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Electron correlations in narrow energy bands
III. An improved solution

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A more accurate solution of the model (of an s-band of interacting electrons) discussed in paper I is obtained. The new solution predicts a finite lifetime for the pseudo-particles and also the 'Mott' insulator-conductor transition. A physical interpretation of the theory based upon an analogy with the theory of alloys is given, and a special case in which the predictions of the theory can be worked out in some detail is studied.

1. Introduction

In two previous papers (Hubbard 1963, 1964; these papers will be referred to as I and II respectively) a theory of electron correlations in narrow energy bands has been described. The particular feature of this theory is that it yields the exact solutions in the two opposite limiting cases of very weakly interacting electrons, in which case band theory is good, and very strongly interacting electrons, in which case Heitler–London theory is good, thus providing a bridge between band theory and Heitler–London theory. It was suggested that the theory might be usefully applied to d-bands in transition metals, their alloys and salts.

In I the theory was developed for the especially simple case of an s-band. In the course of this development certain approximations were introduced. It is the purpose of this paper to describe a more accurate theory of the s-band case based upon less drastic approximations. This improved theory has the advantage as compared to the theory of I that certain unsatisfactory features of the latter are no longer present in the new theory. The nature of these unsatisfactory features will be explained at once.

One of the most striking predictions of the theory of I is that the pseudo-particle spectrum consists of two sub-bands separated by an energy gap. This result has important implications regarding the properties of a half-filled s-band. On the one hand, band theory predicts that a substance with such a half-filled band will be a metallic conductor; on the other, Heitler–London theory predicts that it will be an insulator with just one electron attached to each atom. It is tempting to suggest that in the case of a half-filled band the lower of the two pseudo-particle bands is just full and the upper empty, thus accounting for the insulating properties predicted in the Heitler–London limit.

Unfortunately, the theory of I does not bear out this suggestion in at least two important respects. First, if one calculates (for the case of a half-filled band) the number of pseudo-particle states in each of the two sub-bands, one does not in general find that each sub-band contains exactly one state per atom (although the

total number of pseudo-particle states in both sub-bands taken together is exactly two states per atom as required). The developments described in this paper do not appear to throw any new light on this problem. One can advance strong arguments to show that this failing is merely a consequence of the approximations introduced, but the author is not aware of any computational technique which will guarantee the correctness of the theory in this respect.

Secondly, the theory of I predicts that the pseudo-particle spectrum splits into two bands however weak the interaction between the electrons. The incorrectness of this prediction has already been noted in § 8 of I. What one expects on physical grounds has been discussed by Mott (1949 and later papers, particularly that of 1961), who suggests that when the bandwidth is sufficiently small the system does indeed behave as an insulator, but that there is a critical bandwidth such that when it is exceeded the system behaves as a conductor. Thus one would expect that for sufficiently small bandwidths the pseudo-particle spectrum consists of two bands, but that for large bandwidths the spectrum consists of a single band; this is exactly the result found in this paper.

A further unsatisfactory feature of the theory of I is that it predicts an infinite lifetime for the pseudo-particles; the theory of the present paper leads to a finite pseudo-particle lifetime.

The general plan of the paper is as follows. In § 2 the physical interpretation of the theory is discussed, and in particular the nature of the new effects taken into account by the theory of this paper are indicated. In §§ 3 to 5 the mathematical details of the theory are developed using a Green function technique. Finally, in § 6 the general theory developed in the preceding sections is applied to a special case (a special band structure) which can be worked out in considerable detail and serves to illustrate the nature of the results to be expected from the general theory.

2. The alloy analogy

The expression derived in I for the electron propagator may be written

$$G^{\sigma}_{\mathbf{k}}(E) = \frac{1}{2\pi}\frac{1}{F^{\sigma}_{0}(E)-(\epsilon_{\mathbf{k}}-T_{0})}, \tag{1}$$

where

$$\frac{1}{F^{\sigma}_{0}(E)} = \frac{1-n_{-\sigma}}{E-T_{0}} + \frac{n_{-\sigma}}{E-T_{0}-I}; \tag{2}$$

$\mathbf{k}$ is the (crystal) momentum and $\epsilon_{\mathbf{k}}$ the corresponding band energy, $\sigma(=\pm 1)$ is the electron spin, n_{σ} is the number of electrons per atom of spin σ present, T_0 is the binding energy of the atomic level from which the s-band arises, and I is the energy of interaction of two electrons on the same atom.

The formulae (1) and (2) can be interpreted along the lines indicated in § 9 of II. The quantity $\epsilon_{\mathbf{k}}-T_0$ may be thought of as describing the propagation of electrons between atoms and the function $F^{\sigma}_{0}(E)$ the resonant properties of the atoms. The formula (2) for $F^{\sigma}_{0}(E)$ can be understood by reference to figure 1 which depicts the energy level system for a single atom. If an electron of spin σ is incident on an atom with no electron present already, then that atom must undergo a transition of

type a to absorb the σ spin electron, the corresponding resonant energy being T_0. On the other hand, if the atom already has a $-\sigma$ spin electron present, then it must undergo a transition of type b with resonant energy T_0+I. The probabilities that any atom does or does not have a $-\sigma$ spin electron present are $n_{-\sigma}$ and $1-n_{-\sigma}$ respectively, so the form of (2) follows.

An analogy between formulae (1) and (2) and those describing the propagation of light in solids may be drawn. In the latter case the ordinary free space dispersion law $\omega = ck$ plays the same role as $\epsilon_{\mathbf{k}}$. The analogue of the function $F_0^\sigma(E)$ is the dielectric constant of the medium which is related to the atomic resonances for the absorption of a photon by a formula similar to (2).

An alternative analogy may be drawn between the formulae (1) and (2) and those describing the propagation of electrons in alloys. Indeed, the interpretation given above amounts to saying that the theory of I describes the propagation of an electron

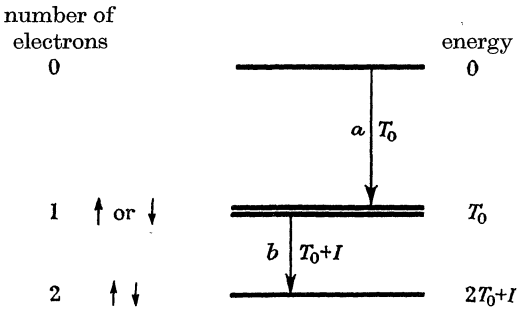

FIGURE 1. The energy levels of an atom.

of spin σ as though it were moving through an alloy consisting of two species of atom randomly distributed in the proportions $n_{-\sigma}:1-n_{-\sigma}$, the binding energies of the s-levels on the two atomic species being T_0+I and T_0. This analogy would be exact if by some magic the $-\sigma$ spin electrons were fixed at particular atoms.

This alloy analogy suggests two directions in which the theory of I might be improved. First, even if the $-\sigma$ spin electrons were somehow fixed, the theory of I does not describe very accurately the propagation of the σ-spin electrons in the resulting alloy, e.g. it gives no account of the damping of the electron wave which results from disorder scattering in the alloy. Thus one direction for improvement lies in development along the lines of better theories of alloys; in particular, it is desirable to develop the theory to the point at which it takes into account the damping due to disorder scattering. Secondly, since the $-\sigma$ spin electrons are not fixed, but do in fact move about, the theory of I might be improved so as to take into account the effects of this motion.

Actually, the theory developed in §§ 3 to 5 of this paper is based upon a generalization of the method of approximation used in I which was in turn based upon the notion that the correlations of electrons on the same atom are of dominant importance. When this generalized method of approximation is employed, it is found that the new terms which arise can be quite naturally divided into two kinds. It turns out that one of these kinds produces corrections to the theory of I which

correspond to an improvement of the 'alloy' theory to include the effects of disorder scattering, while the other kind produces corrections which take account of the effects of the motion of the $-\sigma$ spin electrons. Thus corrections of both the types suggested above are found. They are referred to as the 'scattering' and the 'resonance broadening' corrections respectively. Theories of these two types of correction are developed separately in §§ 4 and 5, and their combined effect is also considered in § 5.

It has been explained above that the main physical effect included by the introduction of the 'scattering' correction to the theory of I is the analogue of damping by disorder scattering in an alloy; this analogue is essentially the phenomenon sometimes referred to as 'spin disorder scattering'. One may now enquire: what physical phenomena, resulting from the movement of the $-\sigma$ spin electrons, are described by the 'resonance broadening' correction discussed in § 5?

The effect of the motion of the $-\sigma$ spin electrons on the propagation of a σ spin electron may be discussed in the following terms. If an atom has a $-\sigma$ spin electron on it, then (so far as a σ spin electron is concerned) that atom is resonant at energy T_0+I. If the $-\sigma$ spin electron now moves away, the atom becomes resonant at energy T_0, and if another $-\sigma$ spin electron later moves onto it, it again becomes resonant at energy T_0+I, and so on. The effect of the motion of the $-\sigma$ spin electrons is that any given atom switches back and forth between being resonant at energies T_0 and T_0+I so far as σ spin electrons are concerned.

The net effect of this switching between resonances depends upon whether the rate of switching is fast or slow compared with $I/\hbar$, since I is the energy separation of the two resonances. If the switching rate is slow compared to $I\hbar$, then the effect is to broaden the two resonances at T_0 and T_0+I, the breadth being $\hbar/\tau$ where τ is the mean lifetime of the atom in either of the resonant states; $\hbar/\tau$ will be of the order of the bandwidth. On the other hand, if the switching rate is fast compared to $I/\hbar$, the separate resonances at T_0 and T_0+I disappear and are replaced by a single narrow resonance at the average energy $T_0+In_{-\sigma}$. This is an example of the well-known 'motional line narrowing' effect. It is these effects which are included by the introduction of the 'resonance broadening' correction to the theory of I.

The new developments to be described in this paper have been interpreted above in terms of the alloy analogy. There are, however, alternative interpretations. Consider figure 2 which shows a σ spin electron incident on an atom and three possible subsequent developments: the atom may emit a σ spin or a $-\sigma$ spin electron, or absorb a $-\sigma$ spin electron. From the point of view of the alloy analogy the process of figure 2 (a) is interpreted as a scattering of the σ spin electron and is included in the 'scattering' correction, while the processes of figure 2 (b) and (c) involve the movement of $-\sigma$ spin electrons and are included in the 'resonance broadening' correction. However, adopting a viewpoint closer to that discussed in § 9 of II, one may think of all three processes as possible modes of decay of the atom after the attachment of the σ spin electron, and so regard all three processes as giving rise to a broadening of the atomic resonance. The mathematics lends itself equally well to this interpretation. Finally, one may adopt a quite opposite view, and think of all three processes formally as scattering processes, figure 2 (a) showing an ordinary scattering process, figure 2 (b) a 'spin-exchange' scattering and figure 2 (c)

a process in which a σ spin electron is scattered into a $-\sigma$ spin hole. That these different interpretations of the same mathematical theory are possible is an indication of the degree of fusion between the band theory and the Heitler–London theory obtained in the present theory; those approaches which stress the scattering nature of the processes shown in figure 2 are adopting a band theory view, while those approaches which regard the processes of figure 2 as modes of decay of the atomic state are adopting a Heitler–London view.

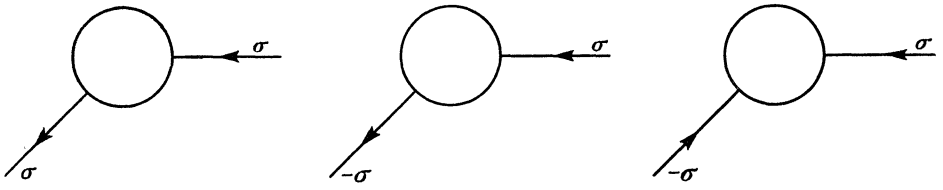

FIGURE 2. Various modes of decay of an atom after absorbing an electron.

3. THE BASIC THEORY

In this section the theory of paper I is briefly reviewed and re-derived by a technique differing slightly from that used in I. The new technique is suggested by the alloy analogy discussed in § 2, and the notation to which it leads will be of use throughout the remainder of the paper. Within the context of this paper the theory developed here may be regarded as a first approximation; in the next three sections the second order corrections to this theory are derived.

As explained in the Introduction, the theory of I and of this paper applies to an s-band of interacting electrons. As in I, for the reasons discussed there, it will be assumed that a useful approximation to the correct theory may be obtained by neglecting the effects of the interaction of electrons on different atoms. Then, as was shown in I, the Hamiltonian of the system may be written

$$H = \sum_{i,j}\sum_{\sigma} t_{ij}\, c^{+}_{i,\sigma} c_{j,\sigma} + T_0 \sum_{i,\sigma} n_{i,\sigma} + \tfrac{1}{2} I \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma}. \tag{3}$$

Here $c_{i,\sigma}$ is the destruction operator for an electron of spin σ in the orbital $\phi(\mathbf{x}-\mathbf{R}_i)$ on the ith atom, where $\phi(\mathbf{x})$ is the Wannier function appropriate to the s-band and $\mathbf{R}_i$ the position vector of the ith atom; $c^{+}_{i,\sigma}$ is the corresponding creation operator and $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$ the corresponding number operator;

$$t_{ij} = \mathcal{N}^{-1} \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - T_0)\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}, \tag{4}$$

where $\mathcal{N}$ is the total number of atoms in the crystal; since $T_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$ one has $t_{ii} = 0$; T_0, $\epsilon_{\mathbf{k}}$ and I have already been defined in § 2. The term in T_0 gives the atomic binding energy, that in I the interaction energy, and the terms in t_{ij} are responsible for the band motion of the electrons.

The theory is developed using the Green function technique described by Zubarev (1960; see also paper I, § 5). Particular attention will be given to the calculation of the electron propagator

$$G^{\sigma}_{ij}(E) = \langle\langle c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E \quad (\eta = -1), \tag{5}$$

from which the most important properties of the system can be calculated.

It is convenient to resolve G_{ij}^{σ} into two components in a certain manner suggested by the alloy analogy. To this end the notation

$$\left.\begin{aligned} n_{i,\sigma}^{+} &\equiv n_{i,\sigma}, \\ n_{i,\sigma}^{-} &\equiv 1-n_{i,\sigma}, \end{aligned}\right\} \tag{6}$$

is introduced. The quantities $n_{i\sigma}^{\pm}$ behave like projection operators since one has

$$n_{i,\sigma}^{\alpha} n_{i,\sigma}^{\beta} = \delta_{\alpha\beta} n_{i,\sigma}^{\alpha} \quad (\alpha, \beta = \pm). \tag{7}$$

Also

$$\sum_{\alpha=\pm} n_{i,\sigma}^{\alpha} = 1. \tag{8}$$

In view of (8) one can now write

$$G_{ij}^{\sigma}(E) = \sum_{\alpha=\pm} \langle\langle n_{i,}^{\alpha}{}_{\sigma} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E}, \tag{9}$$

the resolution of G_{ij}^{σ} into components alluded to above. The component

$$\langle\langle n_{i,-\sigma}^{+} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E}$$

is non-vanishing only on those atoms which have a $-\sigma$ spin electron on them and are therefore resonant to σ spin electrons at energy $T_0 + I$ according to the discussion of § 2. Similarly, $\langle\langle n_{i,-\sigma}^{-} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E}$ is non-vanishing only on atoms without a $-\sigma$ spin electron which are resonant at energy T_0.

The general Green function $\langle\langle A; B\rangle\rangle_{E}$ satisfies the equation of motion (see I, § 5)

$$E\langle\langle A; B\rangle\rangle_{E} = \frac{1}{2\pi}\langle [A, B]_{\eta}\rangle + \langle\langle [A, H]; B\rangle\rangle_{E}, \tag{10}$$

where $[A, B]_{\eta} = AB - \eta BA$. Using the Hamiltonian (3), one finds that the Green functions $\langle\langle n_{i-\sigma}^{\alpha} c_{i\sigma}; c_{j\sigma}^{+}\rangle\rangle_{E}$ $(\alpha = \pm)$ satisfy the equations of motion

$$E\langle\langle n_{i,-\sigma}^{\alpha} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E} = \frac{n_{-\sigma}^{\alpha}}{2\pi}\delta_{ij} + \epsilon_{\alpha}\langle\langle n_{i,-\sigma}^{\alpha} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E} + \sum_{k} t_{ik}\langle\langle n_{i,-\sigma}^{\alpha} c_{k,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E}$$
$$+ \xi_{\alpha}\sum_{k} t_{ik}\{\langle\langle c_{i,-\sigma}^{+} c_{k,-\sigma} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E} - \langle\langle c_{k,-\sigma}^{+} c_{i,-\sigma} c_{i,\sigma}; c_{j,\sigma}^{+}\rangle\rangle_{E}\} \tag{11}$$

where

$$n_{\sigma}^{+} \equiv n_{\sigma}, \quad n_{\sigma}^{-} \equiv 1 - n_{\sigma}, \tag{12}$$

n_{σ} is the mean number of σ spin electrons per atom present in the band,

$$\epsilon_{+} \equiv T_0 + I, \quad \epsilon_{-} \equiv T_0 \tag{13}$$

are the two resonant energies, $\xi_{\pm} = \pm 1$, and use has been made of the identities (7) and the definitions (6).

The theory of I is now obtained if one introduces approximations for the various terms on the right-hand side of (11) according to the following rule: all Green functions involving more than two atomic sites are to be approximated to in terms of Green functions involving not more than two sites. This rule embodies mathematically the physical notion that correlations between electrons on the same

atom are of dominant importance. When applied to (11) this rule leads to the approximations

$$\langle\langle n^{\alpha}_{i,-\sigma} c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E \simeq n^{\alpha}_{-\sigma} \langle\langle c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E \quad (i \neq k), \tag{14}$$

$$\left.\begin{aligned} \langle\langle c^{+}_{i,-\sigma} c_{k,-\sigma} c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle &\simeq 0 \quad (i \neq k), \\ \langle\langle c^{+}_{k,-\sigma} c_{i,-\sigma} c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle &\simeq 0 \quad (i \neq k). \end{aligned}\right\} \tag{15}$$

When these approximations are used (11) becomes (remembering that $t_{ii} = 0$)

$$E\langle\langle n^{\alpha}_{i,-\sigma} c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E = n^{\alpha}_{-\sigma}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_k t_{ik}\langle\langle c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E\right\} + \epsilon_\alpha \langle\langle n^{\alpha}_{i,-\sigma} c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E, \tag{16}$$

whence

$$\langle\langle n^{\alpha}_{i,-\sigma} c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E = \frac{n^{\alpha}_{-\sigma}}{E-\epsilon_\alpha}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_k t_{ik}\langle\langle c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E\right\}. \tag{17}$$

If this result is now substituted into (9) one obtains

$$\langle\langle c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E = \frac{1}{F^{\sigma}_0(E)}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_k t_{ik}\langle\langle c_{k\sigma}; c^{+}_{j\sigma}\rangle\rangle_E\right\}, \tag{18}$$

where $F^{\sigma}_0(E)$ is given by (2). This equation may be solved by introducing the Fourier transform

$$G^{\sigma}_{ij}(E) = \mathcal{N}^{-1}\sum_{\mathbf{k}} G^{\sigma}_{\mathbf{k}}(E)\, e^{i\mathbf{k}.(\mathbf{R}_i - \mathbf{R}_j)}. \tag{19}$$

The solution obtained for $G^{\sigma}_{\mathbf{k}}(E)$ is that given by (1), so the results of paper I are reproduced.

4. The scattering correction

The equation of motion (11) for the component $\langle\langle n^{\alpha}_{i,-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E$ of G^{σ}_{ij} may be rewritten

$$\begin{aligned} E\langle\langle n^{\alpha}_{i,-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E &= n^{\alpha}_{-\sigma}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_k t_{ik}\langle\langle c_{k\sigma}; c^{+}_{j\sigma}\rangle\rangle_E\right\} + \epsilon_\alpha\langle\langle n^{\alpha}_{i,-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E \\ &\quad + \sum_k t_{ik}\langle\langle (n^{\alpha}_{i,-\sigma} - n^{\alpha}_{-\sigma}) c_{k\sigma}; c^{+}_{j\sigma}\rangle\rangle_E + \xi_\alpha \sum_k t_{ik}\{\langle\langle c^{+}_{i,-\sigma} c_{k,-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E \\ &\quad - \langle\langle c^{+}_{k,-\sigma} c_{i,-\sigma} c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E\}. \end{aligned} \tag{20}$$

The approximation described in the preceding section (and I) corresponds to neglecting the last two terms on the right-hand side of (20). The remainder of this paper is essentially concerned with the corrections which arise from these terms. It turns out that the third term on the right-hand side of (20) (which arises from the commutator $[c_{i\sigma}, H]$ in the equation of motion) leads to the effects described as the 'scattering correction' in § 2, while the last term (which arises from the commutator $[n_{i,-\sigma}, H]$) leads to the 'resonance broadening' correction.

In this section only the scattering correction is considered, so the last term on the right-hand side of (20) is neglected, and an approximate expression for the Green function $\langle\langle (n^{\alpha}_{i,-\sigma} - n^{\alpha}_{-\sigma}) c_{i\sigma}; c^{+}_{j\sigma}\rangle\rangle_E$ sought. Using (8) this Green function can be resolved into two components according to

$$\langle\langle (n^{\alpha}_{i,-\sigma} - n^{\alpha}_{-\sigma}) c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E = \sum_{\beta=\pm}\langle\langle (n^{\alpha}_{i,-\sigma} - n^{\alpha}_{-\sigma}) n^{\beta}_{k,-\sigma} c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E. \tag{21}$$

These components obey the equations of motion

$$E\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{k,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_E=\frac{1}{2\pi}\delta_{jk}\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}\rangle$$
$$+\epsilon_\beta\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{k,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_E+\sum_l t_{kl}\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{l,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_E$$
$$+\text{other terms},\tag{22}$$

where the 'other terms' are those arising from the commutators $[n^{\alpha}_{i,-\sigma},H]$ and $[n^{\beta}_{k,-\sigma},H]$.

Equations (22) may be simplified by introducing approximations to the terms on the right-hand side. The 'other terms' and the correlation function

$$\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}\rangle=\langle n^{\alpha}_{i,-\sigma}n^{\beta}_{k,-\sigma}\rangle-n^{\alpha}_{-\sigma}n^{\beta}_{-\sigma}$$

are neglected since they give rise to higher order corrections than those considered here. Further, the approximation

$$\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{l,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle\simeq n^{\beta}_{-\sigma}\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{l,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_E\tag{23}$$

is introduced in the third term. The choice of these particular approximations has been guided by the physical interpretation of the Green functions which is explained later. When these approximations are made, (22) is replaced by the approximate equation

$$E\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E\simeq\epsilon_\beta\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E$$
$$+n^{\beta}_{-\sigma}\sum_l t_{kl}\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{l\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E.\tag{24}$$

It is to be understood that, because of the approximations involved in its derivation, this equation is only valid when $i\neq k$.

If (24) is now solved for $\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,n^{\beta}_{k,-\sigma}c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E$ in terms of the

$$\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{l\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E,$$

and the solution substituted into (21), one obtains (for $i\neq k$) the equation

$$\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E=\frac{1}{F^{\sigma}_0(E)}t_{ki}\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{i\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E$$
$$+\frac{1}{F^{\sigma}_0(E)}\sum_{l\neq i}t_{kl}\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{l\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E,\tag{25}$$

where $F^{\sigma}_0(E)$ is given by (2).

Next, the equations (25) are solved for $\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle$ $(i\neq k)$ in terms of $\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{i\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E$. In the appendix it is shown that the solution can be written (for $i\neq k$)

$$\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E=\sum_l W^{\sigma}_{kl,\,i}(E)\,t_{li}\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{i\sigma};\,c^{+}_{j\sigma}\rangle\rangle_E,\tag{26}$$

where

$$W^{\sigma}_{kl,\,i}(E)=2\pi\left\{g^{\sigma}_{kl}(E)-\frac{g^{\sigma}_{ki}(E)\,g^{\sigma}_{il}(E)}{g^{\sigma}_{ii}(E)}\right\},\tag{27}$$

in which

$$g^{\sigma}_{ij}(E)=\frac{1}{2\pi}\sum_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}}{F^{\sigma}_0(E)-(\epsilon_{\mathbf{k}}-T_0)}\tag{28}$$

is simply the approximation to the propagator $G^{\sigma}_{ij}(E)$ calculated in § 3 (cf. (1) and (19)).

Equation (26) gives the sought for approximation to $\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{k\sigma};\,c^{+}_{j\sigma}\rangle\rangle_{E}$. If this approximation is substituted into the right-hand side of (20), and the last term in that equation dropped (since it gives rise to the resonance broadening correction), one obtains

$$E\langle\langle n^{\alpha}_{i,-\sigma}c_{i,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_{E} \doteq n^{\alpha}_{-\sigma}\left\{\frac{1}{2\pi}\delta_{ij}+\sum_{k}t_{ik}\langle\langle c_{k,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_{E}\right\}$$
$$+\epsilon_{\alpha}\langle\langle n^{\alpha}_{i,-\sigma}c_{i,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_{E}+\lambda'_{\sigma}(E)\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{i,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_{E}, \quad (29)$$

where

$$\lambda'_{\sigma}(E)=2\pi\sum_{k,l}t_{ik}\left\{g^{\sigma}_{kl}(E)-\frac{g^{\sigma}_{ki}(E)\,g^{\sigma}_{il}(E)}{g^{\sigma}_{ii}(E)}\right\}t_{li}. \quad (30)$$

Equation (29) is very similar to (16). The main difference lies in the replacement of ϵ_{α} in (16) by $\epsilon_{\alpha}+\lambda'_{\sigma}(E)$ in (29); it is as though one had corrected the resonant energies ϵ_{α} by the addition of a 'self energy' $\lambda'_{\sigma}(E)$. This interpretation is born out by an

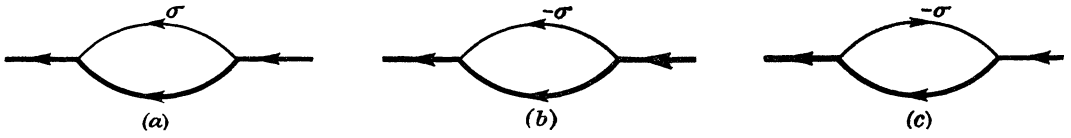

FIGURE 3. Atomic self-energy diagrams.

examination of the physical meaning of the various equations and approximations used in deriving (29). The term in $\lambda'_{\sigma}(E)$ may be interpreted as the self-energy of an atom corresponding to the process shown diagrammatically in figure 3 (*a*), in which the heavy lines represent 'atomic' propagators and the thin line an electron propagator. Figure 3 (*a*) shows a process in which the atom emits an electron (into the rest of the solid) and then re-absorbs it. The propagation of the incoming and outgoing atoms is described by the Green function $\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{i\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_{E}$, and the propagation of the system in the intermediate state in which the electron has been emitted is described by the Green function $\langle\langle(n^{\alpha}_{i,-\sigma}-n^{\alpha}_{-\sigma})\,c_{k,\sigma};\,c^{+}_{j,\sigma}\rangle\rangle_{E}$, where $k\neq i$. It may be noticed that $W^{\sigma}_{kl,i}(E)$ is simply the propagator $g^{\sigma}_{kl}(E)$ modified to take into account the exclusion of the electron from atom i.

Equation (29) may be formally obtained from (16) by the substitutions

$$\epsilon_{\alpha}\rightarrow\epsilon_{\alpha}+\lambda'_{\sigma}(E),\quad t_{ik}\rightarrow t_{ik}-\delta_{ik}\lambda'_{\sigma}(E),$$

so the solution for G^{σ}_{ij} may be obtained at once from (29) by following the procedure explained after (16). The result is

$$G^{\sigma}_{ij}(E)=\frac{1}{2\pi}\frac{1}{f^{\sigma}_{s}(E)-(\epsilon_{\mathbf{k}}-T_{0})}, \quad (31)$$

where

$$\frac{1}{f^{\sigma}_{s}(E)}=\frac{E-(n^{+}_{-\sigma}\epsilon_{-}+n^{-}_{-\sigma}\epsilon_{+})-\lambda'_{\sigma}(E)}{[E-\epsilon_{-}-n^{+}_{-\sigma}\lambda'_{\sigma}(E)]\,[E-\epsilon_{+}-n^{-}_{-\sigma}\lambda'_{\sigma}(E)]-n^{-}_{-\sigma}n^{+}_{-\sigma}\lambda'^{2}_{\sigma}(E)}. \quad (32)$$

The solution (31) has the same form as (1), the only difference being the replacement of $F^{\sigma}_{0}(E)$ by $f^{\sigma}_{s}(E)$. These two functions differ in one respect which is of major importance as regards the predictions of the theory, namely in their analytic

properties regarded as functions of E. To see the analytic properties of f_s^σ one should note that from (27), (28) and (30) one may deduce the formulae

$$\lambda_\sigma(E) = F_0^\sigma(E) - \frac{1}{2\pi g_{ii}^\sigma(E)}, \tag{33}$$

$$g_{ii}^\sigma(E) = \mathcal{N}^{-1} \sum_{\mathbf{k}} g_{\mathbf{k}}^\sigma(E) = \frac{\mathcal{N}^{-1}}{2\pi} \sum_{\mathbf{k}} \frac{1}{F_0^\sigma(E) - (\epsilon_{\mathbf{k}} - T_0)}, \tag{34}$$

where $g_{\mathbf{k}}^\sigma(E)$ is given by (1). From (34) it follows that for real E

$$\lim_{\eta \to 0+} g_{ii}^\sigma(E \pm \mathrm{i}\eta) = \bar{g}_{ii}^\sigma(E) \mp \mathrm{i}\rho_0^\sigma(E), \tag{35}$$

where $\rho_0^\sigma(E)$ is the pseudo-particle density of states calculated in the approximation of paper I, so the function $g_{ii}^\sigma(E)$ and therefore the functions $\lambda_\sigma'(E)$, $f_s^\sigma(E)$ and $G_{\mathbf{k}}^\sigma(E)$ have a branch cut along the real axis for those values of E for which $\rho_0^\sigma(E) > 0$. Thus the analytic properties of the solution (31) are quite different from those of the solution (1), which has poles on the real axis as its only singularities.

The physical implications of these analytic properties of the solution (31) are well known: a propagator with a branch cut along the real axis describes pseudo-particles with finite lifetimes (as opposed to a propagator with poles which describe pseudo-particles with infinite lifetimes); the damping is related to the discontinuity across the branch cut which in turn depends upon $\rho_0^\sigma(E)$. These results are exactly what one expects upon the basis of the discussion given in § 2. The electron wave is damped as a consequence of spin-disorder scattering of the kind indicated in figure 2 (a); the quantity $\rho_0^\sigma(E)$ enters because it measures the density of final states into which an electron of energy E may be scattered. It may be noticed that by analogy with the diagrammatic analysis of perturbation series one would expect that the imaginary part of the 'self-energy' corresponding to the diagram of figure 3 (a) would be related to the damping due to the process of figure 2 (a).

This interpretation draws attention to a logical inconsistency in the above theory. While the solution (31) is more accurate than that calculated in I, the damping is being calculated in terms of $\rho_0^\sigma(E)$, the pseudo-particle density of states calculated in the approximation of I. It would be more logical if the damping were determined by the density of pseudo-particle states calculated self-consistently from the more accurate solution (31). The appearance of $\rho_0^\sigma(E)$ may be traced to the occurrence in (30) of the propagators g_{ij}^σ calculated in the approximation of I. This suggests that it might be more correct to replace the function $\lambda_\sigma'(E)$ everywhere by the function

$$\Omega_\sigma'(E) = 2\pi \sum_{k,l} t_{ik} \left\{ G_{kl}^\sigma(E) - \frac{G_{ki}^\sigma(E)\, G_{il}^\sigma(E)}{G_{ii}^\sigma(E)} \right\} t_{li}, \tag{36}$$

where g_{ij}^σ has been replaced by the actual propagator G_{ij}^σ. This change would have the effect of determining the damping self-consistently in terms of the actual pseudo-particle density of states. It will be assumed throughout the remainder of this paper that this substitution of Ω_σ' for λ_σ' is correct, although no formal justification has been given.

If $\lambda'_\sigma(E)$ is replaced by $\Omega'_\sigma(E)$, the solution for $G^\sigma_{\mathbf{k}}(E)$ is determined by the equations

$$G^\sigma_{\mathbf{k}}(E) = \frac{1}{2\pi}\frac{1}{F^\sigma_s(E)-(\epsilon_{\mathbf{k}}-T_0)}, \tag{37}$$

$$\frac{1}{F^\sigma_s(E)} \quad \frac{E-(n^+_{-\sigma}\epsilon_- + n^-_{-\sigma}\epsilon_+)-\Omega'_\sigma(E)}{[E-\epsilon_- - n^+_{-\sigma}\Omega'_\sigma(E)]\,[E-\epsilon_+ - n^-_{-\sigma}\Omega'_\sigma(E)]-n^+_{-\sigma}n^-_{-\sigma}[\Omega'_\sigma(E)]^2}, \tag{38}$$

$$\Omega'_\sigma(E) = F^\sigma_s(E) - \frac{1}{2\pi G^\sigma_{ii}(E)}, \tag{39}$$

$$G^\sigma_{ii}(E) = \mathcal{N}^{-1}\sum_{\mathbf{k}} G^\sigma_{\mathbf{k}}(E), \tag{40}$$

which are the analogues of (31), (32), (33) and (34). These equations have to be solved simultaneously; the solution of a similar set in a special case is described in § 6, where the nature of the pseudo-particle spectrum to which they lead is discussed.

5. The resonance broadening correction

In the preceding section the 'scattering correction' was studied by retaining the third and dropping the fourth term on the right-hand side of equation (20). Here the opposite procedure is followed, i.e. the third term is dropped and the fourth retained, in order to develop the theory of the 'resonance broadening correction' discussed in § 2.

Expressions for the Green functions

$$\langle\langle c^+_{k,-\sigma}c_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E$$

and

$$\langle\langle c^+_{i,-\sigma}c_{k,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E = -\langle\langle c^+_{k,-\sigma}c_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E$$

which appear in the fourth term of (20) are now sought. These two Green functions may be calculated simultaneously by making a slight departure from conventional notation; one has merely to understand that (where it appears) $c^-_{i,\sigma}$ stands for the destruction operator ordinarily written $c_{i,\sigma}$ (while $c^+_{i,\sigma}$ continues to stand for the corresponding creation operator). Then the two Green functions sought correspond to the two choices of sign of the expression $\langle\langle c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E$.

By the use of (8) the Green function $\langle\langle c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E$ may be resolved into two components according to

$$\langle\langle c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E = \sum_{\alpha=\pm}\langle\langle n^\alpha_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E. \tag{41}$$

These two components satisfy an equation of motion of the form

$$\begin{aligned}
E\langle\langle n^\alpha_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E &= \frac{1}{2\pi}\delta_{ij}\langle n^\alpha_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}\rangle \\
&-\frac{1}{2\pi}\delta_{jk}\xi_\alpha\langle c_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma}\rangle + (\epsilon_\pm \pm \epsilon_- \mp \epsilon_\alpha)\langle\langle n^\alpha_{k,-\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E \\
&+\xi_\alpha\sum_l t_{kl}\langle\langle c^+_{k,\sigma}c_{l,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E - \xi_\alpha\sum_l t_{kl}\langle\langle c^+_{l,\sigma}c_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E \\
&\mp\sum_l t_{kl}\langle\langle n^\alpha_{k,\sigma}c^\pm_{l,-\sigma}c^\mp_{i,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E \pm \sum_l t_{il}\langle\langle n^\alpha_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{l,-\sigma}c_{i,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E \\
&+\sum_l t_{il}\langle\langle n^\alpha_{k,\sigma}c^\pm_{k,-\sigma}c^\mp_{i,-\sigma}c_{l,\sigma};\, c^+_{j,\sigma}\rangle\rangle_E.
\end{aligned} \tag{42}$$

This equation is now simplified by introducing the following approximations: the terms involving correlation functions, the two terms involving a Green function multiplied by a factor ξ_α, and the last term are all neglected; in the remaining terms the approximations

$$\langle\langle n^\alpha_{k,\sigma} c^\pm_{l,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle \simeq n^\alpha_\sigma \langle\langle c^\pm_{l,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E, \tag{43}$$

$$\langle\langle n^\alpha_{k,\sigma} c^\pm_{k,-\sigma} c^\mp_{l,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle \simeq \delta_{kl} n^\alpha_\sigma n^\pm_{-\sigma} \langle\langle c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \tag{44}$$

are introduced. These approximations serve to eliminate corrections of higher order than those to be considered here; the terms remaining are those which lead to the atomic self-energies corresponding to the diagrams shown in figures 3 (*b*) and 3 (*c*), which give the lowest order (in the t_{ik}) self-energy corrections arising from the movement of $-\sigma$ spin electrons.

When these various approximations have been made in (42), that equation is replaced by the approximate equation

$$\begin{aligned} E\langle\langle n^\alpha_{k,\sigma} c^\pm_{k,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \simeq{}& (\epsilon_\pm \pm \epsilon_- \mp \epsilon_\alpha)\langle\langle n^\alpha_{k,\sigma} c^\pm_{k,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \\ &\mp n^\alpha_\sigma t_{ik}\langle\langle (n^\pm_{i,-\sigma} - n^\pm_{-\sigma}) c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \mp n^\alpha_\sigma \sum_{l\neq i} t_{kl}\langle\langle c^\pm_{l,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E, \end{aligned} \tag{45}$$

whence one has, using (41)

$$\begin{aligned} \langle\langle c^\pm_{k,-\sigma} c^\mp_{i,-\sigma} c_{i\,\sigma}; c^+_{j,\sigma}\rangle\rangle_E = \frac{1}{F^{-\sigma}_0(\epsilon_- \pm \epsilon_\pm \mp E)} \{ & t_{ik}\langle\langle (n^\pm_{i,-\sigma} - n^\pm_{-\sigma}) c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \\ &+ \sum_{l\neq i} t_{kl}\langle\langle c^\pm_{l,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E\}, \end{aligned} \tag{46}$$

where $F^\sigma_0(E)$ is given by (2). Equation (46) may now be solved as described in the appendix to give

$$\langle\langle c^\pm_{k,-\sigma} c^\mp_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E = \sum_l W^{-\sigma}_{kl,i}(\epsilon_- \pm \epsilon_\pm \mp E) t_{li}\langle\langle (n^\pm_{i,-\sigma} - n^\pm_{-\sigma}) c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E, \tag{47}$$

where $W^\sigma_{kl,i}(E)$ is given by (27). If the solutions (47) are now substituted into the last term of (20), and the third term in that equation dropped, one obtains after some rearrangement (using $n^+_{i,\sigma} + n^-_{i,\sigma} = n^+_\sigma + n^-_\sigma = 1$)

$$\begin{aligned} E\langle\langle n^\alpha_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \simeq{}& n^\alpha_{-\sigma}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_k t_{ik}\langle\langle c_{k,\sigma}; c^+_{j,\sigma}\rangle\rangle_E\right\} + \epsilon_\alpha\langle\langle n^\alpha_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \\ &- \xi_\alpha n^+_{-\sigma}[\lambda'_{-\sigma}(E) + \lambda''_{-\sigma}(E)]\langle\langle n^-_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \\ &+ \xi_\alpha n^-_{-\sigma}[\lambda'_{-\sigma}(E) + \lambda''_{-\sigma}(E)]\langle\langle n^+_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E, \end{aligned} \tag{48}$$

where $\lambda'_\sigma(E)$ is given by (30) and

$$\lambda''_\sigma(E) = -\lambda'_\sigma(\epsilon_+ + \epsilon_- - E).$$

It will now be assumed, for the reasons already discussed in the preceding section, that it is better to use $\Omega'_\sigma(E)$ given by (36) than $\lambda'_\sigma(E)$ in (48); therefore Ω'_σ will be substituted for λ'_σ and $\Omega''_\sigma(E) = -\Omega'_\sigma(\epsilon_+ + \epsilon_- - E)$ for λ''_σ. The resulting equation may be written in matrix form as

$$\begin{aligned} &\begin{bmatrix} E - \epsilon_- - n^+_{-\sigma}(\Omega'_{-\sigma} + \Omega''_{-\sigma}) & n^-_{-\sigma}(\Omega'_{-\sigma} + \Omega''_{-\sigma}) \\ n^+_{-\sigma}(\Omega'_{-\sigma} + \Omega''_{-\sigma}) & E - \epsilon_+ - n^-_{-\sigma}(\Omega'_{-\sigma} + \Omega''_{-\sigma}) \end{bmatrix} \begin{bmatrix} \langle\langle n^-_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \\ \langle\langle n^+_{i,-\sigma} c_{i,\sigma}; c^+_{j,\sigma}\rangle\rangle_E \end{bmatrix} \\ &\qquad = \begin{bmatrix} n^-_{-\sigma} \\ n^+_{-\sigma} \end{bmatrix}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_k t_{ik}\langle\langle c_{k,\sigma}; c^+_{j,\sigma}\rangle\rangle_E\right\}, \end{aligned} \tag{49}$$

which may be solved for the $\langle\langle n^{\alpha}_{i,-\sigma} c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E$ in terms of $\langle\langle c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E$. If the solution is substituted into (9) one obtains

$$\langle\langle c_{i,\sigma}; c^{+}_{j,\sigma}\rangle\rangle E = \frac{1}{F^{\sigma}_{r}(E)}\left\{\frac{1}{2\pi}\delta_{ij} + \sum_{k} t_{ik}\langle\langle c_{k,\sigma}; c^{+}_{j,\sigma}\rangle\rangle_E\right\}, \tag{50}$$

where

$$\frac{1}{F^{\sigma}_{r}(E)} = \frac{E-(n^{+}_{-\sigma}\epsilon_{-}+n^{-}_{-\sigma}\epsilon_{+})-(\Omega'_{-\sigma}+\Omega''_{-\sigma})}{[E-\epsilon_{-}-n^{+}_{-\sigma}(\Omega'_{-\sigma}+\Omega''_{-\sigma})][E-\epsilon_{+}-n^{-}_{-\sigma}(\Omega'_{-\sigma}+\Omega''_{-\sigma})]-n^{-}_{-\sigma}n^{+}_{-\sigma}(\Omega'_{-\sigma}+\Omega''_{-\sigma})^{2}}. \tag{51}$$

Equation (50) is of the same form as (18), and may be solved at once to give

$$G^{\sigma}_{k}(E) = \frac{1}{2\pi}\frac{1}{F^{\sigma}_{r}(E)-(\epsilon_{\mathbf{k}}-T_0)}. \tag{52}$$

The solution (52) again has the same form as (1) and (37). $F^{\sigma}_{r}(E)$ may be obtained from $F^{\sigma}_{s}(E)$ by simply replacing $\Omega'_{\sigma}(E)$ in $F^{\sigma}_{s}(E)$ by the combination $\Omega'_{-\sigma}(E)+\Omega''_{-\sigma}(E)$ and so has similar analytic properties, i.e. a branch cut along the real axis for those values of E for which either $\rho_{-\sigma}(E) > 0$ or $\rho_{-\sigma}(\epsilon_{+}+\epsilon_{-}-E) > 0$, where $\rho_{\sigma}(E)$ is the density of pseudo-particle states calculated from (52). Thus the solution (52) also describes pseudo-particles with a finite lifetime. The two branch cuts correspond to the two damping processes shown in figures 2 (*b*) and 2 (*c*), $\rho_{-\sigma}(E)$ and $\rho_{-\sigma}(\epsilon_{+}+\epsilon_{-}-E)$ measuring the densities of final states for these two processes.

For small bandwidths the $\Omega'_{\sigma}(E)$ and $\Omega''_{\sigma}(E)$ are small, in which case one obtains from (51) or, more directly, from (49) the approximate expression

$$\frac{1}{F^{\sigma}_{r}(E)} \simeq \frac{n^{-}_{-\sigma}}{E-\epsilon_{-}-n^{-}_{-\sigma}(\Omega'_{-\sigma}+\Omega''_{-\sigma})} + \frac{n^{+}_{-\sigma}}{E-\epsilon_{+}-n^{-}_{-\sigma}(\Omega'_{-\sigma}+\Omega''_{-\sigma})}, \tag{53}$$

which is similar to (2), and shows clearly the 'resonance broadening' effect discussed in § 2. The breadths of the two resonances are proportional to $n^{\pm}_{-\sigma}\mathscr{I}(\Omega'_{-\sigma}+\Omega''_{-\sigma})$. This result may be interpreted as follows. The resonance at ϵ_{-} corresponds to atoms with no $-\sigma$ spin electron, and its breadth is proportional to the probability of a $-\sigma$ spin electron moving on to such an atom; but this probability is directly proportional to the number of $-\sigma$ spin electrons present, i.e. to $n^{+}_{-\sigma}$. Similarly, the breadth of the resonance at ϵ_{+} is proportional to $n^{-}_{-\sigma}$ which measures the availability of atoms with no $-\sigma$ spin electron to which a $-\sigma$ spin electron can jump when moving away from a given atom.

The behaviour in the opposite limit of large bandwidth and, therefore, large Ω'_{σ} and Ω''_{σ} is most conveniently discussed by re-arranging the expression (51) into the form

$$\frac{1}{F^{\sigma}_{r}(E)} = \frac{E-(\epsilon_{+}+\epsilon_{-}-\bar{\epsilon}_{-\sigma})-(\Omega'_{-\sigma}+\Omega''_{-\sigma})}{(E-\epsilon_{-})(E-\epsilon_{+})-(E-\bar{\epsilon}_{-\sigma})(\Omega'_{-\sigma}+\Omega''_{-\sigma})}, \tag{54}$$

where

$$\bar{\epsilon}_{\sigma} = n^{+}_{\sigma}\epsilon_{+}+n^{-}_{\sigma}\epsilon_{-} \tag{55}$$

is the weighted mean of the two resonances. From (54) one may see at once that for large bandwidth $F^{\sigma}_{r}(E) \sim E-\bar{\epsilon}_{-\sigma}$, the two resonances in (53) being replaced by the single narrow resonance at $E=\bar{\epsilon}_{-\sigma}$. As mentioned in § 2, this is an example of 'motional line-narrowing'. In fact, the case discussed here, of an atom switching to

and fro between two resonances, is almost exactly the same as an example discussed by Anderson (1954) and Kubo (1954). These authors found that the problem could be reduced to the inversion of a certain matrix; the analogue in the present theory is the matrix appearing on the left-hand side of (49).

Finally, the scattering correction discussed in the preceding section will be combined with the resonance broadening correction. This is done simply by using the expressions (26) and (47) in (20). The result can be written in the form

$$E\langle\langle n^{\alpha}_{i,-\sigma}c_{i,-\sigma};c^{+}_{j,\sigma}\rangle\rangle_E = n^{\alpha}_{-\sigma}\left\{\frac{1}{2\pi}\delta_{ij}+\sum_k t_{ik}\langle\langle c_{k,\sigma};c^{+}_{j,\sigma}\rangle\rangle_E\right\}+\epsilon_\alpha\langle\langle n^{\alpha}_{i,-\sigma}c_{i,\sigma};c^{+}_{j,\sigma}\rangle\rangle_E$$
$$-\xi_\alpha n^{+}_{-\sigma}\Omega_\sigma(E)\langle\langle n^{-}_{i,-\sigma}c_{i,\sigma};c^{+}_{j,\sigma}\rangle\rangle_E+\xi_\alpha n^{-}_{-\sigma}\Omega_\sigma(E)\langle\langle n^{+}_{i,-\sigma}c_{i,\sigma};c^{+}_{j,\sigma}\rangle\rangle_E, \quad (56)$$

where
$$\Omega_\sigma(E)=\Omega'_\sigma(E)+\Omega'_{-\sigma}(E)+\Omega''_{-\sigma}(E), \quad (57)$$

in which Ω'_σ and Ω''_σ have been substituted for λ'_σ and λ''_σ. Equation (56) has the same form as (48), so the solution for $G^\sigma_{\mathbf{k}}$ may be derived from it in the same manner with the result

$$G^\sigma_{\mathbf{k}}(E)=\frac{1}{2\pi}\frac{1}{F^\sigma(E)-(\epsilon_{\mathbf{k}}-T_0)}, \quad (58)$$

where
$$\frac{1}{F^\sigma(E)}=\frac{E-(n^{+}_{-\sigma}\epsilon_{-}+n^{-}_{-\sigma}\epsilon_{+})-\Omega_\sigma(E)}{[E-\epsilon_{-}-n^{+}_{-\sigma}\Omega_\sigma][E-\epsilon_{+}-n^{-}_{-\sigma}\Omega_\sigma]-n^{+}_{-\sigma}n^{-}_{-\sigma}\Omega^2_\sigma}. \quad (59)$$

Most of the remarks concerning the solutions obtained in this and the preceding section apply equally well to the solution (58). That Ω'_σ and Ω''_σ only appear in the combination (57) emphasizes the close relationship between the three processes shown in figure 2.

6. A special solution

The theory of the preceding sections has led to a prescription for the calculation of the propagator $G^\sigma_{\mathbf{k}}(E)$ which is embodied in equations like (57) to (59). In order to gain some impression of the nature of the pseudo-particle spectrum to which the solution of these equations leads, in this section a special (but not atypical) case in which the solution is quite readily obtainable is considered.

The equations one has to solve are given by (57) to (59) together with (cf. (39), (40))

$$\Omega'_\sigma(E)=F^\sigma(E)-\frac{1}{2\pi G^\sigma_{ii}(E)} \quad (60)$$

and
$$G^\sigma_{ii}(E)=\mathcal{N}^{-1}\sum_{\mathbf{k}}G^\sigma_{\mathbf{k}}(E)=\frac{1}{2\pi}\mathcal{N}^{-1}\sum_{\mathbf{k}}\frac{1}{F^\sigma(E)-(\epsilon_{\mathbf{k}}-T_0)}. \quad (61)$$

The special case to be studied may be characterized by the features: (i) the number of electrons present is one per atom, i.e. one has a half-filled s-band; (ii) the system is assumed to be non-ferromagnetic, so one has the same number of electrons of each spin; (iii) it is assumed that the unperturbed band structure $\epsilon_{\mathbf{k}}$ is such that the corresponding density of states function

$$p(E)=\mathcal{N}^{-1}\sum_{\mathbf{k}}\delta(E-\epsilon_{\mathbf{k}}) \quad (62)$$

has the form

$$p(E) = \frac{4}{\pi\Delta}\sqrt{\left\{1-\left(\frac{E-T_0}{\frac{1}{2}\Delta}\right)^2\right\}} \quad \text{if} \quad |E-T_0| < \tfrac{1}{2}\Delta,$$
$$= 0 \quad \text{otherwise}, \tag{63}$$

i.e. the density of states curve has a parabolic form centred on T_0 with a bandwidth Δ.

From assumptions (i) and (ii) above it follows that $n_\sigma^+ = n_\sigma^- = \frac{1}{2}$. This result, together with the property $p(E) = p(2T_0 - E)$ of the density of states function given by (63), leads to a useful symmetry property of the solutions. This symmetry is best exhibited by choosing the origin of energy such that $T_0 + \frac{1}{2}I = 0$, so that

$$\epsilon_+ = -\epsilon_- = \tfrac{1}{2}I;$$

relative to this energy origin one then finds

$$F^\sigma(E) = -F^\sigma(-E), \quad \Omega'_\sigma(E) = -\Omega'_\sigma(-E), \tag{64}$$

from which, together with (57) and assumption (ii), it follows that

$$\Omega_\sigma(E) = 3\Omega'_\sigma(E). \tag{65}$$

If these various results are now used in (59), one obtains after some re-arrangement the relation

$$3\Omega'_\sigma(E) = E - \frac{\frac{1}{4}I^2}{E - F^\sigma(E)}. \tag{66}$$

Combining (61) and (62) one has

$$G^\sigma_{ii}(E) = \frac{1}{2\pi}\int \frac{p(E')\,\mathrm{d}E'}{F^\sigma(E) - (E' - T_0)}. \tag{67}$$

If the form of $p(E)$ given by (63) is now substituted, the integration may be performed with the result

$$G^\sigma_{ii}(E) = \frac{4}{\pi\Delta^2}[F^\sigma(E) - \sqrt{[\{F^\sigma(E)\}^2 - \{\tfrac{1}{2}\Delta\}^2]}]. \tag{68}$$

This function is two-valued; returning to the integral (67) one sees that one must take the branch in the F-plane, with a cut along the real axis from $-\frac{1}{2}\Delta$ to $\frac{1}{2}\Delta$, which has the property that the square root is positive on the real F axis when $|F| > \frac{1}{2}\Delta$. From (60) and (68) one has

$$\Omega'_\sigma(E) = \tfrac{1}{2}[F^\sigma(E) - \sqrt{[\{F^\sigma(E)\}^2 - \{\tfrac{1}{2}\Delta\}^2]}]. \tag{69}$$

If this result is now substituted into (66) one obtains the cubic equation

$$EF^3 - \{\tfrac{7}{3}E^2 + \tfrac{3}{4}(\tfrac{1}{2}\Delta)^2 - \tfrac{1}{4}I^2\}F^2 + \{\tfrac{5}{3}E(E^2 - \tfrac{1}{4}I^2)$$
$$+ \tfrac{3}{2}E(\tfrac{1}{2}\Delta)^2\}F - \tfrac{1}{3}(E^2 - \tfrac{1}{4}I^2)^2 - \tfrac{3}{4}E^2(\tfrac{1}{2}\Delta)^2 = 0 \tag{70}$$

for $F^\sigma(E)$, so the solution of the self-consistent equations has been reduced to the solution of a cubic.

If Δ and I are fixed, then for any given value of E the equation (70) may have either three real roots or one real and two complex roots. In the former case one finds that the density of pseudo-particle states vanishes for that E, in the latter case that it is non-vanishing; $F^\sigma(E)$ must then be taken as given by the appropriate complex

root. Actually, the equation (70) can be reduced to a dimensionless form by the scaling

$$E/I \to e, \quad F/I \to f, \quad \Delta/I \to \delta, \tag{71}$$

in which form it may be seen that (apart from scaling factors) the nature of the solutions is determined only by the ratio Δ/I rather than by Δ and I separately.

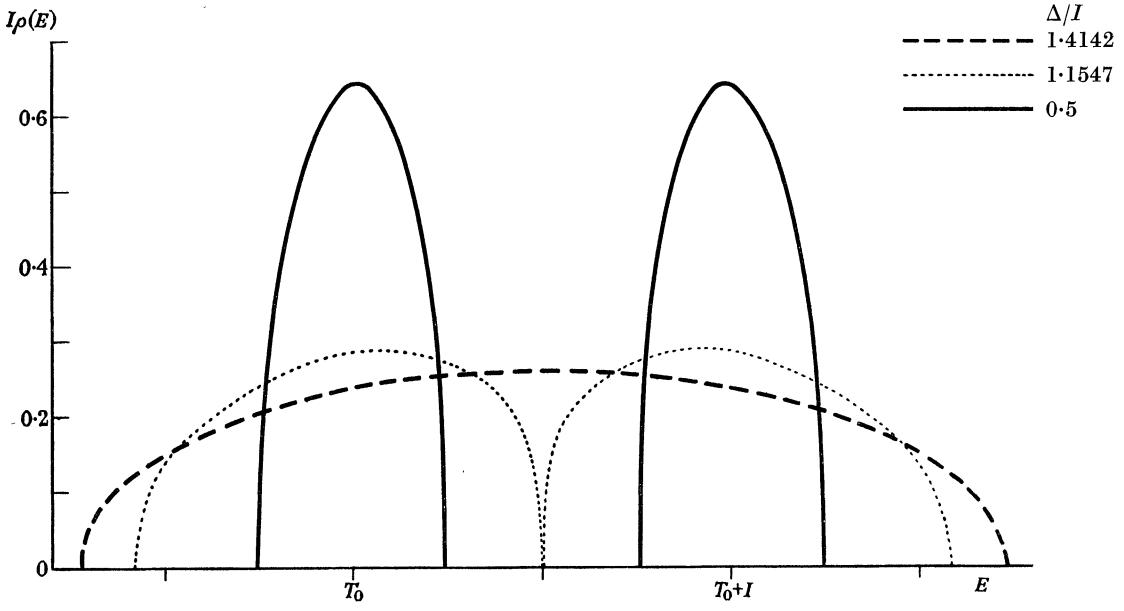

FIGURE 4. Pseudo-particle density of states functions for three ratios Δ/I; $\Delta/I = 1{\cdot}1547$ is the critical Δ/I ratio.

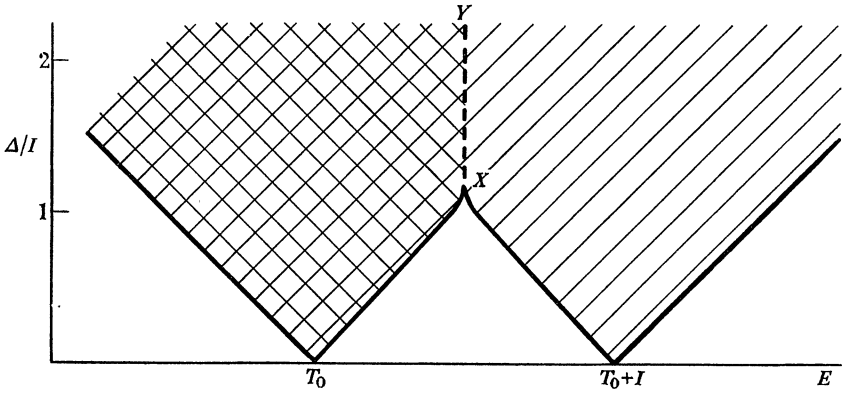

FIGURE 5. The dependence of the pseudo-particle spectrum upon the Δ/I ratio.

In figure 4 the form of the pseudo-particle density of states function is shown for three values of the ratio Δ/I. It will be seen that the spectrum consists of either one or two bands, depending upon the value of Δ/I. This structure of the pseudo-particle spectrum is shown more explicitly in figure 5, where the boundaries of the pseudo-particle bands are plotted as a function of Δ/I, the density of states being non-vanishing in the hatched region of the $(E, \Delta/I)$ plane.

The behaviour of the spectrum as a function of Δ/I shown in figure 5 is exactly that anticipated by Mott and discussed in § 2. For the half-filled band case dealt with here, the pseudo-particle states will be occupied (at the absolute zero of temperature) in the region of the $(E, \Delta/I)$ plane indicated by the double hatching in figure 5, so for values of Δ/I less than the critical value corresponding to the point X one band is full and one empty and the system behaves as an insulator (or semi-conductor), but for values of Δ/I exceeding this critical value there is a Fermi surface at the energy indicated by the line $X\,Y$ and the system is a conductor. The transition

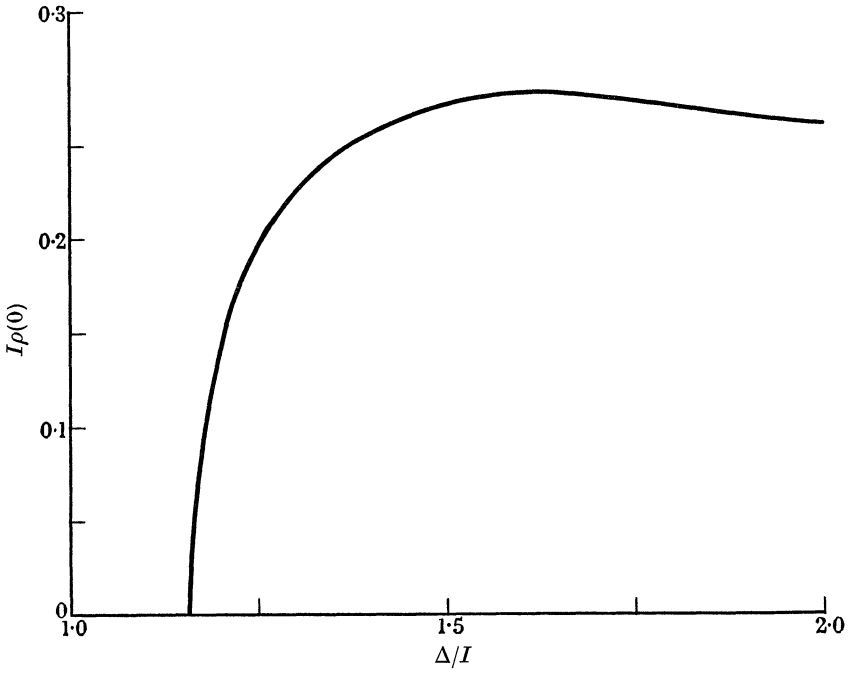

FIGURE 6. The dependence of the pseudo-particle density of states at the Fermi energy upon the Δ/I ratio.

at X from insulator to conductor is what is sometimes referred to as the 'Mott transition'. The critical value of Δ/I for the special case discussed here is

$$(\Delta/I)_{\text{critical}} = 2/\sqrt{3} = 1{\cdot}1547.... \tag{72}$$

There are two comments concerning the nature of the transition as predicted by the above theory which are of interest. First, it will be noticed that as Δ/I approaches the critical value from below the two pseudo-particle bands come continuously together. In fact, when Δ/I is near the critical value the gap between the bands is given by

$$\text{constant} \times [(\Delta/I)_{\text{critical}} - (\Delta/I)]^{\frac{3}{2}}. \tag{73}$$

This behaviour is somewhat different from that predicted by Mott, who advanced arguments to indicate that the transition might be sudden rather than continuous. However, this prediction of the present theory has to be treated with some caution because the theory neglects the interactions of electrons on different atoms. It may

be expected that when these latter interactions are taken into account the results will be somewhat altered; in particular, it can be seen that these interactions lead to effects of the type Mott held to be responsible for the sharpness of the transition, so the continuous nature of the transition found here may be merely an artefact due to the approximations that have been made.

Secondly, for values of Δ/I just above the critical value the density of states at the Fermi surface is very small, but increases rapidly with increasing Δ/I, as may be seen from figure 6. This means that although the system is a conductor, for values of Δ/I just exceeding the critical value it is a rather poor conductor, but that the conductivity increases rapidly as one moves away from the critical value. Again, this prediction of the present theory will be invalidated if the transition turns out to be sharp, since the density of states at the Fermi surface will then be finite when one is just on the conductor side of the transition.

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Appendix

The equations (25) and (46) can both be written in the form

$$X_{k,i}(E) = \frac{1}{F(E)}\{t_{ik}\,Y(E) + \sum_{l\neq i} t_{kl}\,X_{l,i}(E)\} \tag{A 1}$$

by making the identifications

$$X_{k,i} \equiv \langle\langle (n^{\alpha}_{i,-\sigma} - n^{\alpha}_{-\sigma})\,c_{k,\sigma};\, c^{+}_{j,\sigma}\rangle\rangle_E, \quad Y(E) \equiv \langle\langle (n^{\alpha}_{i\,-\sigma} - n^{\alpha}_{-\sigma})\,c_{i,\sigma};\, c^{+}_{j,\sigma}\rangle\rangle_E,$$

in the one case and

$$F(E) \equiv F^{\sigma}_{0}(E)$$

$$X_{k,i}(E) \equiv \langle\langle c^{\pm}_{k,-\sigma} c^{\mp}_{i,-\sigma}\,c_{i,\sigma};\, c^{+}_{j,\sigma}\rangle\rangle_E, \quad Y(E) \equiv \langle\langle (n^{\pm}_{i,-\sigma} - n^{\pm}_{-\sigma})\,c_{i,\sigma};\, c^{+}_{j,\sigma}\rangle\rangle_E,$$

$$F(E) \equiv F^{-\sigma}_{0}(\epsilon_{-} \pm \epsilon_{\pm} \mp E)$$

in the other. To establish the correctness of the solutions (26) and (47) it suffices to show that

$$X_{k,i}(E) = \sum_{m} W_{km,\,i}(E)\,t_{mi}\,Y(E) \tag{A 2}$$

gives a solution of (A 1) when $k \neq i$, where

$$W_{km,\,i}(E) = 2\pi\left\{g_{km}(E) - \frac{g_{ki}(E)\,g_{im}(E)}{g_{ii}(E)}\right\} \tag{A 3}$$

and

$$g_{ij}(E) = \frac{1}{2\pi}\sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}}{F(E) - (\epsilon_{\mathbf{k}} - T_0)}. \tag{A 4}$$

However, using (4), one sees at once by Fourier transformation that the g_{ij} given by (A 4) satisfies

$$\frac{1}{F}\sum_k t_{ik} g_{kj} = g_{ij} - \frac{1}{2\pi F}\delta_{ij}. \tag{A 5}$$

Using this result, and noting from (A 3) that $W_{ij,\,i} = 0$, one has

$$\begin{aligned}\frac{1}{F}\sum_{l\neq i} t_{kl} W_{ij,\,i} &= \frac{1}{F}\sum_l t_{kl} W_{ij,\,i} \\ &= W_{kj,\,i} - \frac{1}{F}\delta_{kj} + \delta_{ik}\frac{g_{ij}}{g_{ii}},\end{aligned} \tag{A 6}$$

from which

$$\frac{1}{F}\sum_{k\neq l}\sum_m t_{kl} W_{im,\,i} t_{mi}\, Y = \sum_m W_{km,\,i} t_{mi}\, Y - \frac{1}{F} t_{ik}\, Y + \delta_{ik}\sum_m \frac{g_{im}}{g_{ii}} t_{mi}\, Y. \tag{A 7}$$

This equation shows at once that the $X_{k,\,i}(E)$ given by (A 2) does indeed satisfy (A 1) when $k \neq i$.