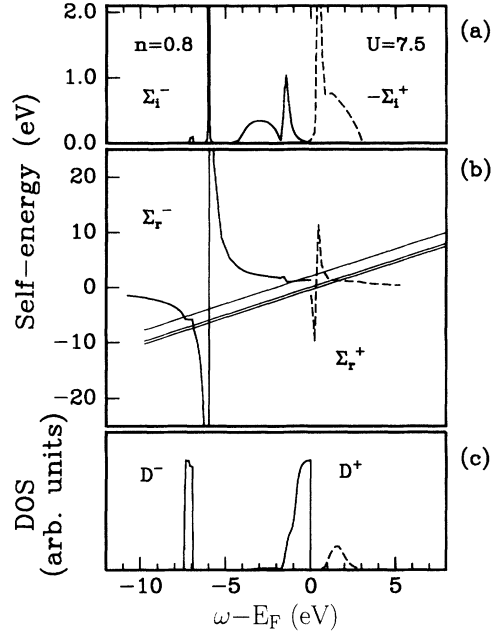FIG. 8. Same as Fig. 7 with $\frac{U}{W} = 1$.

FIG. 9. Same as Fig. 7 with $\frac{U}{W} = 3$.

differences between the two calculated spectra become negligible. Even if the t-matrix approach is commonly believed to be valid only in the case of either almost filled or almost empty bands, this comparison shows that its range of validity is much wider and it depends on the value of the correlation parameter.

VII. CONCLUSIONS

The approach we have described provides a general framework to introduce Hubbard corrections into band
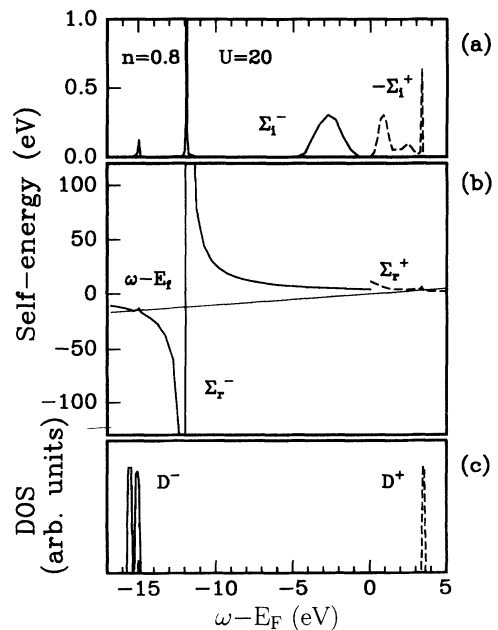

FIG. 10. Same as Fig. 7 with $\frac{U}{W} = 8$. The straight line corresponding to $\omega - E_f$ is reported.
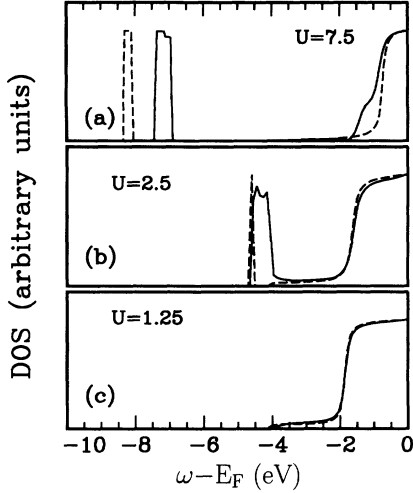
FIG. 11. Density of quasiparticle hole states obtained by the present theory (continuous line) and by the t-matrix approach (dashed line) for a constant density of states and (a) $\frac{U}{W} = 3$, (b) $\frac{U}{W} = 1$, and (c) $\frac{U}{W} = 0.5$.

structure calculations without any limitation on the value of U and of the carrier density. For a single band or for highly symmetric systems the only quantity that is needed is the density of band states which enters the definition of self-energy through Eqs. (A13) and (5.23). The theory can be extended to the more general case of many bands with different symmetry along the lines followed to extend the t-matrix approach[31] and to deal with magnetic phases, provided a local approximation is adopted.

The numerical results we have presented illustrate the general features of the predicted behavior for a single-band system as a function of the U value and of the band filling and, in particular, the presence of satellite struvctures and the occurrence of the metal-insulator transition. We have shown the conditions under which the transition can occur when only configurations with $m_{\max} = 1$ are considered in the expansion of the states for $(N_e \pm 1)$-particle system. It is not clear at present how these conditions are modified if configurations with a higher electron-hole couple number are considered. As we pointed out, in the low U limit, where perturbation theory is expected to hold, the discontinuity at the Fermi level should go to zero as a consequence of the fact that the correction to the ground state energy of the N_e-particle system is introduced by four-particle states. On the other hand, in the large U range the discontinuity has to be found in order to recover the atomic limit and even if the values for which the metal-insulator transition takes place might be slightly different from those predicted by the present theory, we do not expect dramatic changes in the qualitative behavior of the system.

The present theory with $m = 1$ and with the local approximations can be used to study realistic systems with many hybridizing bands. It will be interesting to apply it to transition metal oxides which have a large U value and show a metal-insulator transition.

APPENDIX A:
FORM OF THE INTEGRAL EQUATION

According to (5.5) what is actually needed is the sum

$$\sum_{tt'} V_{st} F_{3tt'} V_{t's} = \left(\frac{U}{N}\right)^2 \sum_{tt'} [\hat{F}_3^D + \hat{F}_3^D (J_{31}$$

$$+ \hat{T}_{33} + \hat{T}_{33} \hat{F}_3^D J_{31}) \hat{F}_3^D]_{tt'} \qquad (A1)$$

and therefore it is useful to express the previous quantities in terms of matrix elements between three-particles states $|t\rangle$ (here $|t\rangle = |\mathbf{Q}_1 \uparrow, \mathbf{Q}_2 \downarrow, \mathbf{Q}_3 \uparrow\rangle$ and we consider the case of an electron removed from $\mathbf{k}_0 \downarrow$). For the diagonal resolvent one has

$$\langle t|\hat{F}_3^D|t\rangle$$

$$= \frac{U}{N} \frac{1}{z - E_0 - \epsilon_{\mathbf{Q}_1\uparrow} + \epsilon_{\mathbf{Q}_2\downarrow} + \epsilon_{\mathbf{Q}_3\uparrow} - \frac{U}{N} N_{e\uparrow}(N_{e\downarrow} - 1)}.$$
$$(A2)$$

One can easily determine from (5.11) and (5.12) the elements of the scattering matrices in the form

$$T_{33}(z - \epsilon_{\mathbf{Q}_1\uparrow}) = \langle t|\hat{T}_{33}|t'\rangle$$
$$= \frac{U}{N} \frac{1}{1 - U g_3(z - \epsilon_{\mathbf{Q}_1\uparrow})} \delta_{\mathbf{Q}_1, \mathbf{Q}_1'}, \qquad (A3)$$

$$T_{31}(z + \epsilon_{\mathbf{Q}_3\uparrow}) = \langle t|\hat{T}_{31}|t'\rangle$$
$$= -\frac{U}{N} \frac{1}{1 + U g_1(z + \epsilon_{\mathbf{Q}_3\uparrow})} \delta_{\mathbf{Q}_3, \mathbf{Q}_3'}, \qquad (A4)$$

having defined

$$g_3(z - \epsilon_{\mathbf{Q}_1\uparrow}) = \frac{1}{N} \sum_{\mathbf{Q}_3} \sum_{\mathbf{Q}_2} f(\epsilon_{\mathbf{Q}_3\uparrow}) f(\epsilon_{\mathbf{Q}_2\downarrow}) \langle t|\hat{F}_3^D|t\rangle$$
$$\times \delta_{\mathbf{Q}_3 + \mathbf{Q}_2, \mathbf{Q}_1 + \mathbf{k}_0}, \qquad (A5)$$

$$g_1(z + \epsilon_{\mathbf{Q}_3\uparrow}) = \frac{1}{N} \sum_{\mathbf{Q}_1} \sum_{\mathbf{Q}_2} [1 - f(\epsilon_{\mathbf{Q}_1\uparrow})] f(\epsilon_{\mathbf{Q}_2\downarrow})$$
$$\times \langle t|\hat{F}_3^D|t\rangle \delta_{\mathbf{Q}_3 + \mathbf{Q}_2, \mathbf{Q}_1 + \mathbf{k}_0}. \qquad (A6)$$

In the following

$$g_2(z - \epsilon_{\mathbf{Q}_1\uparrow} + \epsilon_{\mathbf{Q}_3\uparrow}) = \frac{1}{N} \sum_{\mathbf{Q}_2} f(\epsilon_{\mathbf{Q}_2\downarrow}) \langle t|\hat{F}_3^D|t\rangle \delta_{\mathbf{Q}_3 + \mathbf{Q}_2, \mathbf{Q}_1 + \mathbf{k}_0}$$
$$(A7)$$

will also be used. All these matrix elements, involving the free resolvent can be easily determined from properties of the noninteracting system.

We introduce now the quantity

$$A(z - \epsilon_{\mathbf{Q}_1\uparrow}) = \sum_{\mathbf{Q}_2\mathbf{Q}_3} \sum_{\mathbf{Q}_1'\mathbf{Q}_2'\mathbf{Q}_3'} \langle t|\hat{F}_3^D|t\rangle \langle t|\hat{J}_{31}|t'\rangle \langle t'|\hat{F}_3^D|t'\rangle \delta_{\mathbf{Q}_1+\mathbf{Q}_2,\mathbf{Q}_3+\mathbf{k}_0} \delta_{\mathbf{Q}_1'+\mathbf{Q}_2',\mathbf{Q}_3'+\mathbf{k}_0},$$ (A8)

which allows us to write Eq. (A1) as

$$\sum_{tt'} V_{st} F_{3tt'} V_{t's} = \left(\frac{U}{N}\right)^2 \sum_{\mathbf{Q}_1}[1 - f(\epsilon_{\mathbf{Q}_1\uparrow})] \{g_3(z - \epsilon_{\mathbf{Q}_1\uparrow}) + A(z - \epsilon_{\mathbf{Q}_1\uparrow})$$

$$+g_3(z - \epsilon_{\mathbf{Q}_1\uparrow})T_{33}(z - \epsilon_{\mathbf{Q}_1\uparrow})g_3(z - \epsilon_{\mathbf{Q}_1\uparrow}) + g_3(z - \epsilon_{\mathbf{Q}_1\uparrow})T_{33}(z - \epsilon_{\mathbf{Q}_1\uparrow})A(z - \epsilon_{\mathbf{Q}_1\uparrow})\}.$$ (A9)

One can derive from the Fadeev equations an integral equation for $A(z-\epsilon_{\mathbf{Q}_1\uparrow})$ by (i) inserting (5.13) into (5.14); (ii) multiplying each member of the resulting equation by $\langle t|\hat{F}_3^D|t\rangle$, and $\langle t'|\hat{F}_3^D|t'\rangle$; and finally (iii) summing up over $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_1', \mathbf{Q}_2'\mathbf{Q}_3'$ to get

$$A(z - \epsilon_{\mathbf{Q}_1\uparrow}) = B(z - \epsilon_{\mathbf{Q}_1\uparrow})$$
$$+ \sum_{\mathbf{Q}_1'}[1 - f(\epsilon_{\mathbf{Q}_1'\uparrow})]$$
$$\times K(z, \epsilon_{\mathbf{Q}_1\uparrow}, \epsilon_{\mathbf{Q}_1'\uparrow})A(z - \epsilon_{\mathbf{Q}_1'\uparrow})$$ (A10)

with

$$B(z - \epsilon_{\mathbf{Q}_1\uparrow}) = \sum_{\mathbf{Q}_3'} f(\epsilon_{\mathbf{Q}_3'\uparrow})g_2(z + \epsilon_{\mathbf{Q}_3'\uparrow} - \epsilon_{\mathbf{Q}_1\uparrow})$$
$$\times T_{31}(z + \epsilon_{\mathbf{Q}_3'\uparrow})\{g_1(z + \epsilon_{\mathbf{Q}_3'\uparrow})$$
$$+ \sum_{\mathbf{Q}_1'}[1 - f(\epsilon_{\mathbf{Q}_1'\uparrow})]g_2(z + \epsilon_{\mathbf{Q}_3'\uparrow} - \epsilon_{\mathbf{Q}_1'\uparrow})$$
$$\times g_3(z - \epsilon_{\mathbf{Q}_1'\uparrow})T_{33}(z - \epsilon_{\mathbf{Q}_1'\uparrow})\}$$ (A11)

and

$$K(z, \epsilon_{\mathbf{Q}_1\uparrow}, \epsilon_{\mathbf{Q}_1'\uparrow}) = \sum_{\mathbf{Q}_3'} f(\epsilon_{\mathbf{Q}_3'\uparrow})g_2(z + \epsilon_{\mathbf{Q}_3'\uparrow} - \epsilon_{\mathbf{Q}_1\uparrow})$$
$$\times T_{31}(z + \epsilon_{\mathbf{Q}_3'\uparrow})g_2(z + \epsilon_{\mathbf{Q}_3'\uparrow} - \epsilon_{\mathbf{Q}_1'\uparrow})$$
$$\times T_{33}(z - \epsilon_{\mathbf{Q}_1'\uparrow}).$$ (A12)

A comment concerning the choice of single-particle energies is now in order. The energies $\epsilon_{\mathbf{k}\sigma}$ that have been used up to now are eigenvalues of the $\hat{H}_0$ Hamiltonian and are the so-called *bare energies*: it is supposed that they have been obtained from a single-particle self-consistent field calculation *neglecting the correlation contribution*. In a real band structure calculation the $\hat{H}'$ term is treated by some sort of mean-field approximation. Therefore the band energies $\epsilon_{\mathbf{k}\sigma}^b$ are related to the bare energies by the equation

$$\epsilon_{\mathbf{k}\sigma}^b = \epsilon_{\mathbf{k}\sigma} + \frac{U}{N}N_{e,-\sigma}.$$ (A13)

If instead of the bare energies one wants to use the band energies, as is often the case, the constant shift of (A13) must be included in all the expressions which involve single-particle energies. Having done that and after transforming all the summations over Q vectors in integrals over the density of band states, using where necessary the so-called local approximation,[18] one gets all

the previous quantities in the form that has been adopted for the present calculations.

APPENDIX B: COMPARISON WITH PREVIOUS THEORETICAL WORK

We show how some methods adopted up to now in the self-energy calculation can be derived as approximations of the present theory. Most of the previous theoretical work has been based on one of the following approaches: (a) the t-matrix approach[17,19,23,31] or (b) the second order perturbation theory.[18,21,22,26,34,42]

The t-matrix approach relies on the assumption, adopted also to get expressions (5.23) and (5.25), that only configurations with $m \leq 1$ enter the expansion of the many-body wave functions, but with the additional assumption that the electron-hole scattering term in $\hat{V}_3$ can be neglected. It can be applied under the condition that the band is nearly full. With this further approximation the quantity $A(\omega - \epsilon)$ defined in (A8) is zero and the self-energies (5.23) and (5.25) turn out to be

$$\Sigma^{(-)}(\omega) = \frac{U}{N}(N_e - N_{e\uparrow}) - \int_{E_f}^{\infty} d\epsilon\ n(\epsilon)T_{33}(\omega - \epsilon),$$ (B1)

$$\Sigma^{(+)}(\omega) = -\frac{U}{N}N_{e\uparrow} + \int_{-\infty}^{E_f} d\epsilon\ n(\epsilon)T_{33}(\omega - \epsilon),$$ (B2)

which coincide with the expression of Ref. 31, except for the constant term.

In order to obtain the expression of the self-energy evaluated to the second order in the Coulomb repulsion parameter U, it is necessary to consider configurations with $m_{\max} = 2$, but replacing the resolvents $\hat{F}_i$ appearing in Eq. (5.2) by the free resolvents $\hat{F}_i^D$. This leads to write the hole self-energy referred to "bare" single particle states as

$$\Sigma^{(-)}(\omega) = \frac{U}{N}N_{e\uparrow} - \sum_t V_{st}F_{3tt}^D V_{ts} + \sum_f V_{0f}'F_{4ff}^D V_{f0}'$$
$$- \sum_v V_{sv}''F_{5vv}^D V_{vs}.$$ (B3)

This amounts to neglecting all the scattering processes between configurations having the same number of electron-hole couples, i.e., setting the $\hat{V}_i$ potentials of Sec. III equal to zero. By replacing the matrix elements in Eq. (B3) by their explicit expression one can easily obtain

$$\Sigma^{(-)}(\epsilon_{k_0\downarrow}) = \frac{U}{N}N_{e\uparrow} - \left(\frac{U}{N}\right)^2 \sum_{k_1 k_2 k_3} \frac{f(\epsilon_{k_1\uparrow})f(\epsilon_{k_2\downarrow})[1 - f(\epsilon_{k_3\uparrow})]}{\epsilon_{k_1\uparrow} + \epsilon_{k_2\downarrow} - \epsilon_{k_3\uparrow} - \epsilon_{k_0\downarrow}}\delta_{k_1 + k_2, k_3 + k_0}$$

$$+ \left(\frac{U}{N}\right)^2 \sum_{k_1 k_3 k_2} \frac{f(\epsilon_{k_1\uparrow})[1 - f(\epsilon_{k_3\uparrow})][1 - f(\epsilon_{k_2\downarrow})]}{\epsilon_{k_1\uparrow} + \epsilon_{k_0\downarrow} - \epsilon_{k_3\uparrow} - \epsilon_{k_2\downarrow}}\delta_{k_1 + k_0, k_3 + k_2} \tag{B4}$$

and for the electron case

$$\Sigma^{(+)}(\epsilon_{k_0\downarrow}) = \frac{U}{N}N_{e\uparrow} + \left(\frac{U}{N}\right)^2 \sum_{k_1 k_2 k_3} \frac{f(\epsilon_{k_3\uparrow})[1 - f(\epsilon_{k_2\downarrow})][1 - f(\epsilon_{k_1\uparrow})]}{\epsilon_{k_3\uparrow} + \epsilon_{k_0\downarrow} - \epsilon_{k_1\uparrow} - \epsilon_{k_2\downarrow}}\delta_{k_1 + k_2, k_3 + k_0}$$

$$- \left(\frac{U}{N}\right)^2 \sum_{k_1 k_3 k_2} \frac{f(\epsilon_{k_3\uparrow})[1 - f(\epsilon_{k_1\uparrow})]f(\epsilon_{k_2\downarrow})}{\epsilon_{k_2\downarrow} + \epsilon_{k_3\uparrow} - \epsilon_{k_1\uparrow} - \epsilon_{k_0\downarrow}}\delta_{k_1 + k_0, k_3 + k_2}, \tag{B5}$$

which are the expressions first used by Treglia and co-workers.[18] In the modified form of second order theory recently proposed by Steiner and co-workers[26,43] as an expansion in the fluctuations around mean-field solutions, the second order term has the same form as the U^2 contribution entering Eqs. (B4) and (B5) while the linear term accounts for the change in the orbital occupancies of the fluctuating state compared to the mean-field case.

There is an important difference between Eqs. (B1) and (B2) and the perturbative expressions (B4) and (B5) of the self-energies. In the perturbation theory the real part of the self-energy is continuous at the Fermi level, i.e., if we remove or create an electron with energy $\epsilon_{k_0\downarrow} = E_F$. The same is not true for the t-matrix case: if we put $\omega = E_F$ in Eqs. (B1) and (B2) we get different values for the electron and hole self-energies. As shown in Sec. VI, the discontinuity at E_F occurs for $m_{max} = 1$ even when the electron-hole scattering is taken into account and is essential in order to reproduce the metal-insulator transition at large U values and the atomic limit behavior of the Hubbard Hamiltonian.[41]

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