Interatomic and intra-atomic electron correlation in narrow band solids

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Abstract. Effect of interatomic electron correlation has been studied in narrow band solids using one-particle Green function method. We follow Hubbard in drawing an analogy with an alloy and find a self-consistent solution which predicts a finite lifetime for pseudoparticles. A specific case of a (non-magnetic) model system with half-filled parabolic band has been considered to calculate the pseudoparticle density of states function. Unlike the result in the presence of intra-atomic correlations alone, we find that this particular system is never an insulator, however large intra-atomic correlations may be.

1. Introduction

During the past decade there have been numerous studies of the electron correlation in narrow band solids (Hubbard 1963, 1964a, 1964b, Gutzwiller 1963, 1964, 1965, Kanamori 1963, Kemeny 1965a, 1965b). The Hubbard model of the electron correlation is based on the assumption that despite the band motion of d electrons, the electrons at any site are strongly correlated with each other. The Hubbard model is too simple to represent the real situation in the transition metals and their chalcogenides. For real systems one must consider the degeneracy of the d-band, the interatomic interaction, and the presence of the s band (s–d hybridization) together with the intra-atomic interaction. However, treatment of all these effects simultaneously is not a practical proposition at the moment. The problem of degeneracy in d band has been discussed by Hubbard (1964a), Chao (1971) and Seigel and Kemeny (1972). The presence of the s band has been considered by Kishore and Joshi (1970a, 1970b, 1970c, 1971) by taking into account the effect of hybridization of s and d bands on the Hubbard Model.

The Hubbard model is characterized by the absence of intersite electron correlation. The validity of this assumption of the Hubbard model is doubtful. There will be of the order of $\frac{1}{2}Nz$ pairs of nearest neighbours in a system if z is the number of nearest neighbours which a given site has. Since interatomic interaction will be approximately one-sixth the intra-atomic interaction, it is clear that the interatomic term can have an appreciable contribution. With this in mind the study of the contribution of the interatomic interaction together with the intra-atomic interaction is necessary. Caron and Pratt (1968) studied the effect of interatomic interaction on the magnetic properties of the system using a generalized self-consistent cluster treatment. Kemeny (1965a) included this interaction and studied the metal-insulator transition in narrow

band solids by finding out the conditions for an electron and a hole to form a bound pair. But in the actual estimate of the binding energy of the pair, he took only intra-atomic interaction into account. Therefore, the contribution of intersite interaction could not be known. Later Kishore and Joshi (1969) studied the effect of intersite inter-action using the Hubbard type decoupling method. It was found there that intra-atomic and interatomic correlations working together split the original band into three sub-bands. The middle band occurs only because of the consideration of the inter-atomic interaction. The decoupling method used there creates an obvious difficulty similar to that in the first paper of Hubbard (Hubbard 1963) i.e., however small the interactions may be, the original band due to these interactions always splits into three separate sub-bands. Physically this does not seem to be justified. Here we will try to get rid of this difficulty by treating the electron-correlation problem in a self-consistent way as Hubbard did in his third paper (Hubbard 1964b).

Following Hubbard we introduce an alloy analogy. Hubbard considered intrasite correlation only and his problem was analogous to that of the binary alloy. Since we consider intersite correlation too, we have to draw an analogy with a ternary alloy. We use the one electron Green function method and by truncating the hierarchy of Green function equations, we arrive at a self-consistent formulation of the problem. Firstly we decouple the equation of motion of the Green function in a very approximate way where no account is taken of the fluctuation effects as well as motional-broaden-ing-effects. These effects are then discussed and taken into account in sections 3 A and 3 B. Finally in section 4 we present results of the calculation of the perturbed density of states for a model system with a half-filled parabolic band.

The requirement of the self-consistency, for the description of the electron correla-tion in narrow bands, may be obtained via an alternative approach—the coherent potential approximation (Velicky *et al* 1968). We will discuss it for our problem in the appendix.

2. Mathematical preliminaries and basic definitions

A. The Hamiltonian

The Hamiltonian of the system under consideration in the Wannier representation and in second quantization form is (Hubbard 1963)

$$\mathcal{H} = \sum_{ij} \sum_{\sigma} T_{ij} \, c^{\dagger}_{i\sigma} \, c_{j\sigma} + \frac{1}{2} \sum_{ijkl} \sum_{\sigma\sigma'} \langle ij | \frac{1}{r} | kl \rangle \, c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'} c_{l\sigma'} c_{k\sigma} \tag{1}$$

We use the usual notation. The first term is the band theory Hamiltonian. This term describes the individual motion of the electrons. The second term takes care of the correlations. Here

$$\langle ij | \frac{1}{r} | kl \rangle = e^2 \int \frac{\varphi^*(r-R_i) \, \varphi^*(r'-R_j) \varphi(r'-R_l) \, \varphi(r-R_k)}{|r-r'|} \, dr dr' \tag{2}$$

One can easily evaluate the terms given by (2) by using known atomic functions; the approximate magnitude of various terms for d electrons in transition metals is given by

$$\langle ii | \frac{1}{r} | ii \rangle \simeq 15 \, \text{eV}; \quad \langle ij | \frac{1}{r} | ij \rangle \simeq 3 \, \text{eV}$$

$$\langle ii | \frac{1}{r} | ij \rangle \simeq \tfrac{1}{2} \, \text{eV}; \quad \langle ij | \frac{1}{r} | ik \rangle \simeq \tfrac{1}{10} \, \text{eV} \tag{3}$$

where i, j and k are all nearest neighbours. Neglecting all correlation terms but $\langle\, ii \mid \frac{1}{r} \mid ii\, \rangle$ and $\langle\, ij \mid \frac{1}{r} \mid ij\, \rangle$, the Hamiltonian becomes

$$\mathcal{H} = \sum_{ij} \sum_{\sigma} T_{ij}\, c_{i\sigma}^{\dagger}\, c_{j\sigma} + \tfrac{1}{2} I \sum_{i} \sum_{\sigma} n_{i\sigma}\, n_{i-\sigma} + \tfrac{1}{2} \sum_{ij} \sum_{\sigma\sigma'} K_{ij}\, n_{i\sigma}\, n_{j\sigma'} \qquad (4)$$

where $\qquad I = \langle\, ii \mid \frac{1}{r} \mid ii\, \rangle$

$$K_{ij} = \langle\, ij \mid \frac{1}{r} \mid ij\, \rangle = K, \text{ (if } i \text{ and } j \text{ are nearest neighbours)}$$

$$= 0, \text{ otherwise} \qquad (5)$$

B. The Green function

The double-time temperature dependent retarded (+) and advanced (−) Green functions for the operators A and B are defined by (Zubarev 1960),

$$\langle\!\langle A(t);\, B(t') \rangle\!\rangle^{(\pm)} = \mp\, i\theta\left\{\pm(t-t')\right\} \langle\, [A(t),\, B(t')]\, \eta\, \rangle \qquad (6)$$

where $\qquad\qquad [A, B]_{\eta} = AB - \eta BA$

$$\eta = \pm 1 \text{ (whichever is convenient)}$$

$$A(t) = \exp(i\mathcal{H}t)\, A(0) \exp(-i\mathcal{H}t)$$

$\theta(t)$ is the step function. Notation $\langle\, \dots . X\, \rangle$ denotes the average of the operator X over grand canonical ensemble at temperature T. In our analysis we work with the operators $A(t) = c_{i\sigma}$, $B(t) = c_{j\sigma}^{\dagger}$; hence the Green function is

$$G_{ij}^{\sigma}(E) = \langle\!\langle c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle_E \qquad (\eta = -1) \qquad (7)$$

The Fourier transformation gives

$$G_{ij}^{\sigma}(E) = \frac{1}{N} \sum_{k} e^{ik\,(R_i - R_j)}\, G^{\sigma}(k, E) \qquad (8)$$

The equation of motion of the Green function $\langle\!\langle c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle_E$ is

$$E \langle\!\langle c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle_E = \frac{1}{2\pi} \langle\, [c_{i\sigma},\, c_{j\sigma}^{\dagger}]_{+} \rangle + \langle\!\langle [c_{i\sigma},\, \mathcal{H}]_{-};\, c_{j\sigma}^{\dagger} \rangle\!\rangle_E \qquad (9)$$

From the knowledge of the Green function the density of states per atom of spin σ, $\rho^{\sigma}(E)$ and the mean number of electrons per atom of spin σ, $n_{\sigma}(E)$ can be evaluated from the usual relations.

3. An approximate self-consistent solution

The equation of motion (9) of the Green function $G_{ij}^{\sigma}(E)$ with the Hamiltonian (4) becomes

$$EG_{ij}^{\sigma}(E) = \frac{\delta_{ij}}{2\pi} + \sum_{m} T_{im}\, G_{mj}^{\sigma}(E) + I \langle\!\langle n_{i-\sigma}\, c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle$$

$$+ \sum_{m} \sum_{\sigma'} K_{im} \langle\!\langle n_{m\sigma'}\, c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle \qquad (10)$$

The higher order Green functions $\langle\!\langle n_{i-\sigma}\, c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle$ and $\langle\!\langle n_{m\sigma'} c_{i\sigma};\, c_{j\sigma}^{\dagger} \rangle\!\rangle$ obey the equations of motion

$$(E - T_0) \langle\!\langle n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{\delta_{ij}}{2\pi} \langle n_{i-\sigma} \rangle + \langle n_{i-\sigma} \rangle \sum_{r \neq i} T_{ir} \langle\!\langle c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ I \langle\!\langle n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle + \sum_r T_{ir} \langle\!\langle n_{i-\sigma} - \langle n_{i-\sigma} \rangle c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ \sum_r T_{ir} \{ \langle\!\langle c_{i-\sigma}^\dagger\, c_{r-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle - \langle\!\langle c_{r-\sigma}^\dagger\, c_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \}$$

$$+ \sum_r \sum_{\sigma'} K_{ir} \langle\!\langle n_{r\sigma'}\, n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \tag{11}$$

and

$$(E - T_0) \langle\!\langle n_{m\sigma'}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{\delta_{ij}}{2\pi} \langle n_{m\sigma'} \rangle + \langle n_{m\sigma'} \rangle \sum_{r \neq i} T_{ir} \langle\!\langle c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ I \langle\!\langle n_{i-\sigma}\, n_{m\sigma'}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle + \sum_r T_{ir} \langle\!\langle n_{m\sigma'} - \langle n_{m\sigma'} \rangle c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ \sum_r T_{mr} \{ \langle\!\langle c_{m\sigma'}^\dagger\, c_{r\sigma'}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle - \langle\!\langle c_{r\sigma'}^\dagger\, c_{m\sigma'}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \}$$

$$+ \sum_r \sum_{\sigma''} K_{ir} \langle\!\langle n_{m\sigma'}\, n_{r\sigma''}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \tag{12}$$

where

$$T_0 = T_{ii} = \frac{1}{N} \sum_k \epsilon_k \tag{13}$$

Now neglecting the fourth and fifth terms on the right hand side of Eq. (11) and using the approximation

$$\langle\!\langle n_{r\sigma'}\, n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \simeq \langle n_{r\sigma'} \rangle \langle\!\langle n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

we get the approximate expression for $\langle\!\langle n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ (Kishore and Joshi 1969):

$$\langle\!\langle n_{i-\sigma}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{n_{-\sigma}}{(E - T_0 - I - Knz)} \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r \neq i} T_{ir}\, G_{rj}^\sigma (E) \right\} \tag{14}$$

Here we have written $\langle n_{i-\sigma} \rangle = n_{-\sigma}$, which follows from the translational symmetry of the problem. $n = n_\sigma + n_{-\sigma}$. Similarly we may find out an approximate expression for $\langle\!\langle n_{m\sigma'}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ from Eq. (12);

$$\langle\!\langle n_{m\sigma'}\, c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{n_{\sigma'}}{(E - T_0 - I n_{-\sigma} - Knz)} \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r \neq i} T_{ir}\, G_{rj}^\sigma (E) \right\} \tag{15}$$

Now putting these approximate values from (14) and (15) in (10) we have

$$(E - T_0)\, G_{ij}^\sigma (E) = \left\{ 1 + \frac{I n_{-\sigma}}{(E - T_0 - I - Knz)} + \frac{Knz}{(E - T_0 - I n_{-\sigma} - Knz)} \right\}$$

$$\times \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r \neq i} T_{ir}\, G_{rj}^\sigma (E) \right\} \tag{16}$$

The Fourier transform of the Green function $G_{ij}^\sigma (E)$ may be written as

$$G^\sigma (k, E) = \frac{1}{2\pi} \frac{1}{F_0^\sigma (E) - (\epsilon_k - T_0)} \tag{17}$$

where

$$\frac{1}{F_0^\sigma (E)} = \left\{ 1 + \frac{I n_{-\sigma}}{(E - T_0 - I - Knz)} + \frac{Knz}{(E - T_0 - I n_{-\sigma} - Knz)} \right\} \frac{1}{(E - T_0)} \tag{18}$$

Expression for $F_0^\sigma(E)$ may also be written as

$$\frac{1}{F_0^\sigma(E)} = \frac{\dfrac{I^2 n_{-\sigma}(1-n_{-\sigma})}{(I+Knz)\ (In_{-\sigma}+Knz)}}{(E-T_0)} + \frac{\dfrac{I n_{-\sigma}}{(I+Knz)}}{(E-T_0-I-Knz)} + \frac{\dfrac{Knz}{(In_{-\sigma}+Knz)}}{(E-T_0-In_{-\sigma}-Knz)} \qquad (19)$$

The propagation of σ spin electron is described by the electron propagator $G^\sigma(k, E)$ given by Eq. (17). Here the quantity $(\epsilon_k - T_0)$ describes the propagation of electrons between atoms and the function $F_0^\sigma(E)$ describes the resonant properties of the atoms. The alloy analogy suggests the above treatment to be improved in two directions. Firstly, let $-\sigma$ spin electrons be fixed. Then for the accurate description of σ spin electron propagation in the resulting alloy, the damping of the electron wave resulting from disorder scattering should be considered. And secondly, since the $-\sigma$ spin electrons are not really fixed, the effect of their motion should be considered. Corrections corresponding to these effects are referred to as the 'scattering correction' and 'motional broadening correction' respectively (Hubbard 1964b). Both of these corrections will be calculated below.

A. *The scattering correction*

While finding out the expression for $G_{ij}^\sigma(E)$, the fourth and fifth terms on the right hand sides of Eqs. (11) and (12) were neglected. These two terms lead to the 'scattering correction' as well as 'motional broadening correction' respectively. We first consider the 'scattering correction' and therefore neglect the fifth term in both the Eqs. (11) and (12). Firstly we consider Eq. (11) and proceed to find out an approximate expression for the Green function $\langle\!\langle (n_{i-\sigma}-n_{-\sigma})\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$. The Green function $\langle\!\langle n_{i-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ obeys the equation of motion

$$E \langle\!\langle n_{i-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{\delta_{ij}}{2\pi} n_{-\sigma} + I \langle\!\langle n_{i-\sigma}\, n_{r-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ \sum_m T_{rm} \langle\!\langle n_{i-\sigma}\, c_{m\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ \sum_m T_{im}\{ \langle\!\langle c_{i-\sigma}^\dagger\, c_{m-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle - \langle\!\langle c_{m-\sigma}^\dagger\, c_{i-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle\}$$

$$+ \sum_m \sum_{\sigma'} K_{mr} \langle\!\langle n_{i-\sigma}\, n_{m\sigma'}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \qquad (20)$$

The equation of motion of the Green function appearing in the second term of the above equation may be written as;

$$E \langle\!\langle n_{i-\sigma}\, n_{r-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{\delta_{rj}}{2\pi} \langle n_{i-\sigma}\, n_{r-\sigma} \rangle + I \langle\!\langle n_{i-\sigma}\, n_{r-\sigma}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ \sum_m T_{rm} \langle\!\langle n_{i-\sigma}\, n_{r-\sigma}\, c_{m\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$+ \sum_m \sum_{\sigma'} K_{mr} \langle\!\langle n_{i-\sigma}\, n_{r-\sigma}\, n_{m\sigma'}\, c_{r\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \qquad (21)$$

This equation may be simplified by introducing the approximations

$$\langle n_{i-\sigma} n_{r-\sigma} \rangle \simeq \langle n_{i-\sigma} \rangle \langle n_{r-\sigma} \rangle$$

and

$$\langle\!\langle n_{i-\sigma} n_{r-\sigma} n_{m\sigma'} c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \simeq \langle n_{m\sigma'} \rangle \langle\!\langle n_{i-\sigma} n_{r-\sigma} c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$$

Thus we get

$$\langle\!\langle n_{i-\sigma} \; n_{r-\sigma} \; c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle = \frac{n_{-\sigma}}{(E - T_0 - I - Knz)} \left\{ \frac{\delta_{rj}}{2\pi} n_{-\sigma} + \sum_{m \neq r} T_{rm} \langle\!\langle n_{i-\sigma} \; c_{m\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \right\} \tag{22}$$

Similarly we may get the expression for the Green function $\langle\!\langle n_{i-\sigma} n_{m\sigma'} c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$ appearing in the last term of (20),

$$\langle\!\langle n_{i-\sigma} \; n_{m\sigma'} \; c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle = \frac{n_{\sigma'}}{(E - T_0 - In_{-\sigma} - Knz)}$$

$$\times \left\{ \frac{\delta_{rj}}{2\pi} n_{-\sigma} + \sum_{n \neq r} T_{rn} \langle\!\langle n_{i-\sigma} \; c_{n\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \right\} \tag{23}$$

Neglecting the fourth term of (20) and substituting the values of Green functions $\langle\!\langle n_{i-\sigma} n_{r-\sigma} c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$ and $\langle\!\langle n_{i-\sigma} n_{m\sigma'} c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$ from (22) and (23) in that equation, we get

$$\langle\!\langle n_{i-\sigma} \; c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle = \frac{1}{F_0^{\sigma}(E)} \left\{ \frac{\delta_{rj}}{2\pi} n_{-\sigma} + \sum_{m \neq r} T_{rm} \langle\!\langle n_{i-\sigma} \; c_{m\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \right\} \tag{24}$$

Where $F_0^{\sigma}(E)$ is given by Eq. (18).

Now from Eqs (24) and (16) we get

$$\langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle = \frac{1}{F_0^{\sigma}(E)} T_{ri} \langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$$

$$+ \frac{1}{F_0^{\sigma}(E)} \sum_{m \neq r, \, i} T_{rm} \langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{m\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \tag{25}$$

It was shown by Hubbard (1964b) that Eq. (25) may be solved for

$$\langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \quad (i \neq r) \text{ in terms of } \langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$$

in the following way.

$$\langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle = \sum_m W_{rm, \, i}^{\sigma}(E) T_{mi} \langle\!\langle (n_{i-\sigma} - n_{-\sigma}) \; c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \tag{26}$$

where

$$W_{rm, \, i}^{\sigma}(E) = 2\pi \left\{ g_{rm}^{\sigma}(E) - \frac{g_{ri}^{\sigma}(E) \, g_{im}^{\sigma}(E)}{g_{ii}^{\sigma}(E)} \right\} \tag{27}$$

and

$$g_{ij}^{\sigma}(E) = \frac{1}{2\pi} \sum_k \frac{\exp i k \cdot (R_i - R_j)}{F_0^{\sigma}(E) - (\epsilon_k - T_0)} \tag{28}$$

If this approximate solution is substituted into the right hand side of Eq. (11) and the fifth term in that equation (which gives rise to the motional broadening correction) is dropped, we obtain

$$[E - T_0 - I - Knz - \lambda_{\sigma}(E)] \langle\!\langle n_{i-\sigma} \; c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle$$

$$= n_{-\sigma} \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r \neq i} T_{ri} \langle\!\langle c_{r\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \right\} - n_{-\sigma} \lambda_{\sigma}(E) \langle\!\langle c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\!\rangle \tag{29}$$

where
$$\lambda_\sigma(E) = 2\pi \sum_{r,m} T_{ir} \left\{ g^\sigma_{rm}(E) - \frac{g^\sigma_{ri}(E)\, g^\sigma_{im}(E)}{g^\sigma_{ii}(E)} \right\} \tag{30}$$

It may easily be seen that Eq. (29) is very similar to Eq. (14). Merely the substitution $[T_0 + I + Knz + \lambda_\sigma(E)]$ for $(T_0 + I + Knz)$ and $[T_{ik} - \delta_{ik}\lambda_\sigma(E)]$ for T_{ik} would bring Eq. (14) in the form of Eq. (29).

We now consider Eq. (12) and proceed to find out an expression for $\langle\!\langle (n_{m\sigma'} - n_{\sigma'}) c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$. The Green function $\langle\!\langle n_{m\sigma'} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$ obeys the equation of motion

$$E \langle\!\langle n_{m\sigma'} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle = \frac{\delta_{rj}}{2\pi} n_{\sigma'} + I \langle\!\langle n_{m\sigma'} n_{r-\sigma} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$$

$$+ \sum_n T_{rn} \langle\!\langle n_{m\sigma'} c_{n\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$$

$$+ \sum_n T_{mn} \left\{ \langle\!\langle c^\dagger_{m\sigma'} c_{n\sigma'} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle - \langle\!\langle c^\dagger_{n\sigma'} c_{m\sigma'} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \right\}$$

$$+ \sum_{n\sigma''} K_{rn} \langle\!\langle n_{m\sigma'} n_{n\sigma''} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \tag{31}$$

The equation of motion of the Green function appearing in the second term of the above equation may be written as;

$$E \langle\!\langle n_{m\sigma'} n_{r-\sigma} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle = \frac{\delta_{rj}}{2\pi} \langle n_{m\sigma'} n_{r-\sigma} \rangle + I \langle\!\langle n_{m\sigma'} n_{r-\sigma} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$$

$$+ \sum_n T_{rn} \langle\!\langle n_{m\sigma'} n_{r-\sigma} c_{n\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$$

$$+ \sum_{n\sigma''} K_{rn} \langle\!\langle n_{m\sigma'} n_{r-\sigma} n_{n\sigma''} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \tag{32}$$

We may simplify this equation by introducing the approximations

$$\langle n_{m\sigma'} n_{r-\sigma} \rangle \simeq \langle n_{m\sigma'} \rangle \langle n_{r-\sigma} \rangle \text{ and}$$

$$\langle\!\langle n_{m\sigma'} n_{r-\sigma} n_{n\sigma''} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \simeq \langle n_{n\sigma''} \rangle \langle\!\langle n_{m\sigma'} n_{r-\sigma} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$$

Thus we get

$$\langle\!\langle n_{m\sigma'} n_{r-\sigma} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle = \frac{n_{-\sigma}}{(E - T_0 - I - Knz)} \left\{ \frac{\delta_{rj}}{2\pi} n_{\sigma'} + \sum_{n \neq r} T_{rn} \langle\!\langle n_{m\sigma} c_{n\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \right\} \tag{33}$$

Similarly we may get the expression for the Green function $\langle\!\langle n_{m\sigma'} n_{n\sigma''} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle$ appearing in the last term of (31);

$$\langle\!\langle n_{m\sigma'} n_{n\sigma''} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle = \frac{n_{\sigma''}}{(E - T_0 - I n_{-\sigma} - Knz)} \left\{ \frac{\delta_{rj}}{2\pi} n_{\sigma'} + \sum_{s \neq r} T_{rs} \langle\!\langle n_{m\sigma'} c_{s\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \right\} \tag{34}$$

Now substituting these two expressions in Eq. (31) and neglecting its fourth term we get

$$\langle\!\langle n_{m\sigma'} c_{r\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle = \frac{1}{F_0^\sigma(E)} \left\{ \frac{\delta_{rj}}{2\pi} n_{\sigma'} + \sum_{n \neq r} T_{rn} \langle\!\langle n_{m\sigma'} c_{n\sigma}; c^\dagger_{j\sigma} \rangle\!\rangle \right\} \tag{35}$$

With the help of (35) and (16) we have

$$\langle\!\langle (n_{m\sigma'}-n_{\sigma'})\,c_{r\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle = \frac{1}{F^\sigma_0(E)}\,T_{ri}\,\langle\!\langle (n_{m\sigma'}-n_{\sigma'})c_{i\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle$$

$$+ \frac{1}{F^\sigma_0(E)}\sum_{n\neq r,\,i} T_{rn}\,\langle\!\langle (n_{m\sigma'}-n_{\sigma'})c_{n\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle \tag{36}$$

As before, we may write the solution of this equation in the following way

$$\langle\!\langle (n_{m\sigma'}-n_{\sigma'})c_{r\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle = \sum_n W^\sigma_{rn,\,i}(E)\,T_{ni}\,\langle\!\langle (n_{m\sigma'}-n_{\sigma'})c_{l\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle \tag{37}$$

Substituting this approximate solution into the right hand side of (12) and dropping the fifth term, we have

$$[E - T_0 - I\,n_{-\sigma} - Knz - \lambda_\sigma(E)]\,\langle\!\langle n_{m\sigma'}\,c_{i\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle$$

$$= n_{\sigma'}\left\{\frac{\delta_{ij}}{2\pi} + \sum_{r\neq i} T_{ri}\,\langle\!\langle c_{r\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle\right\} - n_{\sigma'}\lambda_\sigma(E)\,\langle\!\langle c_{i\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle \tag{38}$$

Putting the values of $\langle\!\langle n_{l-\sigma}c_{i\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle$ and $\langle\!\langle n_{m\sigma'}c_{i\sigma}; c^\dagger_{j\sigma}\rangle\!\rangle$ from (29) and (38) in (10) we find the expression for $G^\sigma(k, E)$;

$$G^\sigma(k, E) = \frac{1}{2\pi}\cdot\frac{1}{F^\sigma_s(E)-(\epsilon_k-T_0)} \tag{39}$$

where

$$\frac{1}{F^\sigma_s(E)} = \frac{1 + \dfrac{In_{-\sigma}}{[E-T_0-I-Knz-\lambda_\sigma(E)]} + \dfrac{Knz}{[E-T_0-In_{-\sigma}-Knz-\lambda_\sigma(E)]}}{(E-T_0) + \dfrac{In_{-\sigma}\cdot\lambda_\sigma(E)}{[E-T_0-I-Knz-\lambda_\sigma(E)]} + \dfrac{Knz\cdot\lambda_\sigma(E)}{[E-T_0-In_{-\sigma}-Knz-\lambda_\sigma(E)]}} \tag{40}$$

$\lambda_\sigma(E)$, defined by the relation (30) may be cast into the form

$$\lambda_\sigma(E) = F^\sigma_0(E) - \frac{1}{2\pi g^\sigma_{ii}(E)} \tag{41}$$

where

$$g^\sigma_{ii}(E) = \frac{1}{N}\sum_k g^\sigma_k(E) = \frac{1}{2\pi N}\sum_k \frac{1}{F^\sigma_0(E)-(\epsilon_k-T_0)} \tag{42}$$

The propagator $G^\sigma(k, E)$, described by (39) and (40), has a branch cut along the real axis for those values of E for which $\rho^\sigma_0(E)$ (the density of states corresponding to the propagator given by (17)) is positive. Thus this propagator describes pseudoparticles with finite lifetimes. As we are interested in the self-consistent solution, we replace $\lambda_\sigma(E)$ everywhere by the function

$$\Omega_\sigma(E) = 2\pi\sum_{r,\,m} T_{lr}\left\{G^\sigma_{rm}(E) - \frac{G^\sigma_{ri}(E)\,G^\sigma_{im}(E)}{G^\sigma_{ii}(E)}\right\} \tag{43}$$

where the actual propagator $G^\sigma_{ij}(E)$ has been put for $g^\sigma_{ij}(E)$. With this replacement Eqs. (40), (41) and (42) take the form,

$$\frac{1}{F_s^\sigma(E)} = \frac{1 + \dfrac{I_{n-\sigma}}{[E - T_0 - I - Knz - \Omega_\sigma(E)]} + \dfrac{Knz}{[E - T_0 - I_{n-\sigma} - Knz - \Omega_\sigma(E)]}}{(E - T_0) + \dfrac{I_{n-\sigma} \cdot \Omega_\sigma(E)}{[E - T_0 - I - Knz - \Omega_\sigma(E)]} + \dfrac{Knz}{[E - T_0 - I_{n-\sigma} - Knz - \Omega_\sigma(E)]}}$$

(44)

$$\Omega_\sigma(E) = F_s^\sigma(E) - \frac{1}{2\pi G_{ii}^\sigma(E)}$$

(45)

and
$$G_{ii}^\sigma(E) = \frac{1}{N} \sum_k G^\sigma(k, E)$$

(46)

B. Motional broadening correction

We have found out the expression for the ' scattering correction ' in the previous sub-section. Till now we have assumed $-\sigma$ spin electrons to be fixed while studying the motion of σ spin electron. However, now we proceed to take into account the effect of the motion of $-\sigma$ spin electron. The Green functions $\langle\!\langle c_{r-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ and $\langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ appearing in the fifth term of Eq. (11) respectively contain the information about the events in which $-\sigma$ spin electron reaches and departs from the ith site at the time when σ spin electron comes on the ith site. Thus the complete expression $\{\langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle - \langle\!\langle c_{r-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \}$ of eq. (11) tells us about the effect of motion of $-\sigma$ electron through the ith site and thereby gives the motional or resonance correction. The Green functions $\langle\!\langle c_{r\sigma'}^\dagger c_{m\sigma'} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ and $\langle\!\langle c_{m\sigma'}^\dagger c_{r\sigma'} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$ appearing in the fifth term of eq. (20) respectively give the information about the events in which σ' (σ or $-\sigma$) spin electron reaches and departs from the mth site (which is the nearest neighbour to the ith site) at the time when σ electron comes on the ith site. Thus the complete expression $\{\langle\!\langle c_{m\sigma'}^\dagger c_{r\sigma'} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle - \langle\!\langle c_{r\sigma'}^\dagger c_{m\sigma'} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \}$ of (12) tells about the effect of the motion of σ' electron through the mth site and thereby shares the resonance correction.

1. Motional broadening correction due to the motion of $-\sigma$ electron through the ith site.

Firstly we consider the departure of $-\sigma$ electron from the ith site together with the arrival of σ electrons on the ith site i.e. we consider the Green function $\langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$, which satisfies the equation of motion

$$E \langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle = \frac{\delta_{ij}}{2\pi} \langle c_{i-\sigma}^\dagger c_{r-\sigma} \rangle + \sum_m T_{im} \langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{m\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$- \sum_m T_{im} \langle\!\langle c_{m-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle + \sum_m T_{rm} \langle\!\langle c_{i-\sigma}^\dagger c_{m-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

$$\div I \langle\!\langle n_{r\sigma} c_{i-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle + \sum_{m,\sigma'} K_{im} \langle\!\langle c_{i-\sigma}^\dagger n_{m\sigma'} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

(47)

This equation may be simplified by introducing some approximations; the first term on the right hand side involving correlation function is neglected; in the second and third terms the following approximations are introduced.

$$\langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{m\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle \simeq \delta_{mi} \langle\!\langle c_{i-\sigma}^\dagger c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^\dagger \rangle\!\rangle$$

and
$$\langle\langle c_{m-\sigma}^{\dagger} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle \simeq \delta_{rm} n_{-\sigma} \langle\langle c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$$

With these approximations eq. (47) may be written as;

$$(E-T_0)\langle\langle c_{i-\sigma}^{\dagger} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle = T_{ir}\langle\langle (n_{i-\sigma}-n_{-\sigma})c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$$

$$+ \sum_{m\neq i} T_{rm}\langle\langle c_{i-\sigma}^{\dagger} c_{m-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$$

$$+ I\langle\langle n_{r\sigma} c_{i-\sigma}^{\dagger} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle + \sum_{m\sigma'} K_{im}\langle\langle c_{i-\sigma}^{\dagger} n_{m\sigma'} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle \qquad (48)$$

Putting the approximate values of the Green functions $\langle\langle n_{r\sigma} c_{i-\sigma}^{\dagger} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$ and $\langle\langle c_{i-\sigma}^{\dagger} n_{m\sigma'} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$ in (48) we have

$$\langle\langle c_{i-\sigma}^{\dagger} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle = \frac{1}{F_\sigma^0(E)}\left\{ T_{ir}\langle\langle (n_{i-\sigma}-n_{-\sigma}) c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle + \sum_{m\neq i} T_{rm}\langle\langle c_{i-\sigma}^{\dagger} c_{m-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle\right\}$$

$$(49)$$

This equation may be solved as follows:

$$\langle\langle c_{i-\sigma}^{\dagger} c_{r-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle = \sum_m W_{rm,i}^{-\sigma}(E)\, T_{mi}\langle\langle (n_{i-\sigma}-n_{-\sigma}) c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle \qquad (50)$$

Now we consider the arrival of $-\sigma$ electron at the ith site together with the arrival of σ electron, i.e. we consider the propagator $\langle\langle c_{r-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$. With the approximations used above, the equation of motion of this Green function may be written as

$$(E-T_0-I)\langle\langle c_{r-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle = -T_{ir}\langle\langle (n_{i-\sigma}-n_{-\sigma}) c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$$

$$- \sum_{m\neq i} T_{rm}\langle\langle c_{m-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle - I\langle\langle n_{r\sigma} c_{r-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$$

$$+ \sum_{m\sigma'} K_{im}\langle\langle c_{r-\sigma}^{\dagger} n_{m\sigma'} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle \qquad (51)$$

Putting the approximate values of the Green functions $\langle\langle n_{r\sigma} c_{r-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$ and $\langle\langle c_{r-\sigma}^{\dagger} n_{m\sigma'} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle$ in (51) we have

$$\langle\langle c_{r-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle = \frac{1}{F_0^{'-\sigma}(E)}\left\{ -T_{ir}\langle\langle (n_{i-\sigma}-n_{-\sigma}) c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle\right.$$

$$\left. - \sum_{m\neq i} T_{rm}\langle\langle c_{m-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle\right\} \qquad (52)$$

where
$$\frac{1}{F_0^{'-\sigma}(E)} = \frac{1}{(E-T_0-I)}\left\{ 1 - \frac{In_\sigma}{(E-T_0-I)} + \frac{Knz}{[E-T_0-I(1-n_\sigma)-Knz]}\right\} \qquad (53)$$

This equation has the solution

$$\langle\langle c_{r-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle = -\sum_m W_{rm,i}^{'-\sigma}(E)\, T_{mi}\langle\langle (n_{i-\sigma}-n_{-\sigma}) c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\rangle \qquad (54)$$

where
$$W_{rm,i}^{'\sigma}(E) = 2\pi\left\{ g_{rm}^{'\sigma}(E) - \frac{g_{ri}^{'\sigma}(E)\, g_{im}^{'\sigma}(E)}{g_{ii}^{'\sigma}(E)}\right\} \qquad (55)$$

and

$$g_{ij}^{'\sigma}(E) = \frac{1}{2\pi} \sum_k \frac{\exp\{i\mathbf{k}\cdot(R_i-R_j)\}}{F_0^{'\sigma}(E)-(\epsilon_k-T_0)} \tag{56}$$

Substituting (50) and (54) into the fifth term of (11) and neglecting the fourth term in that equation (as we are considering now only the resonance correction), we get after some rearrangements:

$$[E-T_0-I-\lambda_{-\sigma}(E)-\lambda'_{-\sigma}(E)-Knz]\langle\langle n_{i-\sigma}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$$

$$=n_{-\sigma}\left\{\frac{\delta_{ij}}{2\pi}+\sum_{r\neq i}T_{ri}\langle\langle c_{r\sigma};\,c_{j\sigma}^\dagger\rangle\rangle\right\}-n_{-\sigma}[\lambda_{-\sigma}(E)+\lambda'_{-\sigma}(E)]$$

$$\times\langle\langle c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle \tag{57}$$

We observe that when interatomic correlations are absent (i.e. $K=0$), the contribution towards the motional broadening correction due to the $-\sigma$ electron arriving at the ith site is equal to the contribution due to the $-\sigma$ electron departing from the ith site. But in the present case (K finite) the contribution $\lambda'_{-\sigma}(E)$ due to the $-\sigma$ electron arriving at the ith site is somewhat different from the contribution $\lambda_{-\sigma}(E)$ due to the $-\sigma$ electron departing from the ith site. To a first approximation we suppose $\lambda'_{-\sigma}(E)$ to be equal to $\lambda_{-\sigma}(E)$. With this approximation (57) may be written as:

$$[E-T_0-I-2\lambda_{-\sigma}(E)-Knz]\langle\langle n_{i-\sigma}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$$

$$=n_{-\sigma}\left\{\frac{\delta_{ij}}{2\pi}+\sum_{r\neq i}T_{ri}\langle\langle c_{r\sigma};\,c_{j\sigma}^\dagger\rangle\rangle\right\}-2n_{-\sigma}\lambda_{-\sigma}(E)\langle\langle c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle \tag{58}$$

2. *Motional broadening correction due to the motion of σ' (σ or $-\sigma$) electron through the mth site.* As in the preceding situation, firstly we consider the departure of σ' electron from the mth site together with the arrival of σ electron on the ith site, i.e. we consider the Green function $\langle\langle c_{m\sigma'}\,c_{r\sigma'}c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$. With approximations similar to those used in writing (48), the equation of motion of this Green function may be written as

$$(E-T_0)\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle = T_{rm}\langle\langle(n_{m\sigma'}-n_{\sigma'})\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$$

$$+\sum_{n\neq m}T_{rn}\langle\langle c_{m\sigma'}^\dagger\,c_{n\sigma'}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle+I\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,n_{i-\sigma}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$$

$$+\sum_{n\sigma''}K_{in}\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,n_{n\sigma''}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle \tag{59}$$

Putting the approximate values of $\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,n_{i-\sigma}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$ and $\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,n_{n\sigma''}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$ in this equation, we have

$$\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle = \frac{1}{F_0^\sigma(E)}\left\{T_{rm}\langle\langle(n_{m\sigma'}-n_{\sigma'})c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle+\sum_{n\neq m}T_{rn}\langle\langle c_{m\sigma'}^\dagger c_{n\sigma'}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle\right\}$$

$$\tag{60}$$

which may be solved in the form

$$\langle\langle c_{m\sigma'}^\dagger\,c_{r\sigma'}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle = \sum_n W_{rn,\,m}^\sigma(E)\,T_{nm}\langle\langle(n_{m\sigma'}-n_{\sigma'})c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle \tag{61}$$

Now we consider the arrival of σ' electron on the mth site together with the arrival of σ electron on the ith site, i.e. we consider the propagator $\langle\langle c_{r\sigma'}^\dagger\,c_{m\sigma'}\,c_{i\sigma};\,c_{j\sigma}^\dagger\rangle\rangle$. Proceed-

ing exactly in the same way as we did in obtaining the expression (61) we get an expression for $\langle\!\langle c_{r\sigma'}^{\dagger} c_{m\sigma'} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle$

$$\langle\!\langle c_{r\sigma'}^{\dagger} c_{m\sigma'} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle = -\sum_{n} W_{rn,m}^{\sigma}(E) \, T_{nm} \langle\!\langle (n_{m\sigma'}-n_{\sigma'}) c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle \tag{62}$$

Substituting the solutions (61) and (62) in the fifth term of eq. (12) and neglecting the fourth term in that equation (as we are considering here only the resonance correction), we get

$$[E-T_0-In_{-\sigma}-Knz-2\lambda_\sigma] \langle\!\langle n_{m\sigma'} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle$$

$$= n_{\sigma'} \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r\neq i} T_{ir} \langle\!\langle c_{r\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle \right\} - 2n_{\sigma'} \lambda_\sigma \langle\!\langle c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle \tag{63}$$

Putting the values of $\langle\!\langle n_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle$ and $\langle\!\langle n_{m\sigma'} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle$ from eqs. (58) and (63) in (10) we find that when only the resonance correction is considered, the expression for the Green function $G^{\sigma}(k, E)$ is given by

$$G^{\sigma}(k, E) = \frac{1}{2\pi} \cdot \frac{1}{F_r^{\sigma}(E) - (\epsilon_k - T_0)} \tag{64}$$

where

$$\frac{1}{F_r^{\sigma}(E)} = \frac{1 + \dfrac{In_{-\sigma}}{[E-T_0-I-Knz-2\Omega_{-\sigma}]} + \dfrac{Knz}{[E-T_0-In_{-\sigma}-Knz-2\Omega_\sigma]}}{(E-T_0) + \dfrac{2In_{-\sigma}\cdot\Omega_{-\sigma}}{[E-T_0-I-Knz-2\Omega_{-\sigma}]} + \dfrac{2Knz\cdot\Omega_\sigma}{[E-T_0-In_{-\sigma}-Knz-2\Omega_\sigma]}} \tag{65}$$

As mentioned earlier, in order to get self consistent solution $\Omega_\sigma(E)$ has been written in place of $\lambda_\sigma(E)$ in Eq. (65). The Green function (64) also has a branch cut along the real axis for those values of E for which $\rho^{\sigma}(E) > 0$, where $\rho^{\sigma}(E)$ is the density of pseudo-particle states calculated from eq. (64).

Till now, the cases of 'scattering correction' and 'motional broadening correction' have been considered separtealy. However both of the corrections may be considered simultaneously. From eqs. (26), (50) and (54), eq. (11) becomes

$$[E-T_0-I-Knz-\Omega_\sigma-2\Omega_{-\sigma}] \langle\!\langle n_{i-\sigma} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle$$

$$= n_{-\sigma} \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r\neq i} T_{ri} \langle\!\langle c_{r\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle \right\} - n_{-\sigma}(\Omega_\sigma + 2\Omega_{-\sigma}) \langle\!\langle c_{i\sigma}; c_j^{\dagger}\rangle\!\rangle \tag{66}$$

Similarly from eqs. (37), (61) and (62), eq. (12) becomes

$$[E-T_0-In_{-\sigma}-Knz-3\Omega_\sigma] \langle\!\langle n_{m\sigma'} c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle$$

$$= n_{\sigma'} \left\{ \frac{\delta_{ij}}{2\pi} + \sum_{r\neq i} T_{ir} \langle\!\langle c_{r\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle \right\} - 3n_{\sigma'}\Omega_\sigma \langle\!\langle c_{i\sigma}; c_{j\sigma}^{\dagger}\rangle\!\rangle \tag{67}$$

With the help of the relations (66) and (67) we get an expression for $G^{\sigma}(k, E)$ from eq. (10) containing both the corrections simultaneously:

$$G^{\sigma}(k, E) = \frac{1}{2\pi} \cdot \frac{1}{F^{\sigma}(E) - (\epsilon_k - T_0)} \tag{68}$$

$$\frac{1}{F^\sigma(E)} = \frac{1 + \dfrac{In_{-\sigma}}{[E-T_0-I-Knz-\Omega_\sigma-2\Omega_{-\sigma})]} + \dfrac{Knz}{[E-T_0-In_{-\sigma}-Knz-3\Omega_\sigma]}}{(E-T_0) + \dfrac{In_{-\sigma}(\Omega_\sigma+2\Omega_{-\sigma})}{[E-T_0-I-Knz-\Omega_\sigma-2\Omega_{-\sigma}]} + \dfrac{3knz\cdot\Omega_\sigma}{[E-T_0-In_{-\sigma}-Knz-3\Omega_\sigma]}} \tag{69}$$

4. A special (nonmagnetic) case

Our main purpose is to find out the value of the pseudoparticle spectrum given by the poles of the Green's function $G^\sigma(k, E)$ given by (68). Calculation of $G^\sigma(k, E)$ means the solution of the three equations (68), (69) and (43) simultaneously. For the purpose of a numerical calculation we consider the simple special case in which the solution is readily obtainable. This special case has the features; (i) $n=1$ i.e., the number of electrons present is one per atom; (ii) $n_{-\sigma}=n_\sigma=\frac{1}{2}$ i.e., we assume the system to be nonferromagnetic; (iii) The density of state function

$$P(E) = \frac{1}{N}\sum_k \delta(E-\epsilon_k) \tag{70}$$

corresponding to the unperturbed band structure ϵ_k, has the following parabolic form centered on T_0 with a band width Δ;

$$P(E) = \frac{4}{\pi\Delta}\sqrt{1-\left(\frac{E-T_0}{\Delta/2}\right)^2} \quad \text{if } |E-T_0| < \Delta/2 \tag{71}$$
$$= 0, \text{ otherwise}$$

From the assumption (ii) it follows that $\Omega_\sigma(E)=\Omega_{-\sigma}(E)$. Now choosing the origin of energy such that $T_0+I/2=0$, equation (69) becomes

$$\frac{1}{F^\sigma(E)} = \frac{1 + \dfrac{I/2}{[E-I/2-Kz-3\Omega_\sigma]} + \dfrac{Kz}{[E-Kz-3\Omega_\sigma]}}{(E+I/2) + \dfrac{\frac{3}{2}I\Omega_\sigma}{[E-I/2-Kz-3\Omega_\sigma]} + \dfrac{3Kz\Omega_\sigma}{[E-Kz-3\Omega_\sigma]}} \tag{72}$$

where

$$\Omega_\sigma(E)=F^\sigma(E)-\frac{1}{2\pi G_{ii}^\sigma(E)} \tag{73}$$

and

$$G_{ii}^\sigma(E) = \frac{1}{N}\sum_k G^\sigma(k,E) = \frac{1}{2\pi N}\sum_k \frac{1}{F^\sigma(E)-(\epsilon_k-T_0)} \tag{74}$$

Combining (74) and (70) we can write

$$G_{ii}^\sigma(E) = \frac{1}{2\pi}\int \frac{P(E')\mathrm{d}E'}{F^\sigma(E)-(E'-T_0)} \tag{75}$$

Putting the form of $P(E)$ from (71) and integrating, we obtain

$$G_{ii}^\sigma(E) = \frac{4}{\pi\Delta^2}[F^\sigma(E)-\sqrt{\{F^\sigma(E)\}^2-\{\Delta/2\}^2}] \tag{76}$$

From (73) and (76) following relation emerges.

$$\Omega_\sigma(E)=\frac{1}{2}[F^\sigma(E)-\sqrt{\{F^\sigma(E)\}^2-\{\Delta/2\}^2}] \tag{77}$$

Substituting this value of $\Omega_\sigma(E)$ into (72) we get

$$F^3+AF^2+BF+C=\sqrt{F^2-\Delta^2/4}\,[F^2+AF+D] \tag{78}$$

where $\quad A = \frac{1}{3}(4Kz - 5E)$

$$B = \frac{1}{9}\left(E - \frac{I}{2} - Kz\right)\left(5E + \frac{3I}{2} - 3Kz\right) + \frac{1}{9}(E - Kz)(3E + I) - \frac{\Delta^2}{8}$$

$$C = \frac{\Delta^2}{8}(E - Kz) - \frac{2}{9}(E - Kz)\left(E + \frac{I}{2}\right)\left(E - \frac{I}{2} - Kz\right)$$

$$D = \frac{1}{3}\left(E - \frac{I}{2} - Kz\right)\left(E + \frac{I}{2} - Kz\right) + \frac{E}{3}(E - Kz)$$

$$\left.\begin{matrix} \\ \\ \\ \\ \\ \\ \\ \end{matrix}\right\} \quad (79)$$

Squaring Eq. (78) we get the quartic equation for $F^\sigma(E)$

$$F^4\left\{2B - 2D + \frac{\Delta^2}{4}\right\} + F^3\left\{2C + 2AB - 2AD + \frac{A\Delta^2}{2}\right\} + F^2\left\{B^2 - D^2 + 2AC\right.$$

$$\left. + \frac{\Delta^2 A^2}{4} - \frac{\Delta^2 D}{2}\right\} + F\left\{2BC + \frac{DA}{2}\Delta^2\right\} + \left\{C^2 + \frac{\Delta^2 D^2}{4}\right\} = 0 \qquad (80)$$

Thus the solution of the self-consistent equations has been reduced to the solution of a quartic.

It may easily been seen that if we put $K = 0$ in (80) it reduces to the equation

$$EF^3 - \left\{\frac{7}{3}E^2 + \frac{3}{4}(\Delta/2)^2 - \frac{I^2}{4}\right\}F^2 + \left\{\frac{5}{3}E\left(E^2 - \frac{I^2}{4}\right) + \frac{3}{2}E(\Delta/2)^2\right\}F$$

$$- \left\{\frac{1}{3}\left(E^2 - \frac{I^2}{4}\right)^2 + \frac{3}{4}E^2(\Delta/2)^2\right\} = 0 \qquad (81)$$

which is the same as Hubbard's eq. (70) (Hubbard 1946b). Thus we get exactly the results of Hubbard in the absence of intersite correlations.

For any fixed values of I, K and E eq. (80) may have either four complex roots, or two complex and two real roots or four real roots. Let one of the roots be

$$F = \alpha + i\beta \qquad (82)$$

then $\quad \sqrt{F^2 - (\Delta/2)^2} = A + iB \qquad (83)$

where $\quad A = \sqrt{\dfrac{[\alpha^2 - \beta^2 - (\Delta/2)^2] + \sqrt{[\alpha^2 - \beta^2 - (\Delta/2)^2]^2 + 4\alpha^2\beta^2}}{2}} \qquad (84)$

and $\quad B = \sqrt{\dfrac{-[\alpha^2 - \beta^2 - (\Delta/2)^2] + \sqrt{[\alpha^2 - \beta^2 - (\Delta/2)^2 + 4\alpha^2\beta^2}}{2}} \qquad (85)$

Now from eq. (76)

$$G^\sigma_{ii} = \frac{4}{\pi\Delta^2}[(\alpha - A) - i(B - \beta)] \qquad (86)$$
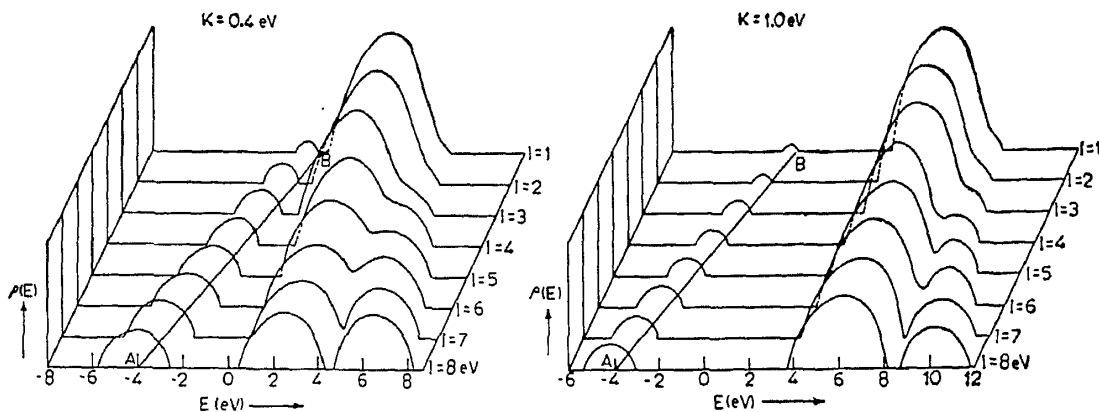
since the pseudo-particle density of states is given in terms of the negative imaginary part of the Green function G^σ_{ii}, the numerical value of $(B - \beta)$ is required for the determination of the density of states function. For this purpose eq. (80) has been solved for $F^\sigma(E)$. A particular case of the simple cubic system ($z = 6$) with band width $= 4{\cdot}0$ eV has been considered. For a particular set of I and K, the appropriate root of $F^\sigma(E)$ (i.e. the root which gives the quantity $(B - \beta)$ to be positive) is chosen from which we get the density of states function $\rho^\sigma(E)$ for this particular set. Various sets of values of I and K have been taken. Keeping K fixed the density-spectrum has been calculated for various values of I (from 1 eV to 8 eV by the step of 1eV). Thus
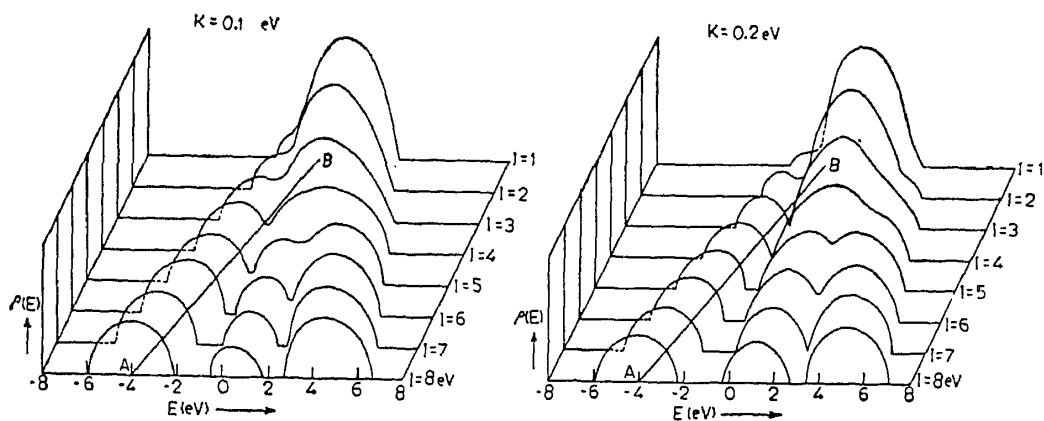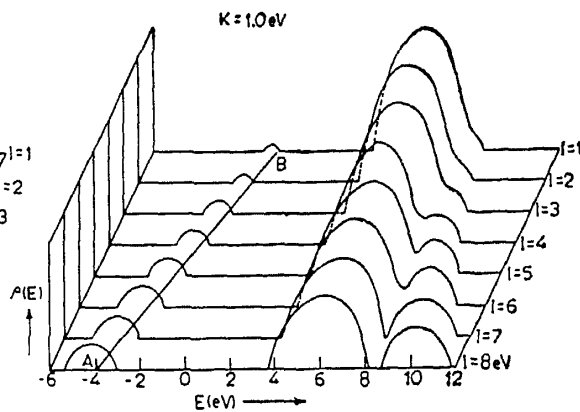
Figure 1. Pseudoparticle density of states function for a number of values of intra-atomic correlation I, with a fixed value $K=0.1$ eV. Line AB meets the energy axis at the centre of the unperturbed band (i.e., at $E=T_0$).
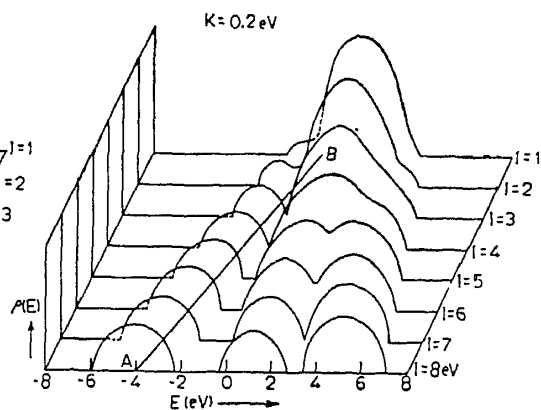
Figure 2. Pseudoparticle density of states function for a number of values of intra-atomic correlation I, with a fixed value $K=0.2$ eV.

Figure 3. Pseudoparticle density of states function for a number of values of intra-atomic correlation I, with a fixed value $K=0.4$ eV.

Figure 4. Pseudoparticle density of states function for a number of values of intra-atomic correlation I, with a fixed value $K=1.0$ eV.

we get a set of density-spectra which shows the effect of the variation of I. Four sets with $K=0.1$, 0.2, 0.4 and 1.0 eV have been obtained and shown graphically in figures 1, 2, 3 and 4 respectively.

5. Discussion

The above calculation shows that when we take intersite correlations K into account together with the intrasite correlations I, the unperturbed band splits into three bands. For large values of I and K these three bands are all separated from each other. As the values of I and K are decreased, bands come nearer and below certain crtical values these merge into one band. There are innumerable sets of the critical values of I and K, because a new choice of K will lead to a change in the value of I at which the merger gets in.

The effect of the variation of the parameter I alone has been seen by keeping K fixed and calculating pseudoparticle density of states function for various values of I.
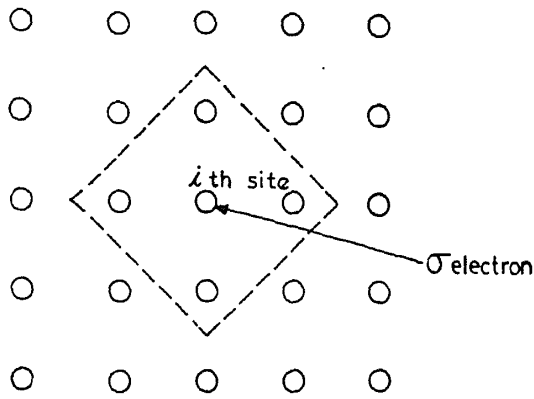
Figure 5. Atomic arrangement in a lattice. The ith atom may be resonant at any one of the $2(2z+1)$ energy values depending upon the electron occupancy of the sites inside the cluster.

We see that if I is increased in small steps, the band first splits into two at some value $I_1(K)$. When I is increased further we get three separate sub-bands at some higher value $I_2(K)$. Effect of the variation of the parameter K is observed by calculating density of states at different values of K. It is seen that $I_1(K)$ decreases with the increase of K. $I_2(K)$ does not appear to depend much on K. Unlike the result in the presence of intra-atomic correlations alone, we find that a nonmagnetic system, with a half-filled band, is never an insulator however large the intra-atomic correlations may be (i.e., even in the split-band-region it is not an insulator).

We have not investigated the magnetic properties of the system in detail. But we can easily see the effect of intersite correlations on the magnetic behaviour of the system, at least for a zero bandwidth (i.e., atomic limit) case. In this limit $T_{ij} = T_0 \, \delta_{ij}$

and hence $\epsilon_k = T_0$ for all k. Then from eq. (74) we have $G_{ii}^\sigma (E) = G^\sigma (k, E) = \dfrac{1}{2\pi F^\sigma (E)}$

which when put in eq. (73) gives $\Omega_\sigma(E) = 0$ and we may write $F^\sigma(E) = F_0^\sigma(E)$ in eq. (68) where $F_0^\sigma (E)$ is given by eq. (19). For this particular case it may be shown (Kishore and Joshi 1969) that the energy of the ferromagnetic state is lower than that of the paramagnetic state. While in the Hubbard model one finds that for $n=1$ and in the atomic limit the energies of both the paramagnetic and ferromagnetic states are the same.

It is to be noted that several approximations have been made during the course of the treatment. Without these approximations the mathematics of the problem becomes quite complicated and it is extremely difficult to arrive at a solution. But keeping the mathematical derivations aside, we can see by a simple physical reasoning that the unperturbed single band should split exactly into $2(2z+1)$ sub-bands. In figure 5 we schematically show the atoms in a lattice. It can be easily seen from the figure that (as far as the arrival of a σ spin electron is concerned) ith atom may be resonant at any one of the energies: T_0, T_0+K, T_0+2K......, T_0+2zK; T_0+I, T_0+I+K, T_0+I+2K, ..., $T_0+I+2zK$, depending upon the electron occupancy of the sites inside the cluster. This shows that in the atomic limit, for the Hamiltonian (4), an atomic level located at T_0 (in the absence of electronic correlations) will be split into $2(2z+1)$ levels. Thus the two bands of Hubbard model should increase in number to $2(2z+1)$ bands when we take into account the interatomic correlations with z nearest neighbours alone. The approximations used during the course of the treatment have reduced the number of perturbed bands from $2(2z+1)$ to three. So our predictions regarding the metallic (or nonmetallic and magnetic behaviours are not exact results

for the Hamiltonian (4), but are artifacts of the approximation scheme we have to resort to in order to arrive at a solution. Nevertheless, it may be concluded that while studying the electrical or magnetic properties of the narrow energy band systems, one should not overlook the role of the intersite correlations.

Acknowledgements

Appendix

We consider a ternary alloy described in the tight binding approximation. A single atomic orbital $|n\rangle$ is associated with each site n. The one-particle Hamiltonian in the Wannier representation is

$$\mathcal{H} = \sum_{m \neq n} |m\rangle h_{mn} \langle n| + \sum_n |n\rangle \epsilon_n \langle n| = W + D \tag{1A}$$

where W is the kinetic energy part and D is the sum of contributions from all sites of the crystal having random potentials. The single particle Hamiltonian refers to a particular configuration and in order to study the macroscopic properties of the system, an averaging over all configurations is to be performed. We define the Green function $G(z)$ corresponding to the Hamiltonian $\mathcal{H}$ by

$$G(z) = (z - \mathcal{H})^{-1} \tag{2A}$$

All the macroscopic quantities of interest may be determined by the configurationally averaged Green function $\langle G(z) \rangle$, which has the full symmetry of the empty lattice. The effective Hamiltonian which has full crystal symmetry is defined by

$$\langle G(z) \rangle = (z - \mathcal{H}_{eff})^{-1} \tag{3A}$$

where
$$\mathcal{H}_{eff} = W + \Sigma(z) \tag{4A}$$

Here $\Sigma(z)$ is the average atomic potential (i.e., the self-energy) associated with each site, an unknown of the problem.

With the help of multiple scattering theory we can determine the self energy $\Sigma(z)$, choosing the self-consistent condition*

$$\langle T_n \rangle = 0 \tag{5A}$$

where T_n in the case of a ternary alloy may be written,

$$\frac{x_1[\epsilon_1 - \Sigma(z)]}{1 - [\epsilon_1 - \Sigma(z)]f(z)} + \frac{x_2[\epsilon_2 - \Sigma(z)]}{1 - [\epsilon_2 - \Sigma(z)]f(z)} + \frac{x_3[\epsilon_3 - \Sigma(z)]}{1 - [\epsilon_3 - \Sigma(z)]f(z)} = 0 \tag{6A}$$

where x_1, x_2, x_3 are the concentrations of the three components and ϵ_1, ϵ_2 and ϵ_3 are the atomic potentials of the components. Eq. (6A) may be cast into the form

$$\Sigma(z) = \epsilon + \frac{f(z)[\Sigma(z)\{\epsilon_1 + \epsilon_2 + \epsilon_3 - \epsilon\} - \{\epsilon_1\epsilon_2 + \epsilon_2\epsilon_3 + \epsilon_1\epsilon_3\}]}{[1 + \Sigma(z)f(z)]}$$

$$+ \frac{f(z)[x_1\epsilon_2\epsilon_3 + x_2\epsilon_1\epsilon_3 + x_3\epsilon_1\epsilon_2 + \epsilon_1\epsilon_2\epsilon_3 \cdot f(z)]}{[1 + \Sigma(z)f(z)]^2} \tag{7A}$$

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*A detailed description of the method of evaluating the self-energy $\Sigma(z)$ using the self-consistent condition (5A) is given by Velicky *et al* (1968). The expression for T_n is given in eq. (4.8) of that paper. Our $f(z)$ here stands for the $F(z)$ of that paper which is defined in eq. (3.16).

here $\varepsilon = x_1\epsilon_1 + x_2\epsilon_2 + x_3\epsilon_3$ is the mean atomic energy.

Now if we regard the down spin electron as fixed to randomly distributed sites, then we see that the motion of the up spin electron is identical to the motion of electrons in an alloy. With the replacement given below in going over from alloy problem to the present problem, it is very easy to show that eq. (44) is identical to the eq. (7A).

$$G_{ii}^{\sigma}(E) \longrightarrow f(z)$$

$$F_s^{\sigma}(E) \longrightarrow [z - f(z)]$$

$$T_0 \longrightarrow \epsilon_1$$

$$(T_0 + I n_{-\sigma} + Knz) \longrightarrow \epsilon_2$$

$$(T_0 + I + Knz) \longrightarrow \epsilon_3$$

$$\frac{I^2 n_{-\sigma}(1 - n_{-\sigma})}{(I + Knz)(I n_{-\sigma} + Knz)} \longrightarrow x_1$$

$$\frac{Knz}{(I n_{-\sigma} + Knz)} \longrightarrow x_2$$

$$\frac{I n_{-\sigma}}{(I + Knz)} \longrightarrow x_3$$

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