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Abstract. The spectra of two-hole and two-electron excitations are calculated for a single-band Hubbard Hamiltonian. These spectra are directly connected with the intensity of CVV Auger spectra and with the appearance potential spectra of transition metals with strong electron–electron interactions. The theory is based on a local decoupling procedure applied to the retarded two-particle double-time Green functions in the site representation. It is exact in four important limiting cases: in the non-interacting limit ($U \to 0$), in the atomic limit (band width $W \to 0$), in the limit of low concentration of electrons ($n \to 0$) and holes ($n \to 2$), and it provides a physically reasonable interpolation between these limits. In contrast with previous similar theories, it has proper transformation properties under the electron–hole transformation. The theory is illustrated numerically in a simplified model.

1. Introduction

The spectrum of two-particle excitations in systems of correlated electrons is an important quantity that determines many physical properties of these systems. Particularly, the intensity of the CVV Auger spectrum is proportional to the density of the two-hole excitations below the Fermi level in the valence band. Similarly, the appearance potential spectra are connected with the density of the two-electron excitations above the Fermi level in the valence band.

For systems with completely filled, or empty bands, an exact solution (sometimes called Kanamori's solution, Kanamori 1963) is possible (see also Beeby 1967, and Drchal and Velický 1976). This theory was employed by Cini (1976) and by Sawatzky (1977) to explain the CVV Auger spectra of transition metals, and by Drchal and Velický (1976) in studies of the electronic structure of disordered alloys. However, most transition metals have partially filled d-bands. In this case, various approximate treatments were used:

(i) Perturbation theory. The two-particle Green function (GF) was constructed as a sum of ladder graphs, the one-particle propagators in the ladder were calculated either within second order (in U/W, where U is the strength of electron–electron interactions and W is the band width) perturbation theory (Tréglia *et al* 1981), or within the non-self-consistent T-matrix approximation (NSC-TMA) (Penn 1979, Cini 1979). The validity of the second-order theory is limited to weak pair interactions (U/W small). The NSC-TMA is valid for very low particle concentrations and, of course, also for weak pair interactions

at arbitrary particle concentrations. Considerable improvements were made when the self-consistency was introduced into the TMA (SC-TMA) (Babanov *et al* 1971, 1973a, b, Drchal 1979, Drchal and Kudrnovský 1984). The validity of the SC-TMA is still limited to low particle concentrations, not exceeding 0.3 per one spin sub-band (Caron and Kemeny 1971).

　　(ii) The cluster approach (Cini and Verdozzi 1987) is based on the configuration interaction (CI) method applied to a finite cluster (containing, say, 125 atoms) and it yields very accurate and reliable results. However, with increasing number of holes, the dimensionality of the configurational space increases very rapidly. Consequently, the method can be efficiently used only for systems with low concentration of particles (either holes or electrons).

　　(iii) Decoupling procedures are used to simplify the higher-order GF entering the equation of motion for double-time GF. Presilla and Sacchetti (1987) employed an RPA-like pairing in *k*-space in their study of the multi-band Hubbard-type Hamiltonian. This approximation, however, behaves incorrectly at the electron–hole symmetry operation. In the present work an alternative approach based on the decoupling in the site representation is developed, which eliminates this drawback.

2. Theory

The two-particle excitation spectrum of the single-band Hubbard Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} + U \sum_i a^+_{i\uparrow} a_{i\uparrow} a^+_{i\downarrow} a_{i\downarrow} \tag{1}$$

can be studied using the two-particle double-time retarded GF:

$$G(ijlm, t) = (-i)\theta(t)\langle \Psi^M_0 | [a_{i\downarrow}(t)a_{j\uparrow}(t), a^+_{m\uparrow} a^+_{l\downarrow}] | \Psi^M_0 \rangle \tag{2}$$

where $\theta(t)$ is the Heaviside step function ($\theta(t) = 1$ for $t > 0$; $\theta(t) = 0$ otherwise), and $|\Psi^M_0\rangle$ is the ground state of H with M particles. The Fourier transform of this GF

$$G(ijlm, z) = \int_{-\infty}^{\infty} \mathrm{d}t \exp(izt) G(ijlm, t)$$

$$G(ijlm, t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \exp(-i\omega t) G(ijlm, \omega) \tag{3}$$

is holomorphic in the upper half-plane of complex energy z (Im $z > 0$). It can easily be shown that the spectral representation of the superdiagonal element $G_0(z) = G(0000, z)$ is given by

$$G_0(z) = \sum_\alpha \frac{W^{M+2}_\alpha}{z - (E^M_\alpha - E^{M+2}_0)} - \sum_\beta \frac{W^{M-2}_\beta}{z - (E^M_0 - E^{M-2}_\beta)} \tag{4}$$

where

$$W^{M+2}_\alpha = |\langle \Psi^{M+2}_\alpha | a^+_{0\uparrow} a^+_{0\downarrow} | \Psi^M_0 \rangle|^2 \qquad W^{M-2}_\beta = |\langle \Psi^{M-2}_\beta | a_{0\downarrow} a_{0\uparrow} | \Psi^M_0 \rangle|^2 \tag{5}$$

and E^M_α, $|\Psi^M_\alpha\rangle$ are the eigenvalues and eigenvectors of Hamiltonian (1) corresponding

to states of M electrons. In metallic systems with Fermi level μ, equation (4) can be simplified using the positive excitation energies ω

$$E_\alpha^{M+2} - E_0^M = \omega_\alpha^{M+2} + 2\mu \qquad E_0^M - E_\beta^{M-2} = 2\mu - \omega_\beta^{N-2}. \tag{6}$$

The spectral density

$$A(E) = -\pi^{-1} \operatorname{Im} G_0(E + \mathrm{i}0) \tag{7}$$

has two branches: for $E > 2\mu$ (the first term in (4)) it corresponds to the two-electron excitations (appearance potential spectra), and for $E < 2\mu$ (the second term in (4)) it corresponds to the two-hole excitations (CVV Auger spectra).

The GF $G(ijlm, z)$ obeys the equation of motion

$$z\, G(ijlm, z) = \rho(ijlm) + \sum_n t_{jn} G(inlm, z) + \sum_n t_{in} G(njlm, z)$$

$$+ U\delta_{ij} G(ijlm, z) + U(1 - \delta_{ij})\Gamma(ijlm, z) \tag{8}$$

where

$$\rho(ijlm) = \langle \Psi_0^M | [a_{i\uparrow} a_{j\downarrow}, a_{m\downarrow}^+ a_{l\uparrow}^+] | \Psi_0^M \rangle = \delta_{il}\delta_{jm} - \delta_{jm}\langle a_{l\uparrow}^+ a_{i\uparrow} \rangle - \delta_{il}\langle a_{m\downarrow}^+ a_{j\downarrow} \rangle \tag{9}$$

and $n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$. We shall approximate the higher-order GF $\Gamma(ijlm, z)$ on the RHS of equation (8) using the decoupling

$$\Gamma(ijlm, z) = \langle\!\langle (n_{i\downarrow} + n_{j\uparrow}) a_{i\uparrow} a_{j\downarrow} | a_{m\downarrow}^+ a_{l\uparrow}^+ \rangle\!\rangle \simeq \langle n_{i\downarrow} + n_{j\uparrow} \rangle G(ijlm, z) \tag{10}$$

which corresponds to the local effective-medium approximation for the two-particle states. We assume that the ground state $|\Psi_0^M\rangle$ is translationally invariant. Then $\langle n_{i\sigma} \rangle = \langle n_{j\sigma} \rangle$ and $\langle n_{i\downarrow} + n_{j\uparrow} \rangle = n$, n being the concentration of electrons ($0 \leq n \leq 2$, $n = M/N$, N is the number of sites). The equation of motion (8) then simplifies to the form

$$(z - Un)G(ijlm, z) = \rho(ijlm) + \sum_n t_{jn} G(inlm, z)$$

$$+ \sum_n t_{in} G(njlm, z) + U(1 - n)\delta_{ij} G(ijlm, z). \tag{11}$$

Equation (11) represents an inhomogeneous system of linear equations for the unknown quantities $G(ijlm, z)$. This system can be solved using the exact Kanamori's solution of the two-particle problem (see, e.g., Beeby 1967, Drchal and Velický 1976):

$$G(ijlm, z) = \frac{1}{N^2} \sum_{kq} \exp\{\mathrm{i}[k(R_i - R_l) + q(R_j - R_m)]\} \frac{1 - n_{k\uparrow} - n_{q\downarrow}}{\xi - E(k) - E(q)}$$

$$\times \left(1 + \frac{1}{N} \sum_p \frac{\exp[\mathrm{i}p(R_i - R_j)]}{\xi - E(k+p) - E(q-p)} \frac{V}{1 - V\Psi_0(k + q_1, \xi)}\right). \tag{12}$$

The superdiagonal element $G_0(z)$ of the GF is

$$G_0(z) = \frac{1}{N^2} \sum_{kq} \frac{1}{1 - V\Psi_0(k+q, \xi)} \frac{1 - n_{k\uparrow} - n_{q\downarrow}}{\xi - E(k) - E(q)} \tag{13}$$

where

$$\Psi_0(k, \xi) = \frac{1}{N} \sum_p \frac{1}{\xi - E(k - p) - E(p)} \qquad (14)$$

is the unperturbed two-particle propagator, $n_{k\sigma} = \langle a_{k\sigma} a_{k\sigma} \rangle$ is the average occupancy of the one-electron Bloch state $(k\sigma)$,

$$\xi = z - Un \qquad (15)$$

is the renormalised energy,

$$V = U(1 - n) \qquad (16)$$

is the renormalised strength of the pair interaction,

$$E(k) = \frac{1}{N} \sum_{lm} \exp[-ik(R_l - R_m)] t_{lm} \qquad (17)$$

is the dispersion law of the unperturbed one-particle energy band, and the summations in (12), (13) and (14) run over the first Brillouin zone.

In order to evaluate the accuracy of our solution we compare it with the exact results that may be found in some special cases.

(a) In the non-interacting limit ($U = 0$), expression (13) gives the exact result

$$G_0(z) = \frac{1}{N^2} \sum_{kq} \frac{1 - n_{k\uparrow} - n_{q\downarrow}}{z - E(k) - E(q)}. \qquad (18)$$

This also follows directly from the equation of motion (8), in which $\Gamma(ijlm, z)$ is multiplied by U. Therefore, for $U = 0$, equation (8) holds exactly even if the decoupling (10) yields an incorrect result for $\Gamma(ijlm, z)$.

(b) In the atomic limit ($E(k) = 0$ for all k), formula (13) gives the exact result

$$G_0(z) = (1 - n)/(z - U) \qquad (19)$$

which can also be derived from (8), since the decoupling (10) gives exact expression for $\Gamma(ijlm, z)$ in this limit.

(c) Formula (13) yields the exact result, identical to Kanamori's solution, in the limit of low concentration of electrons ($n \to 0$)

$$G_0(z) = \frac{1}{N} \sum_k \frac{\Psi_0(k, z)}{1 - U\Psi_0(k, z)} \qquad (20)$$

because the decoupling (10) gives an exact value of Γ, $\Gamma(ijlm, z) = 0$.

(d) Similarly, in the limit of low concentration of holes ($n \to 2$), expression (13) is again exact, giving

$$G_0(z) = \frac{1}{N} \sum_k \frac{\check{\Psi}_0(k, z)}{1 - U\check{\Psi}_0(k, z)} \qquad (21)$$

where

$$\check{\Psi}_0(k, z) = \frac{1}{N} \sum_p \frac{1}{2U - z + E(k + p) + E(p)}. \qquad (22)$$

This also follows from (10), since it gives exact result $\Gamma(ijlm, z) = 2G(ijlm, z)$.

(*e*) It can be shown that solution (13) behaves correctly at the electron–hole transformation. It transforms according to the exact relation (cf. Mertsching 1977)

$$G_0(U, n, [E(k)], z) = G_0(U, 2 - n, [-E(k)], 2U - z). \tag{23}$$

The approximation derived by Presilla and Sacchetti (1987) is exact only in cases (*a*), (*b*) and (*d*), but not in (*c*) and (*e*), because it violates the electron–hole symmetry requirements. This can be seen from the single-band version of the Presilla and Sacchetti's result, which reads in our notation as

$$G_0(z) = \frac{1}{N^2} \sum_{kq} \frac{1}{1 - U\tilde{\Psi}_0(k+q, z)} \frac{1 - n_{k\uparrow} - n_{q\downarrow}}{2U - z + E(k) + E(q)}. \tag{24}$$

This resembles our result (13), except that renormalisation of energy, and, more important, the renormalisation of the interaction strength is missing. On the other hand, the ladder approximation combined with the *T*-matrix approximation is correct in cases (*a*), (*c*)–(*e*). In the atomic limit (case *b*) it is correct only for $n = 0$ and $n = 2$.

Expression (13) is an explicit compact formula for the two-particle, single-site GF. It can be directly used for calculation of the Auger intensity. It has very simple structure: the quantities in the denominator have purely two-particle character since they come from the exact (Kanamori's) solution of the two-particle problem, but the energy $\tilde{\xi}$ and the pair interaction V are renormalised quantities. On the other hand, the expression in the numerator is purely of one-particle nature as it contains the information on the occupancy of the one-particle states in the system of correlated electrons.

The occupation numbers $n_{k\sigma}$ can be calculated from the one-particle GF. Our theory, however, gives no prescription how to determine the one-particle GF. We are therefore free to choose a suitable approximation scheme for evaluation of the one-particle GF. Of course, it would be desirable to determine the one-particle GF consistently with the approximate form of the two-particle GF following the method proposed by Baym and Kadanoff (1961) for construction of conserving approximations. This seems hardly possible in our scheme because the double-time, two-particle GF considered here has no direct connection with the one-particle GF. The reason is that the two-particle GF calculated in our theory depends on the time variables as $G(t, t, 0, 0)$, while for the calculation of the one-particle self-energy a different type of GF, namely $G(t, t, t, 0)$, is necessary.

On the other hand, the occupation numbers are rather insensitive to the fine details of the one-particle GF, except a finite jump at the Fermi momentum k_F, which follows from the Luttinger's (1961) theorem. Therefore, it seems that even rough approximations for the one-particle GF that fulfil Luttinger's theorem can yield the two-particle GF with good accuracy.

The renormalised energy $\tilde{\xi}$ (15) and the effective strength of pair interaction V (16) are used to describe the form of the two-particle GF (13). These quantities can be interpreted as follows. The energy shift Un that enters (15) is a sum of the one-particle Hartree–Fock self energies for a pair of electrons: $Un = Un_\uparrow + Un_\downarrow$. In order to explain the physical meaning of the effective interaction $V = U(1 - n)$, we start from the definition (2) of the two-particle GF ($i = j = l = m = 0$), and for simplicity, we consider the two-electron excitations only. At time $t = 0$, we create a pair of particles with opposite spins on the atom at the origin, and after time t we look for the probability amplitude of finding a pair of particles at the same site. In systems with low particle concentrations ($n \ll 1$), the evolution of a pair of particles created at the origin is governed mainly by

the bare repulsion U; they move freely on the lattice except that they tend to avoid each other. The two-particle GF is given by Kanamori's solution, and $V = U$. The situation changes with increasing particle concentrations. For the almost filled band $(2 - n \ll 1)$, the pair of particles created at the origin is bounded to stay there because all the neighbouring sites that can be reached by hopping are fully occupied. Due to the Pauli principle neither of two particles created at the origin can move to this neighbourhood. This situation is described by an effective interaction of attractive type, $V = -U$. In the intermediate case (half-filled band, $n = 1$) the bare repulsion U and the effects of the Pauli exclusion principle compensate each other: the particles behave as if they were free and the effective interaction V goes to zero. We note that in the atomic limit, the two-particle GF (19) is expressed via the energy z and the bare interaction U. This could lead to an incorrect conclusion that the renormalised quantities are inapplicable in this case. Of course, it is not so, because equation (19) can be rewritten as $G_0(z) = (1 - n)/(\xi - V)$.

3. A simplified model

To illustrate our theory numerically we introduce a simplified model. We assume that the dispersion law $E(k)$ corresponds to the semi-elliptic density of states

$$g(E) = 2/\pi(1 - E^2)^{1/2}\theta(1 - E^2) \tag{25}$$

we employ the so-called scaling factor approximation that has been successfully used in numerical calculations of the two-particle spectra of metals and alloys (Drchal and Velický 1976, Drchal and Kudrnovský 1982) and a related interpolation approximation for the occupation numbers

$$E(k - q) + E(q) \simeq [2(1 - E(k))]^{1/2}E(q - \tfrac{1}{2}k) \tag{26a}$$

$$n_{q-k,\sigma} + n_{q,\sigma} \simeq 2n_{q-\frac{1}{2}k,\sigma}. \tag{26b}$$

We approximate the one-particle occupation numbers by their Hartree–Fock values

$$n_{k\sigma} \simeq \theta[\mu - \tfrac{1}{2}Un - E(k)]. \tag{27}$$

Then (13) simplifies to a two-dimensional integral over energy variables

$$G_0(z) = \int_{-1}^{1} dx\, g(x) \int_{-1}^{1} dy\, g(y) \left(1 - \frac{V}{1 - x}[\xi - (\xi^2 - 2 + 2x)^{1/2}]\right)^{-1}$$

$$\times \{\xi - [2(1 - x)]^{1/2}y\}^{-1}[1 - 2\theta(\mu - \tfrac{1}{2}Un - y)]. \tag{28}$$

The integration over y can be done analytically. It yields the one-dimensional integral

$$G_0(z) = \frac{\sqrt{2}}{\pi} \int_{-1}^{1} dx\, \frac{(1 - x)(1 + x)^{1/2}}{1 - x - V[\xi - (\xi - 2 + 2x)^{\frac{1}{2}}]} P\left(\frac{\xi}{[2(1 - x)]^{1/2}}\right) \tag{29}$$

where

$$P(z) = \frac{2}{\pi} \int_{-1}^{1} dy\, \frac{sgn(y - y_0)(1 - y^2)^{1/2}}{z - y} = \frac{4}{\pi}\left\{(1 - y_0^2)^{1/2} - z\sin^{-1} y_0\right.$$

$$\left. + (z^2 - 1)^{1/2}\left[i\ln\left(\frac{1 - zy_0 - i(z^2 - 1)^{1/2}(1 - y_0^2)^{1/2}}{z - y_0}\right) - \tfrac{1}{2}\pi\right]\right\} \tag{30}$$
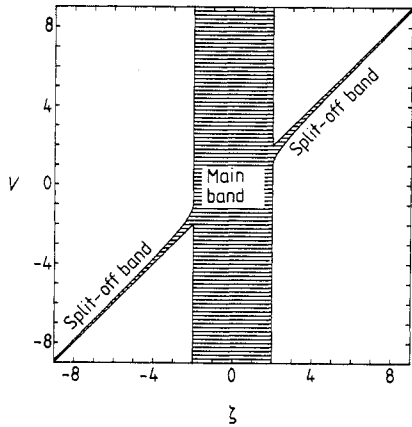
Figure 1. Localisation of the two-particle spectrum calculated within the simplified model. The lines $V =$ constant intersect the regions shown to give the bounds of the two-particle spectrum.

and $y_0 = \mu - \tfrac{1}{2}Un$. Expression (29) is evaluated numerically with the help of the analytical deconvolution technique (Hass *et al* 1984).

The formula (13) for the two-particle GF is simple enough that direct evaluation without additional approximations (i.e., using realistic band structure $E(\mathbf{k})$, full six-dimensional integration over the $\mathbf{k}$-space and more realistic approximation for the one-particle occupation numbers $n_{k\sigma}$ than Hartree–Fock) is also possible.

4. Results and discussion

It may be shown by inspection of formula (28) that the density of the single-site, two-particle states is non-zero for ξ from the interval $(-2, 2)$ if $|V| < 1$ and for ξ lying inside the union of intervals $(-2, 2) \cup (V, V + V^{-1})$ if $|V| > 1$ (see figure 1). The interval $(-2, 2)$ corresponds to the main band, and the interval $(V, V + V^{-1})$ to the split-off band. With increasing $|V|$ an increasing number of states belongs to the split-off band, whose width $(|V|^{-1})$ decreases. The renormalised pair interactions V may be either positive or negative, depending on the particle concentration n. Therefore two split-off bands are found, one above the main band (for $V > 1$), and the other below the main band (for $V < -1$). The energy $\xi = 2\mu$ separates the two-electron states from the two-hole states. A detailed discussion of the bounds of the two-particle spectrum relevant to our simplified model may be found elsewhere (Drchal and Velický 1976).

The densities of the single-site, two-particle states calculated for the simplified model are presented in figures 2 and 3. We have selected the parameters U and n to show the main features of the two-particle spectra:

(1) With increasing strength of the pair interaction U at constant particle concentration n (figure 2) the originally band-like spectrum gradually changes into an atomic-like one.

(2) Varying filling n of the valence band at a constant strength of the pair interaction U (figure 3) has the following effects: (*a*) with increasing particle concentration n the number of two-hole excitations increases, while the number of two-electron excitations decreases; (*b*) the correlation effects are strongly suppressed for n close to 1, as follows from (16); and (*c*) the spectra for the conjugated particle concentrations n and $2 - n$ are related by the electron–hole symmetry (equation (23)).
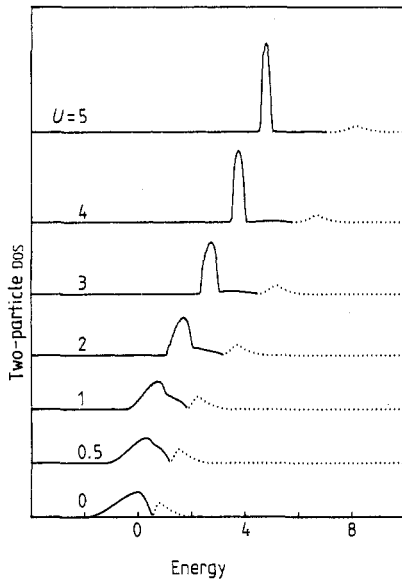
Figure 2. Density of the two-hole (full curves, corresponding to the CVV Auger spectrum) and two-electron excitations (dotted lines corresponding to the appearance potential spectrum) calculated within the simplified model for constant electron concentration $n = 1.5$ and varying the strength of the pair interaction U. The unperturbed one-electron band width is $W = 2$.
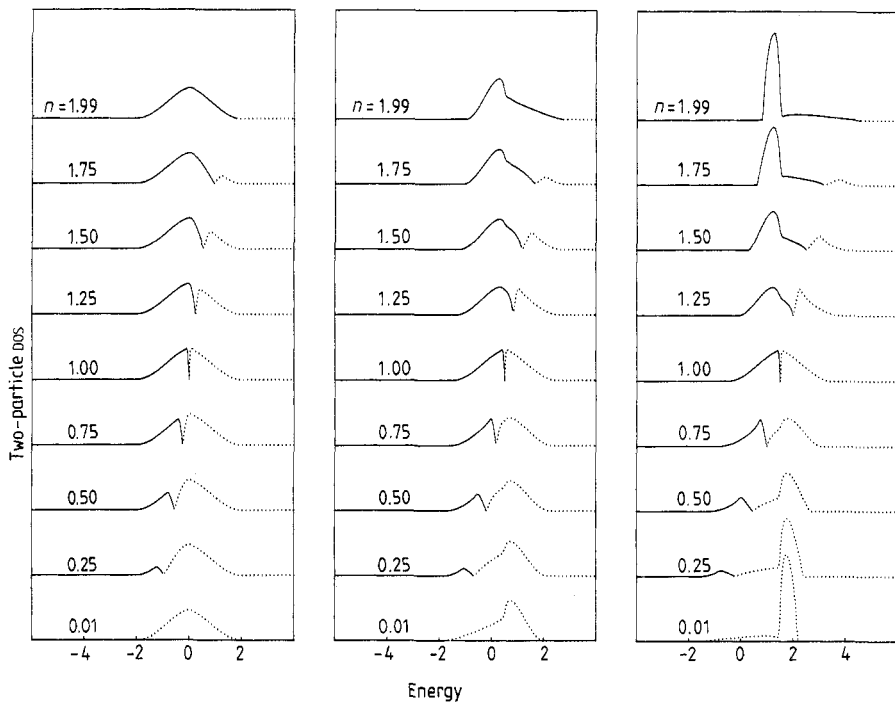

Figure 3. Similar to figure 2, but with three cases of the constant pair interaction, $U = 0$ (left), $U = 0.5$ (centre), and $U = 1.5$ (right) shown for various electron concentrations n.

The most important feature of the present theory is the renormalisation of the strength of pair interaction (equation (16)). It ensures a correct behaviour at the electron–hole transformation. Moreover, it has important consequences for the interpretation of

the Auger spectra. The theory based on the assumption of low hole concentration automatically connects the atomic-like or band-like character of the CVV Auger spectra with the strong or weak intra-atomic Coulomb interaction, respectively. It also makes the conclusion that this interaction is weak for metals in the middle of the 3d series (Mn, Fe, Co). The situation is more complex, however. Direct calculations of the Coulomb integrals for these metals (see Mann 1967) yield lower values (approximately 22–25 eV), but which are still comparable with those for Ni or Cu (approximately 26 eV). The contact pair interaction in the Hubbard Hamiltonian is related to the Coulomb integrals, but it is not identical, due to the screening effects. Finding reliable values of the Hubbard U is a difficult task and it was believed that the value of U is directly connected with the shape of the CVV Auger spectrum. Our theory shows, however, that the character of the Auger spectrum is governed by the renormalised pair interaction $V = U(1 - n)$ instead of the bare interaction U.

5. Conclusions

We have developed a new approximate theory of the two-particle excitations for the single-band Hubbard model. It can be used in studies of the CVV Auger spectra and the appearance potential spectra of metals with incompletely filled narrow bands. The theory is based on the local decoupling scheme applied to the two-particle, double-time GF which corresponds to an effective-medium approximation in the space of the two-particle states. It yields correct results in important limiting cases for which an exact solution is known. Its main limitation is that it includes only one band. It can be generalised, however, to the multi-band case (Kotrla and Drchal 1989). For simplicity, it was formulated for $T = 0$; but extension for the case $T > 0$ is straightforward. The most remarkable feature of the present theory is perhaps that it gives, for the first time, an explicit formula (16) for the strength of renormalised pair interaction which describes well, at least on qualitative level, the dependence of the two-particle spectra on the particle concentration. A detailed comparison of our theory including the multi-band case with other theoretical methods and with the experimental Auger and APS spectra of transition metals is now in preparation.

Acknowledgments

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