One-Electron Green’s Function in Magnetic Insulators

Arisato KAWABATA*

Institute for Solid State Physics
University of Tokyo, Minato-ku, Tokyo

(Received September 30, 1971)

One-electron Green’s function of half-filled Hubbard model is investigated in the atomic limit from the point of view of the relation between the Green’s function and the magnetic properties of the system. It is shown that the Green’s function obtained by Hubbard does not reproduce the known magnetic properties of the system. A new Green’s function is given, which reproduces the Curie law for the magnetic susceptibility in the correct atomic limit (i.e., when the band width is much smaller than the Coulomb repulsion but is still larger than the temperature). The Curie-Weiss law and the antiferromagnetic state is also discussed.

§ 1. Introduction

The electron correlation problem in a narrow band has received considerable attention in recent years. In this paper we deal with a system described by the single-orbital Hubbard model\(^1\) in the half-filled case. In the atomic limit, i.e., in the limit of strong correlation, the system is known to become an antiferromagnetic insulator,\(^2\) which can be well represented by Heisenberg model. However, it is still important to know the properties of the one-particle Green’s function because it is related with many interesting phenomena, e.g., metal-insulator transition or transport of holes or electrons in magnetic insulators. Although the properties of the just half-filled system are very simple, its Green’s function is of no simple matter, since the behavior of one-excess electron or hole is concerned in it.

On the other hand, the Green’s function is closely related to the magnetic properties of the system, e.g., to the magnetic susceptibility. Therefore a properly approximated Green’s function will reproduce the correct behavior of the magnetic susceptibility. In the atomic limit, as is well known, the magnetic susceptibility obeys the Curie law. It is to be emphasised that we must have the Curie law even if the temperature\(^**\) is smaller than the band width; by atomic limit we denotes large Coulomb repulsion and not small band width. The magnetic susceptibility of Hubbard model was calculated by Sakurai,\(^3\) and by Hubbard and Jain,\(^4\) but they obtained the Curie law only when the temperature

\(^*\) Present address: Research Institute for Fundamental Physics, Kyoto University, 606 Kyoto.

\(^**\) We use the system of units in which Boltzmann constant and Planck constant are unity.
is larger than the band width.

The purpose of the present paper is to investigate the properties of the Green's function in the insulating state from the above mentioned point of view.

In § 2 we show the relation between one particle Green's function and magnetic susceptibility in paramagnetic region, and give some conditions which are imposed on the Green's function in order that it reproduces the correct magnetic properties of the system. In § 3 we show that the approximate Green's functions obtained by some investigators do not satisfy these conditions, and in § 4 we give a Green's function which satisfies these conditions, improving the calculation in the Hubbard's paper (to be referred to as HIII). The Green's function will be given as the solution of the coupled equations, which are in general analytically unsoluble, and in § 5 we deal with a special analytically solvable case. The solution in antiferromagnetic state will be discussed in § 6.

§ 2. Spin susceptibility and the Green's function

We consider a system described by the single orbital Hubbard Hamiltonian

\[ \mathcal{H} = \sum_{i,j} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{I}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma}, \]  

(2·1)

where \( c_{i,\sigma}(c_{i,\sigma}) \) is the creation (annihilation) operator of the Wannier state localized at the \( i \)-th site with spin \( \sigma \), \( n_{i,\sigma} \) is the corresponding number operator and \( I \) is the intra-atomic Coulomb repulsion. Here, for the time being, we do not assume that the transfer energy \( t_{ij} \) vanishes except between the nearest-neighbor sites, and we take \( t_{ii} = 0 \).

The retarded Green's function is defined by

\[ G_{\sigma}(i,j; E) = \langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle_E \]

\[ = -i \int_0^\infty dt \; e^{iEt} \langle (c_{i,\sigma}(t) c_{j,\sigma}^\dagger + c_{i,\sigma}^\dagger c_{i,\sigma}(t)) \rangle, \]  

(2·2)

where \( \langle \rangle \) is the grand canonical average and

\[ c_{i,\sigma}(t) = \exp \{it(\mathcal{H} - \mu N)\} c_{i,\sigma} \exp \{-it(\mathcal{H} - \mu N)\}, \]  

(2·3)

\( \mu \) and \( N \) being the chemical potential and the total electron number, respectively. Since the total number of electrons of each spin state is conserved, as is seen from (2.1), the eigen-states of the system can be labeled by \( n_{\sigma} \), the number of electrons of spin \( \sigma \) per atom. Thus we can obtain the correct Green's function in the following way; we construct a Green's function \( G_{\sigma}(i,j; E, n_{\sigma}) \) by taking the average in (2.2) only over the states with a fixed eigenvalue \( n_{\sigma} \), and then put for \( n_{\sigma} \) the correct expectation values (central limit theorem). The values of \( n_{\sigma} \) is to be determined through the self-consistency equation

\[ n_{\sigma} = -\frac{1}{\pi} \int dE f_{\sigma}(E) \operatorname{Im} G_{\sigma}(i,i; E, n_{\sigma}), \]  

(2·4)
where

\[ f_F(E) = \frac{1}{(e^{E/T} + 1)}, \tag{2.5} \]

\( T \) being the temperature. Note that (2.4) is not an identity, but an equation which holds only for equilibrium values of \( n_e \) (see Appendix A).

Hereafter we consider only the half-filled case and write

\[ n_t = \frac{1}{2} + m, \]

\[ n_i = \frac{1}{2} - m \tag{2.6} \]

and

\[ G_{\sigma}(i, i; E, n_{\sigma}) = G_{\sigma}(E, m). \tag{2.7} \]

The spin susceptibility in paramagnetic region is calculated from the Green's function in the following manner; suppose that the magnetic field of magnitude \( H \) is applied along the z-axis. Then, for a fixed value of \( m \), i.e., if we do not consider the redistribution of electrons between the two spin states, the effect of the magnetic field is only to shift the energy by \( \mu_B H \) for up spin and by \( -\mu_B H \) for down spin, and the Green's function can be obtained by replacing \( E \) with \( E + \mu_B H \) or \( E - \mu_B H \) for up or down spin in that in the absence of the magnetic field, where \( \mu_B \) is Bohr magneton (we put the \( g \)-factor of an electron to be 2.0).

Hence from the self-consistency conditions (2.4), (2.6) and (2.7), we get

\[ 2m = -\frac{1}{\pi} \int dE f_F(E) \text{Im} \{G_{\uparrow}(E + \mu_B H, m) - G_{\downarrow}(E - \mu_B H, m)\}, \tag{2.8} \]

where \( G_{\sigma}(E, m) \) is the Green's function in the absence of the magnetic field, and solving this equation we obtain the spin susceptibility \( \chi \) (per atom) from the relation

\[ \chi = \lim_{H \to 0} \frac{\mu_B m}{H}. \tag{2.9} \]

In the atomic limit \( \chi \) must obey the Curie law

\[ \chi = \frac{\mu_B^2}{T} \tag{2.10} \]

and (2.8) must have the solution

\[ 2m = \mu_B H/T. \tag{2.11} \]

Here it should be emphasized that we must have (2.11) irrespective of the value of the ratio of the band width\(^*\) \( \Delta \) and the temperature \( T \) if the condition

\[ I > T > \Delta/I \tag{2.12} \]

is satisfied, because the exchange energy is of order \( \Delta/I \).

\(^*\) It denotes the Bloch energy band due to the first term of (2.1). For simplicity we assume that the state density of this band is symmetric around zero energy and then for a half-filled case it follows that \( \mu = I/2 \) from the electron-hole symmetry.
In the atomic limit \( I \gg \Delta \) the spectrum of \( G_\sigma(E, m) \) generally consists of two sub-bands around \( E = \pm I/2 \) with a width of order \( \Delta^{(0,5)} \) (Fig. 1) and hence, as \( T \ll I \), we have

\[
f_r(E) = 1 - e^{E/\Gamma} \tag{2·13}
\]
in the lower sub-band \( (|E + I/2| \lesssim \Delta) \) and

\[
f_r(E) = e^{-E/\Gamma} \tag{2·14}
\]
in the upper sub-band \( (|E - I/2| \lesssim \Delta) \).

Therefore, putting them into (2·8) and expanding the r.h.s. to the first order in \( H \) and \( m \), we obtain

\[
\left( 1 + \frac{1}{\pi} \mathrm{Im} \int_L dE G'_\sigma(E, 0) \right)
+ \frac{1}{\pi} \mathrm{Im} \int_L dE e^{E/\Gamma} \{ (\mu_B H/Tm) G_\sigma(E, 0) - G'_\sigma(E, 0) \}
+ \frac{1}{\pi} \mathrm{Im} \int_U dE e^{-E/\Gamma} \{ (\mu_B H/Tm) G_\sigma(E, 0) + G'_\sigma(E, 0) \} = 0, \tag{2·15}
\]
where

\[
G'_\sigma(E, 0) = \left. \frac{\partial}{\partial m} G_\sigma(E, m) \right|_{m=0} \tag{2·16}
\]
and \( L \) and \( U \) by the integral sign indicate that the region of the integral is restricted to the lower and the upper sub-band, respectively; in deriving (2·15) we have used the relation

\[
G_\sigma(E, 0) = G'_\sigma(E, 0), \tag{2·17}
\]
\[
G'_\sigma(E, 0) = -G'_\sigma(E, 0). \tag{2·18}
\]

At first sight it seems that the second and the third terms are unimportant because they are of order \( e^{-1/2\Gamma} \), while the first one is of order 1. However, a special case shown below indicates that the first term identically vanishes.

Consider the case when \( t_{\sigma\tau} = 0 \). Then the Green's function can be calculated exactly

\[
G_\sigma(E, m) = \frac{1/2 - m}{E - I/2} + \frac{1/2 + m}{E + I/2}. \tag{2·19}
\]

It is easy to see that

\[
-\frac{1}{\pi} \mathrm{Im} \int_L dE G_\sigma(E, m) = 1/2 + m \tag{2·20}
\]
and that the first term in (2·15) vanishes exactly. Therefore putting (2·19) into (2·15), we obtain
\[ e^{-\frac{1}{2}T} ((\mu_b H/Tm) - 2) = 0, \]
which naturally gives (2·11).

For a finite \( d \) Harris and Lange showed that Eq. (2·20) holds to the order \( (d/l)^1 \). Although we are interested in the case when \( d/l \ll 1 \), it does not lead to the conclusion that the first term in (2·15) is negligible, because the present theory must be applicable to the case \( (d/l)^1 \gg e^{-\frac{1}{2}T} \). However, here we assume* that (2·20) holds to the order \( e^{-\frac{1}{2}T} \). Then the sum of the second and the third terms of the r.h.s. of (2·15) must vanish, while we can easily show that those two terms are identical with the use of the relations
\[ \text{Im} \ G_t(E, 0) = \text{Im} \ G_t(-E, 0), \]  
\[ \text{Im} \ G_t' (E, 0) = -\text{Im} \ G_t' (E, 0), \]
which follow from the electron-hole symmetry
\[ \text{Im} \ G_t(E, m) = \text{Im} \ G_t(-E, -m). \]

Therefore, in order that (2·15) has the solution (2·11), the Green's function must satisfy the relation
\[ \text{Im} \int_{-\infty}^{\infty} dE \text{E} e^{\frac{i}{2}T} \{ 2G_t(E, 0) - G_t' (E, 0) \} = 0. \]  
(2·25)

Generally the Green's function in the atomic limit is not much dependent on the temperature,\(^1,6\) while (2·25) must hold for a very wide range of \( T \) given by (2·12). Therefore, it is natural to expect that the integrand of (2·25) identically vanishes, i.e.,
\[ 2 \text{Im} \ G_t(E, 0) = \text{Im} \ G_t' (E, 0) \]  
\[ 2 \text{Im} \ G_t(E, 0) = -\text{Im} \ G_t' (E, 0) \]
in the lower band, and hence that
\[ 2 \text{Im} \ G_t(E, 0) = -\text{Im} \ G_t' (E, 0) \]  
\[ 2 \text{Im} \ G_t(E, 0) = -\text{Im} \ G_t' (E, 0) \]
in the upper band.

It is clear that the set of Eqs. (2·21), (2·26) and (2·27) is the sufficient

---

*) According to Harris and Lange, for nonzero \( d (< 1) \) satellite bands appear at energies \( E = \pm 3l/2, \) \( E = \pm 5l/2, \ldots \), in the spectrum of \( G_a(E, m) \), in addition to the above-mentioned main sub-bands at \( E = \pm l/2. \) Although the intensity of these satellites is at most of order \( (d/l)^4 \), here we cannot neglect them and they are to be considered as being included in the region of the integration in (2·20). Really (2·20) is correct only to the order \( (d/l)^4 \) if we take account only of the sub-band at \( E = -l/2, \) and we expect that it holds to the order \( e^{-\frac{1}{2}T} \) and in every order in \( (d/l) \) if the contributions of the satellites at \( E = -3l/2, -5l/2 \) are included in it.

On the other hand, the contributions of the satellites to the second and the third terms of the l.h.s. of (2·15) are negligible, because they are at most of order \( e^{-\frac{1}{2}T}(d/l)^4 \).
condition for Eq. (2·15) to have the solution (2·11). However, the argument in this section indicates it to be the necessary condition also.

§ 3. Application to the approximate Green’s functions

In this section we take up some approximate Green’s functions calculated by some investigators to examine whether they satisfy the conditions obtained in § 2. As will be seen, the Green’s function taken up here are independent of temperature, and hence those conditions are the necessary and sufficient conditions.

a) Hubbard’s simple solution

The Green’s function given in the Hubbard’s first paper\(^6\) is of the form

\[ G_\varepsilon(p, E) = \frac{1}{F_\varepsilon(E) - t_p}, \]

\[ \frac{1}{F_\varepsilon(E)} = 1 - \frac{n_{-\varepsilon}}{E + I/2} + \frac{n_{-\varepsilon}}{E - I/2}, \]

where \( G_\varepsilon(p, E) \) and \( t_p \) are the momentum representations of \( G_\varepsilon(i, j; E) \) and \( t_{ij} \), respectively;

\[ G_\varepsilon(p, E) = \sum \exp (-iR_{ij} \cdot p) G_\varepsilon(i, j; E), \]

\[ t_p = \sum \exp (-iR_{ij} \cdot p) t_{ij}, \]

\( R_{ij} \) being the vector drawn from the \( j \)-th site to the \( i \)-th site. The state density \( G_\varepsilon(E) \) is given by\(^*)\)

\[ G_\varepsilon(E) = \frac{1}{N} \sum_p G_\varepsilon(p, E) = \int d\varepsilon \frac{\rho(\varepsilon)}{F_\varepsilon(E) - \varepsilon}, \]

where \( \rho(\varepsilon) \) is the state density of the original band:

\[ \rho(\varepsilon) = \frac{1}{N} \sum_p \delta(\varepsilon - t_p), \]

\( N \) being the total number of the sites. In the atomic limit, we have

\[ F_\varepsilon(E) = \frac{E + I/2}{1 - n_{-\varepsilon}} + O\left(\frac{\Delta}{I}\right) \]

in the lower band, i.e., for \( |E + I/2| \leq \Delta \), and hence from (3·4) we obtain

\[ \text{Im} \ G_\varepsilon(E) = -\pi \rho \left( (E + I/2)/(1 - n_{-\varepsilon}) \right). \]

Thus we find that

\[ \text{Im} \ G_\varepsilon(E, 0) = -\pi \rho (2(E + I/2)), \]

\(* \) Hereafter we drop \( m \) in \( G_m \), except when it is especially necessary to write it explicitly.
One-Electron Green's Function in Magnetic Insulators

\[ \text{Im } G_\varepsilon'(E, 0) = -4\pi(E + I/2)\rho'(2(E + I/2)), \quad (3.10) \]

where

\[ \rho'(\varepsilon) = \frac{d}{d\varepsilon} \rho(\varepsilon). \quad (3.11) \]

If we note the relation

\[ \int d\varepsilon \rho(\varepsilon) = 1, \quad (3.12) \]

we easily see from (3.8) that the condition (2.20) is fulfilled. However, as is seen from (3.9) and (3.10) the condition (2.26) is not satisfied for any realistic functional form of \( \rho(\varepsilon) \).

b) Roth's solution

The solution given by Roth\(^7\) coincides with the Hubbard's simple solution in the atomic limit. Therefore it does not give the correct Curie law either.

c) Hubbard's improved solution

In HIII, the Green's function is given as the solution of the equations

\[ F_\varepsilon(E) = \frac{\{E + I/2 - n_- \varrho_\varepsilon(E)\} \{E - I/2 - (1 - n_-) \varrho_\varepsilon(E)\} - n_- (1 - n_-) \varrho_\varepsilon(E)^2}{E - (I/2)(2n_- - 1) - \varrho_\varepsilon(E)}, \quad (3.13) \]

\[ \varrho_\varepsilon(E) = F_\varepsilon(E) - 1/G_\varepsilon(E) + F_{-\varepsilon}(E) - 1/G_{-\varepsilon}(E) - (F_{-\varepsilon}^*(E) - 1/G_{-\varepsilon}^*(-E)), \quad (3.14) \]

which are to be solved with (3.5). In the lower band, i.e., for \( |E + I/2| \leq 4 \), (3.13) becomes

\[ n_- F_{-\varepsilon}(E) = E + I/2 - n_- \varrho_\varepsilon(E), \quad (3.15) \]

where we have assumed that \( F_\varepsilon \) and \( \varrho_\varepsilon \) are of order \( A \) and neglected the terms of order \( A^2/I \). Since we have assumed that \( \rho(\varepsilon) = \rho(-\varepsilon) \), we have

\[ F_{-\varepsilon}^*(-E) = -F_\varepsilon(E), \quad (3.16) \]

\[ G_{-\varepsilon}^*(-E) = -G_\varepsilon(E) \quad (3.17) \]

and hence, from (3.14) and (3.15), we obtain

\[ 2F_\varepsilon(E, m) - 1/G_\varepsilon(E, m) = (E + I/2)/(1/2 - m) - (F_\varepsilon(E, m) + F_{-\varepsilon}(E, m) - 1/G_{-\varepsilon}(E, m) - 1/G_{-\varepsilon}(E, m)), \quad (3.18) \]

where we put \( n_1 = 1/2 + m, \ n_1 = 1/2 - m \), and explicitly write \( m \) in \( F_\varepsilon \) and \( G_\varepsilon \). Putting \( m = 0 \) in (3.18) and its derivative, we get

\[ F_\varepsilon(E, 0) = E/2 + I/4 + 3/2G_\varepsilon(E, 0), \quad (3.19) \]
A. Kawabata

\[ F'_t(E, 0) = -G'_{t}(E, 0) / 2 \{ G_t(E, 0) \}^2 + 2(E + I/2), \]  

(3·20)

where

\[ F'_t(E, 0) = \frac{\partial}{\partial m} F_t(E, m) \bigg|_{m=0} \]  

(3·21)

and we have used the relation

\[ F'_t(E, 0) = -F_t'(E, 0). \]

In order that the Green's function gives the Curie law, the condition (2·26) must be satisfied for any possible functional form of \( \rho(\varepsilon) \). However, comparing (3·19) and (3·20) with (3·14), it does not seem to be the case for that Green's function. Therefore, Hubbard's improved solution does not correctly describe the magnetic insulators either.

§ 4. Improvement of Hubbard's solution

In this section it will be shown that an improvement of Hubbard's treatment leads to a Green's function which behaves correctly in the atomic limit in the sense stated in § 2.

We proceed in the same way as in III; we assume that the Green's function has the form (3·1). If we introduce notations

\[ n^+_\varepsilon = n_{i, \varepsilon}, \]

\[ n^-\varepsilon = 1 - n_{i, \varepsilon}, \]  

(4·1)

we can write

\[ G_\varepsilon(i, j; E) = \sum_{\alpha=\pm} G_\varepsilon^\alpha(i, j; E), \]  

(4·2)

where

\[ G_\varepsilon^\alpha(i, j; E) = \langle n^\varepsilon - \epsilon c_{t, \varepsilon} c_{j, \varepsilon} \rangle. \]  

(4·3)

The equation of motion for \( G_\varepsilon^\alpha \) is

\[ (E - \varepsilon_\alpha) G_\varepsilon^\alpha(i, j; E) = n^\varepsilon \{ \delta_{ij} + \sum_k t_{ik} G_\varepsilon(k, j; E) \} \]

\[ + \sum_k t_{ik} \langle \langle n^\varepsilon - \epsilon c_{k, \varepsilon} c_{j, \varepsilon} \rangle \rangle \]

\[ + \xi_\varepsilon \sum_k t_{ik} \langle \langle c_{i, \varepsilon} c_{k, \varepsilon} c_{j, \varepsilon} \rangle \rangle - \langle \langle c^\dagger_{k, \varepsilon} c_{k, \varepsilon} c_{j, \varepsilon} \rangle \rangle, \]

(4·4)

where

\[ n^+\varepsilon = n_\varepsilon, \]

\[ n^-\varepsilon = 1 - n_\varepsilon, \]

\[ \xi_\varepsilon = \pm 1 \]  

(4·5)

(4·6)
One-Electron Green’s Function in Magnetic Insulators

\[ \epsilon_{\pm} = \pm I/2. \] (4.7)

For the second term of the r.h.s. of (4.4), we adopt the same approximation as in HIII (scattering correction), and we have

\[ \langle (n^x_{i,-\sigma} - n^{\sigma}_{i,-\sigma})c_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E = \sum_l W_\sigma(k, l; i; E) t_{ij} \langle (n^x_{i,-\sigma} - n^{\sigma}_{i,-\sigma})c_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E, \] (4.8)

where

\[ W_\sigma(k, l; i; E) = G_\sigma(k, l; E) - G_\sigma(k, i; E)G_\sigma(i, l; E)/G_\sigma(E). \] (4.9)

As for the third term in the r.h.s. of (4.4), the treatment in this paper is different from that in HIII. Consider the second Green’s function in the curly bracket of it. It can be written as

\[ \langle c^\dagger_{i,\sigma}c_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E \]
\[ = -i \int_0^\infty dt e^{it\tilde{B}_l} \langle (c^\dagger_{j,\sigma})(-t)c^\dagger_{i,\sigma}c_{i,\sigma}(-t)\rangle. \] (4.10)

In the atomic limit of the half-filled case the states which contribute to the thermal average in (4.10) are those in which each site is occupied by one electron; the probability of finding doubly-occupied or unoccupied sites is of order \( \Delta/I \), and hence we easily see that we can neglect that Green’s function. The same argument cannot be applied to the Green’s function which appears in (4.4), because such combinations of operators as \( c_{i,-\sigma}c_{i,\sigma} \) or \( c^\dagger_{i,-\sigma}c_{i,\sigma} \) do not appear in it. We resolve it into two components:

\[ \langle c^\dagger_{i,\sigma}c_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E = \sum_{\delta = \pm} \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E \] (4.12)

and these two components satisfy an equation of motion of the form

\[ (E - \epsilon_{\pm}) \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E = \delta_{ij} \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E - \delta_{ij} \sum_{\delta'} \langle c^\dagger_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E \]
\[ + \sum_{\delta'} \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E + \sum_{\delta'} \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E \]
\[ - \sum_{\delta'} \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E. \] (4.13)

Here we introduce the same approximation as in HIII; in the r.h.s. of (4.13) we retain only the last two terms. In HIII, Hubbard made further approximations

\[ \langle n^\delta_{i,\sigma}c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E = n^\delta_{i,\sigma}\langle c_{i,\sigma}; c^\dagger_{i,\sigma}; c^\dagger_{j,\sigma}\rangle_E, \] (4.14)
Of these approximations, the first one is reasonable because \( k \) does not coincide with \( l \) nor with \( i \). In the second one, however, the operator \( n^\alpha_\sigma n^-_\sigma \) is replaced by the product of the averages of each operator, and it is clear that this approximation is not reasonable in the atomic limit.

Here we introduce an approximation

\[
\langle n^\alpha_\sigma c_{k,-\sigma} c_{l,\sigma} ; c^\dagger_{j,\sigma} \rangle_E = \delta_{k,l} n^\alpha_\sigma n^-_\sigma \langle c_{i,\sigma} ; c^\dagger_{j,\sigma} \rangle_E .
\]  

(4·15)

and put

\[
\langle n^\alpha_\sigma n^-_\sigma \rangle = 0 \quad \text{for } \alpha = - ,
\]

\[
= n_\sigma \quad \text{for } \alpha = + .
\]  

(4·16)

The approximation (4·17) was led by the consideration that the states which mainly contribute to the average are those in which the each site is occupied by one electron.

Then from (4·12) and (4·13) we obtain

\[
\langle c_{k,-\sigma} c_{l,\sigma} ; c^\dagger_{l,\sigma} , c^\dagger_{j,\sigma} \rangle_E
\]

\[
= \frac{1}{F^0_\sigma (E)} \sum_t t_{kl} \langle c_{i,-\sigma} c^\dagger_{l,\sigma} , c^\dagger_{j,\sigma} \rangle_E - t_{kl} \frac{n_\sigma}{E - \epsilon_+} \langle c_{i,\sigma} ; c^\dagger_{j,\sigma} \rangle_E ,
\]  

(4·17)

where

\[
\frac{1}{F^0_\sigma (E)} = \frac{n_\sigma}{E - \epsilon_+} + \frac{n^-_\sigma}{E - \epsilon_-} .
\]  

(4·18)

For the time being, we confine ourselves to the discussion of the Green's function in the lower band. Then the last term of (4·18) is of order \( 1/I \), and is negligible compared with other terms of order \( 1/A \). Moreover, as in IIIII, we replace \( F^0_\sigma (E) \) in (4·18) by true \( F_\sigma (E) \) which is to be determined self-consistently. Noting that (4·18) is correct for \( k=l=i \) and that the r.h.s. contains the term \( l=i \), we can express its l.h.s. in terms of \( G^-_{\sigma}(i, j; E) \) and we obtain

\[
\sum_k t_{kl} \langle c_{k,-\sigma} c^\dagger_{l,\sigma} , c^\dagger_{i,\sigma} \rangle_E = (F_\sigma (E) - 1/G^-_{\sigma} (E)) G^-_{\sigma}(i, j; E) .
\]  

(4·19)

This equation can be led easily by going over to the momentum representation of both sides of (4·18) with respect to \( R_{kl} \) and by using (3·1) and (3·5) (see Appendix B). In the same way from (4·8) and (4·9) we have

\[
\sum_k t_{kl} \langle (n^\alpha_{k,-\sigma} - n^-_{k,-\sigma}) c_{k,\sigma} ; c^\dagger_{l,\sigma} \rangle_E = (F_\sigma (E) - 1/G_\sigma (E)) \langle (n^\alpha_{l,-\sigma} - n^-_{l,-\sigma}) c_{i,\sigma} ; c^\dagger_{j,\sigma} \rangle_E .
\]  

(4·20)

As can be seen from (4·4), in the lower band, \( G^+_{\sigma}(i, j; E) \) is of order \( 1/I \) and hence we can put

\[
G^-_{\sigma}(i, j; E) = G_{\sigma}(i, j; E) .
\]  

(4·21)
One-Electron Green's Function in Magnetic Insulators

103

to the order $1/\Delta$. Thus, putting $\alpha=-$ in (4.4) and (4.21), using (4.20), and going over to the momentum representation, we obtain

$$G_\sigma(p,E)\{E-\varepsilon_-n_\sigma p-n_\sigma Q_\sigma(E)-Q_-\sigma(E)\}=n_\sigma,$$

(4.23)

where

$$Q_\sigma(E)=F_\sigma(E)-1/G_\sigma(E)$$

(4.24)

Comparing (4.23) with (3.1), we find that the self-consistency equation is given by

$$F_\sigma(E)=(E-\varepsilon_-n_\sigma Q_\sigma(E)-Q_-\sigma(E))/n_\sigma,$$

(4.25)

which is to be solved with (3.4). Unfortunately we cannot explicitly express the dependence of $G_\sigma(E)$ on $n_\sigma$. However, it is easy to show that $G_\sigma(E)$ obtained above satisfies (2.20) and (2.26). Equation (4.25) can be written in the form

$$n_\sigma G_\sigma(E)=E-\varepsilon_-Q_\sigma(E)-Q_-\sigma(E).$$

(4.26)

The r.h.s. of this equation is invariant with respect to the interchange of $\sigma$ with $-\sigma$. Therefore, if we put $n_1=1/2+m$, $n_1=1/2-m$, its derivative in $m$ at $m=0$ vanishes and we have

$$\frac{\partial}{\partial m}\{1/2+m\} \left|_{m=0} \right. = 0,$$

(4.27)

from which (2.26) follows at once.

To show that (2.21) holds for the above-obtained Green's function, we assume that Im $G_\sigma(E)$ vanishes except in the region $|E-\varepsilon_-|\leq\Delta_0$, where $\Delta_0=\Delta$ (later it will be shown to be the case for a special but not unreasonable form of $\rho(\varepsilon)$). So far we have assumed that $E$ is real with an infinitesimal positive imaginary part. Here we extend $G_\sigma(E)$ and $F_\sigma(E)$ to general complex values of $E$, assuming that they are defined by (3.5), (4.24) and (4.26) also. Then $G_\sigma(E)$ has a cut on the part of real axis

$$-\Delta_0 \leq E-\varepsilon_- \leq \Delta_0.$$  

(4.28)

Therefore, since

$$G_\sigma^*(E+i\delta)=G_\sigma(E-i\delta), \quad \delta \to +0$$

(4.29)

for real $E$, we have

$$-\frac{1}{\pi} \text{Im} \int_E dEG_\sigma(E)=-\frac{1}{2\pi i} \int_{\varepsilon_-}^{\varepsilon_+} dE(G_\sigma(E+i\delta)-G_\sigma(E-i\delta))$$

$$=\frac{1}{2\pi i} \int_c dz G_\sigma(z),$$

(4.30)

where the contour $c$ of the integration in $z$ is a circle enclosing clockwise the
cut of \( G_\varepsilon(z) \) shown by (4.28) (Fig. 2).

On the other hand, for \( |z-\varepsilon| \gtrsim \Delta \), from (3.4), (4.24) and (4.26), we obtain

\[
F_\varepsilon(z) \sim \frac{z-\varepsilon_-}{n_{-\varepsilon}},
\]

\[
G_\varepsilon(z) \sim \frac{n_{-\varepsilon}}{z-\varepsilon_-}, \tag{4.31}
\]

and hence, if we let the contour \( c \) in (4.30) very large, we get

\[
-\frac{1}{\pi} \text{Im} \int dE G_\varepsilon(E) = -\frac{1}{2\pi i} \int \frac{n_{-\varepsilon}}{z-\varepsilon_-} = n_{-\varepsilon}. \tag{4.32}
\]

Thus we find that the approximate Green's function obtained above satisfies the conditions (2.21) and (2.26).

In the upper band, i.e., \( |E-\varepsilon_+| \leq \Delta \), from (4.19) we have

\[
\frac{n_{\varepsilon_+}}{E-\varepsilon_+} = \frac{1}{F_\varepsilon^0(E)} \tag{4.33}
\]

if we neglect the terms of order \( 1/I \). Hence, putting (4.33) into (4.18) and replacing \( F_\varepsilon^0(E) \) by \( F_{-\varepsilon}(E) \), we can obtain the self-consistency equation as in the lower band:

\[
n_{-\varepsilon}/G_\varepsilon(E) = E-\varepsilon_- - \Omega_\varepsilon(E) - \Omega_{-\varepsilon}(E). \tag{4.34}
\]

It is obvious that (2.27) follows from this equation.

§ 5. An analytically soluble case

In this section, as in HIII, we consider the case when \( \rho(\varepsilon) \) is given by

\[
\rho(\varepsilon) = \frac{4}{\pi \Delta} \left\{ 1 - \left( \frac{\varepsilon}{\Delta} \right)^2 \right\}^{1/2}. \tag{5.1}
\]

Then from (3.5), we have

\[
G_\varepsilon(E) = \frac{8}{\Delta^2} \left[ F_\varepsilon(E) - \left\{ (F_\varepsilon(E))^2 - \left( \frac{\Delta}{2} \right)^{1/2} \right\} \right] \tag{5.2}
\]

and hence

\[
F_\varepsilon(E) = 1/G_\varepsilon(E) + (\Delta/4)^{3/2} G_\varepsilon(E). \tag{5.3}
\]

Putting it into (4.26) we can easily solve the equation for \( G_\varepsilon(E) \):

\[
G_\varepsilon(E) = 2n_\varepsilon (2/\Delta)^3 \left[ (E-\varepsilon_-) - i \{ (\Delta/2)^2 - (E-\varepsilon_-)^2 \}^{1/2} \right] \tag{5.4}
\]

and we obtain

\[
\text{Im } G_\varepsilon(E) = -2n_\varepsilon (2/\Delta)^3 \{ (\Delta/2)^2 - (E-\varepsilon_-)^2 \}^{1/2} \quad \text{for } |E-\varepsilon_-| \leq \Delta/2 \tag{5.5}
\]
and
\[ \text{Im } G_\varepsilon(E) = 0 \quad \text{for } |E - \varepsilon_\pm| > A/2. \quad (5.6) \]

As is seen from (5.5), the shape of the sub-band is the same as that of the original band \( \rho(\varepsilon) \), and the dependence of \( G_\varepsilon(E) \) on \( n_\varepsilon \) is very simple. However, it seems to be the result of the special choice of \( \rho(\varepsilon) \). At least the author could not prove that it is the case for arbitrary \( \rho(\varepsilon) \). Generally the shape of the sub-band will be different from that of the original band, and \( G_\varepsilon(E) \) will be a very complicated function of \( n_\varepsilon \).

§ 6. Antiferromagnetic solution and the correction of order \( A/I \)

In the calculation made in the preceding sections, we have neglected the contributions of the terms which vanish in the limit \( I \to \infty \). In this section we consider the corrections to the first order in \( 1/I \). If these corrections are properly taken account of, the physical quantities calculated from the Green's function should coincide with those from Heisenberg model, of which the exchange coupling is antiferromagnetic and is of order \( A'/I \).

First we consider the Green's function in antiferromagnetic state, in the same approximation as in § 4.

i) Approximation to the order \( A \)

We consider the case when the crystal lattice is composed of two equivalent interpenetrating sub-lattices \( A \) and \( B \), and assume that \( t_{ij} (\equiv t) \neq 0 \) only between the nearest-neighbor sites, which belong to different sub-lattices. We write the annihilation and the creation operators of atomic orbitals on \( A \)-sites as \( a_{i,\varepsilon} \) and \( a_{i,\varepsilon}^\dagger \), and those on \( B \)-sites as \( b_{i,\varepsilon} \) and \( b_{i,\varepsilon}^\dagger \). We write
\[
\begin{align*}
A_{i,\varepsilon} &= a_{i,\varepsilon}^\dagger a_{i,\varepsilon}, \\
B_{i,\varepsilon} &= b_{i,\varepsilon}^\dagger b_{i,\varepsilon}
\end{align*}
\]
and
\[
\begin{align*}
A_\varepsilon &= \langle A_{i,\varepsilon} \rangle, \\
B_\varepsilon &= \langle B_{i,\varepsilon} \rangle.
\end{align*}
\]

Below we will solve the equation of motion for the Green's function assuming that \( A_\varepsilon \neq B_\varepsilon \). However, strictly speaking we cannot define the Green's function of \( A_\varepsilon \) and \( B_\varepsilon \) in the sense stated in § 2, since the total number of electrons on each sub-lattice is not conserved. Nevertheless, it is generally believed that the sub-lattice magnetization is an approximately good quantum number, and in that sense we can regard the Green's function as the function of \( A_\varepsilon \) and \( B_\varepsilon \). Below we do not write \( A_\varepsilon, B_\varepsilon \) explicitly in \( G_\varepsilon(i,j;E) \).

First consider the Green's function \( \langle a_{i,\varepsilon}; a_{j,\varepsilon}^\dagger \rangle_\varepsilon \). We decompose it into two
components:

\[ \left\langle a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} = \sum_{a=\pm} \left\langle a_{i, -\sigma}^{a} a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E}, \tag{6.3} \]

where \( A_{i, \sigma} = A_{i, \sigma} \) and \( A_{i, \sigma} = 1 - A_{i, \sigma} \). The equation of motion for them is

\[ (E - \varepsilon_{\sigma}) \left\langle a_{i, \sigma}^{a} a_{i, -\sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} = A_{\sigma} a_{\sigma} \mathcal{D}_{ij} + A_{\sigma} \sum_{k} t_{ik} \left\langle b_{k, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \]

\[ + \sum_{k} t_{ik} \left\langle (A_{i, -\sigma} - A_{\sigma}) b_{k, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \]

\[ + \xi_{\sigma} \sum_{k} t_{ik} \left\langle a_{i, -\sigma} b_{k, -\sigma} a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} - \left\langle b_{i, -\sigma} a_{i, -\sigma} a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E}. \tag{6.4} \]

The equation of motion for \( \left\langle b_{i, -\sigma}^{\dagger} b_{k, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \) is

\[ (E - \varepsilon_{\sigma}) \left\langle b_{i, -\sigma}^{\dagger} b_{k, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} = B_{\sigma} \sum_{j} t_{jk} \left\langle a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \]

\[ + \sum_{j} t_{jk} \left\langle (B_{i, -\sigma} - B_{\sigma}) a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \]

\[ + \xi_{\sigma} \sum_{k} t_{ik} \left\langle a_{i, -\sigma}^{\dagger} b_{k, -\sigma} b_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} - \left\langle a_{i, -\sigma} b_{i, -\sigma} b_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E}. \tag{6.5} \]

If we retain only the first and the second terms in the r.h.s. of (6.4) and the first term in (6.5), dropping other terms, we obtain a closed set of equations for \( \left\langle a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \) and \( \left\langle b_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \), and we have

\[ G_{e}^{AA}(p, E) = \frac{F_{e}^{GA}(E)}{F_{e}^{GA}(E) F_{e}^{GB}(E) - t_{p}^{2}}, \tag{6.6} \]

\[ G_{e}^{AB}(p, E) = \frac{t_{p}}{F_{e}^{GA}(E) F_{e}^{GB}(E) - t_{p}^{2}}, \tag{6.7} \]

where

\[ G_{e}^{AA}(p, E) = \sum_{n, \alpha} \left\langle a_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \exp \{-i p \cdot R_{ij} \} \tag{6.8} \]

\[ i \text{ running on the } A \text{ sites}, \]

\[ G_{e}^{AB}(p, E) = \sum_{n, \beta} \left\langle b_{i, \sigma}; a_{j, \sigma}^{\dagger} \right\rangle_{E} \exp \{-i p \cdot R_{ij} \} \tag{6.9} \]

\[ i \text{ running on the } B \text{ sites}, \]

\[ \frac{1}{F_{e}^{AA}(E)} = \frac{A_{+}^{\sigma}}{E - \varepsilon_{+}} + \frac{A_{-}^{\sigma}}{E - \varepsilon_{-}} \tag{6.10} \]

\[ \frac{1}{F_{e}^{AB}(E)} = \frac{B_{+}^{\sigma}}{E - \varepsilon_{+}} + \frac{B_{-}^{\sigma}}{E - \varepsilon_{-}}. \tag{6.11} \]

The present approximation corresponds to the Hubbard's simple solution and is inadequate for our purpose. However, as in § 4 we assume that the correct Green's function is obtained, if in (6.6) and (6.7) \( F_{e}^{AA}(E) \) and \( F_{e}^{GB}(E) \) are replaced by appropriate functions \( F_{e}^{AA}(E) \) and \( F_{e}^{GB}(E) \).

For the Green's function in the third term of the r.h.s. of (6.4), we de-
compose it into two components inserting $B_{k,-\sigma}^\alpha$ in it and introduce the same approximation as in III:

$$(E - \varepsilon_\alpha)\langle (A_{k,-\sigma}^\alpha - A_{-\sigma}^\alpha) B_{k,-\sigma} b_{h,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E = B_{-\sigma}^\alpha \sum_1^T t_{ki} \langle (A_{i,-\sigma}^\alpha - A_{-\sigma}^\alpha) a_{i,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E ,$$

(6.12)

from which we have

$$(6.13)$$

$$\langle (A_{k,-\sigma}^\alpha - A_{-\sigma}^\alpha) b_{k,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E = \frac{1}{F_{-\sigma}^\beta(E)} \sum_1^T t_{ki} \langle (A_{i,-\sigma}^\alpha - A_{-\sigma}^\alpha) a_{i,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E ,$$

where we have replaced $F_{-\sigma}^\alpha$ by $F_{-\sigma}^\beta$. In the same way, for $l \neq i$ we have

$$\langle (A_{k,-\sigma}^\alpha - A_{-\sigma}^\alpha) a_{i,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E = \frac{1}{F_{-\sigma}^\delta(A) \sum_1^T t_{im} \langle (A_{i,-\sigma}^\alpha - A_{-\sigma}^\alpha) b_{m,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E .$$

(6.14)

From these two equations we obtain

$$(6.15)$$

$$\sum_1^T t_{ik} \langle (A_{k,-\sigma}^\alpha - A_{-\sigma}^\alpha) b_{k,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E$$

$$(6.16)$$

$$(6.17)$$

where

and the procedure of the derivation is similar to that in Appendix B.

In (6.4) we neglect the Green's function $\langle b_{k,-\sigma} a_{j,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E$ for the same reason that we have neglected the Green's function of (4.10). As for the Green's function

$$\langle b_{k,-\sigma} a_{i,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E = - \langle a_{i,\sigma}^\dagger b_{k,-\sigma} a_{j,\sigma}; a_{j,\sigma}^\dagger, \alpha \rangle_E ,$$

(6.17)

we again decompose it into two parts by inserting $B_{k,\sigma}^\alpha$ in it, and the equation of motion for them is

$$(6.18)$$

$$(6.19)$$

where we have introduced the same approximation as was applied for (4.13). On the basis of the same argument stated in deriving (4.17), we put

$$\langle B_{-\sigma}^\alpha B_{-\sigma} \rangle = 0 ,$$

$$\langle B_{-\sigma}^\alpha B_{-\sigma} \rangle = B_\sigma ,$$

and from (6.18) we obtain
where we have replaced $F_{\sigma}^{\text{BB}}(E)$ by $F_{\sigma}^{\text{B}}(E)$. In the same way we obtain
\begin{equation}
\langle a_{t_{i}-\sigma}a_{t_{i}}^{\dagger}a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B} = \frac{1}{F_{\sigma}^{\text{A}}(E)} \sum_{\sigma} t_{m} \langle a_{m_{t_{i}}-\sigma}a_{t_{i}}^{\dagger}a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B}. \tag{6.21}
\end{equation}

In the lower band, we neglect the second term of r.h.s. of (6.20), and from these two equations we get, after some manipulations,
\begin{equation}
\sum_{t_{k}} t_{t_{k}} \langle b_{k_{t_{i}}-\sigma}a_{t_{i}}^{\dagger}a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B} = \frac{1}{F_{\sigma}^{\text{A}}(E)} \sum_{\sigma} t_{m} \langle b_{m_{t_{i}}-\sigma}a_{t_{i}}^{\dagger}a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B}. \tag{6.22}
\end{equation}

In the lower band, we can identify $\langle A_{t_{i}-\sigma}a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B}$ with $\langle a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B}$, and putting (6.15) and (6.22) into (6.4) for $\alpha=-$, we obtain
\begin{equation}
\{(E-\varepsilon_{-})-A_{-\sigma}^{2}/F_{\sigma}^{\text{B}}(E)-A_{-\sigma}^{+}Q_{\sigma}^{\text{A}}(E)-Q_{\sigma}^{\text{A}}(E)\} G_{\sigma}^{\text{AA}}(p,E) = A_{-\sigma}, \tag{6.23}
\end{equation}

where
\begin{equation}
Q_{\sigma}^{\text{A}}(E) = F_{\sigma}^{\text{A}}(E) - 1/G_{\sigma}^{\text{A}}(E), \tag{6.24}
\end{equation}
and we have used the relation
\begin{equation}
G_{\sigma}^{\text{BA}}(p,E) = \frac{t_{p}}{F_{\sigma}^{\text{B}}(E)F_{\sigma}^{\text{A}}(E)} = \frac{t_{p}}{F_{\sigma}^{\text{B}}(E)} G_{\sigma}^{\text{AA}}(p,E), \tag{6.25}
\end{equation}
which was assumed above.* Since we have assumed that
\begin{equation}
G_{\sigma}^{\text{AA}}(p,E) = \frac{F_{\sigma}^{\text{B}}(E)}{F_{\sigma}^{\text{A}}(E)F_{\sigma}^{\text{B}}(E)} = \frac{F_{\sigma}^{\text{B}}(E)}{F_{\sigma}^{\text{B}}(E)F_{\sigma}^{\text{B}}(E)} \tag{6.26}
\end{equation}
comparing it with (6.23) we obtain the self-consistency equation
\begin{equation}
A_{-\sigma}^{2}F_{\sigma}^{\text{A}}(E) = E - \varepsilon_{-} - A_{+\sigma}^{+}Q_{\sigma}^{\text{A}}(E) - Q_{\sigma}^{\text{A}}(E), \tag{6.27}
\end{equation}
which can be written as
\begin{equation}
A_{-\sigma}/G_{\sigma}^{\text{A}}(E) = E - \varepsilon_{-} - Q_{\sigma}^{\text{A}}(E) - Q_{\sigma}^{\text{A}}(E). \tag{6.28}
\end{equation}

Thus the Green's function can be determined by the coupled Eqs. (6.16), (6.26), (6.28) and those in which $A$ and $B$ are interchanged.

For the upper band, we replace $B_{\sigma}^{+}/(E-\varepsilon_{+})$ in (6.20) by $1/F_{\sigma}^{\text{A}}(E)$, and identifying $\langle A_{t_{i}-\sigma}a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B}$ with $\langle a_{t_{i}};a_{j_{i}}^{\dagger}\rangle_{B}$, we finally obtain
\begin{equation}
A_{+\sigma}/G_{\sigma}^{\text{A}}(E) = E - \varepsilon_{+} - Q_{\sigma}^{\text{A}}(E) - Q_{\sigma}^{\text{A}}(E). \tag{6.29}
\end{equation}

Since in this sub-section we have neglected the contributions which vanish like

*) We obtain the same result, if we solve (6.5) making use of an approximation similar to the one applied for (6.4) and then solve the coupled equation of $G_{\sigma}^{\text{AA}}$ and $G_{\sigma}^{\text{BA}}$. Therefore the assumption (6.25) is self-consistent in this sense.
1/\Delta I, the obtained Green's function describes only paramagnetic states, and to describe antiferromagnetic states we need to include the terms of order $\Delta^2/\Delta I$.

ii) **Correction of order $\Delta^3/\Delta I$**

Recently Brinkman and Rice\(^9\) investigated the energy spectrum of the single particle excitation in magnetic insulators. According to them, the main change of the energy spectrum due to the correction of order $\Delta^3/\Delta I$ is the shift of the center of the sub-band. Therefore we have assumed that the Green's function correct to the order $\Delta^3/\Delta I$ can be obtained by adding a shift to the energy in the one correct to the order $\Delta$. The shift is equal to the first moment of the sub-band, and it can be easily calculated as in the paper by Brinkman and Rice;\(^9\) the first moment of the lower band of $\sigma$-spin on $A$-site is given by

$$-2zJB\_\sigma$$

and vice versa, where

$$J=\epsilon^2/\Delta I,$$

and $z$ is the number of the nearest-neighbor sites. Thus, if we write the corrected Green's function as $g_{\sigma}^{AA}(p, E)$, $g_{\sigma}^{BB}(p, E)$, etc., we put

\[
g_{\sigma}^{AA}(p, E) = G_{\sigma}^{AA}(p, E + 2zJB\_\sigma),
g_{\sigma}^{BB}(p, E) = G_{\sigma}^{BB}(p, E + 2zJA\_\sigma),
\]

where $G_{\sigma}^{AA}$ and $G_{\sigma}^{BB}$ are given in the preceding sub-section.

Unfortunately the author could not reasonably derive these relations from the equation of motions, but in the following we will see that these Green's functions well reproduce the magnetic properties of the system.

a) **Paramagnetic susceptibility**

In the paramagnetic state we have

\[
A_\epsilon = B_\epsilon = n_\epsilon,
\]

\[
G_\epsilon^A(E) = G_\epsilon^B(E) = G_\epsilon(E),
\]

where $G_\epsilon(E)$ is given in § 4. Therefore if we put

\[
g_\epsilon^A(E) = \frac{1}{N} \sum_p g_{\epsilon}^{AA}(p, E),
g_\epsilon^B(E) = \frac{1}{N} \sum_p g_{\epsilon}^{BB}(p, E),
\]

we have

\[
g_\epsilon^A(E) = g_\epsilon^B(E) = G_\epsilon(E + 2n_\epsilon zJ) = g_\epsilon(E).
\]

Then, putting $n_\epsilon = 1/2 + m$, $n_\epsilon = 1/2 - m$, and replacing $G_\epsilon(E)$ by $g_\epsilon(E)$ in (2.8), we obtain
\[ \int dE \text{Im} G_{\uparrow}(E, m) \exp\left\{ E - \mu_B H - (1-2m)zJ \right\}/T \] 
\[ - \int dE \text{Im} G_{\downarrow}(E, m) \exp\left\{ E + \mu_B H - (1+2m)zJ \right\}/T \] 
\[ - \int dE \text{Im} G_{\uparrow}(E, m) \exp\left\{ - (E - \mu_B H - (1-2m)zJ) \right\}/T \] 
\[ + \int dE \text{Im} G_{\downarrow}(E, m) \exp\left\{ - (E + \mu_B H - (1+2m)zJ) \right\}/T \] 
\[ = 0, \quad (6\cdot36) \]

where the use was made of \((2\cdot21)\). We expand the l.h.s. of this equation to the first order in \(H\) and \(m\), and then using \((2\cdot17), (2\cdot18), (2\cdot25)\) and \((2\cdot26)\) we find

\[ 2m(T+zJ) = \mu_B H \]

and hence

\[ \chi = \frac{2m\mu_B}{H} = \frac{\mu_B^2}{T+zJ}. \] \[ (6\cdot37) \]

\[ (6\cdot38) \]

b) Staggard susceptibility in paramagnetic regions

In this case we put

\[ A_{\uparrow} = B_{\downarrow} = 1/2 + m, \]
\[ A_{\downarrow} = B_{\uparrow} = 1/2 - m \]

and assume that the Green's functions in the presence of the staggard field are given by

\[ g_{\sigma}^A(E + \sigma \mu_B H) \]

and

\[ g_{\sigma}^B(E - \sigma \mu_B H), \] \[ (6\cdot40) \]

where \(\sigma\) in the bracket takes 1 or \(-1\) according as \(\sigma = \uparrow\) or \(\downarrow\). Note that this assumption is correct only approximately and equivalent to the approximation that we regard \(A_{\sigma}\) and \(B_{\sigma}\) as good quantum numbers.

Next we show that the equation

\[ -\frac{1}{\pi} \int dE \text{Im} G_{\sigma}^A(E) = 1 - A_{-\sigma} \]

holds identically for arbitraly \(A_{\sigma}\) and \(B_{\sigma}\); as in § 4, we extend \(G_{\sigma}^A\) and \(G_{\sigma}^B\) for complex values of \(E\), and from \((6\cdot16), (6\cdot26), (6\cdot28)\) and those in which \(A\) and \(B\) are interchanged, we easily find that for \(|E-\varepsilon_-| > \Delta\)

\[ F_{\sigma}^A(E) = 1/G_{\sigma}^A(E) = (E-\varepsilon_-)/A_{-\sigma}. \]

Therefore \((6\cdot41)\) can be proved by the same argument as was used in proving
One-Electron Green's Function in Magnetic Insulators

(2.21). It is clear that (6.41) holds for B-sites also.
Moreover it is easy to see from (6.26) and (6.28) that (2.26) and (2.27) holds for \( G_+^a(E) \) also.

Then from the equation

\[
2m = A_1^\gamma - A_1^\delta = - \frac{1}{\pi} \int dE f_\tau(E) \text{Im} \{ \tau_1^\delta (E + \mu B H) - \tau_1^\gamma (E - \mu B H) \},
\]

(6.43)

using (6.41), we find that the staggered susceptibility is given by

\[
\chi_s = \frac{\mu_B^2}{T - zJ}. \tag{6.44}
\]

c) Sub-lattice magnetization in antiferromagnetic state

In (6.43), we put \( H = 0 \). Then, using (6.41) we find

\[
0 = \frac{1}{\pi} \int L dE \text{Im} G_+^\delta (E) \exp \left[ \frac{(1 + 2m) z J}{T} \right]
- \frac{1}{\pi} \int L dE \text{Im} G_+^\gamma (E) \exp \left[ \frac{(1 - 2m) z J}{T} \right]
- \frac{1}{\pi} \int U dE \text{Im} G_+^\delta (E) \exp \left[ \frac{- (1 + 2m) z J}{T} \right]
+ \frac{1}{\pi} \int U dE \text{Im} G_+^\gamma (E) \exp \left[ \frac{- (1 - 2m) z J}{T} \right]. \tag{6.45}
\]

From (6.28) and (6.29) we find that

\[
A_1^- G_+^\delta (E) = A_1^\delta G_+^\delta (E) \tag{6.46}
\]

in the lower band, and that

\[
A_1^+ G_+^\delta (E) = A_1^\delta G_+^\delta (E) \tag{6.47}
\]

in the upper band. Hence (6.45) becomes

\[
0 = \frac{1}{\pi} \int L dE \text{Im} G_+^\delta (E) e^{(2zJ)/T} \left( e^{-2m z J / T} - \frac{1 - 2m}{1 + 2m} \right)
- \frac{1}{\pi} \int U dE \text{Im} G_+^\gamma (E) e^{-(2zJ)/T} \left( e^{2m z J / T} - \frac{1 + 2m}{1 - 2m} \right), \tag{6.48}
\]

and this equation has the solution

\[
(1 + 2m) e^{-(2m z J / T)} = (1 - 2m) e^{2m z J / T}, \tag{6.49}
\]

which can be written as

\[
2m = \tanh(2m z J / T). \tag{6.50}
\]

As is well known, relations (6.38), (6.44) and (6.50) can be led by ap-
plying the molecular field approximation to the Heisenberg model, of which the exchange coupling is $J$ (antiferromagnetic). It is natural that we obtain the results of molecular field approximation, for in this approximation we replace many-body effects by some appropriate one-body potential, which will give only a uniform shift to the energy of electrons. Thus we see that the Green's functions (6·31) well reproduce the magnetic properties of the system.

§ 7. Summary and discussion

We have derived the conditions imposed on the one-electron Green's function in magnetic insulators in their insulating limit, where the magnetic susceptibility must obey the Curie law. The investigation in § 2 indicates that these are necessary as well as sufficient conditions, although we could not prove it rigorously. A Green's function which satisfies these conditions was obtained in § 4, and it was shown that it well reproduces the magnetic properties of the antiferromagnet if the corrections of order $\mathcal{A}^2/\mathcal{I}$ were included in it. It is to be noted that the Green's function obtained in § 4 is not exact to the order $\mathcal{A}$, although it correctly reflects the magnetic properties of the system, and hence the inclusion of all the corrections of order $\mathcal{A}^2/\mathcal{I}$ will not necessarily lead to a correct result. It seems to be one of the reasons why we could not pick up appropriate correction terms from the equations of motion.

Acknowledgements

The author wishes to thank Professor Tôru Moriya for suggesting this problem and for reading the manuscript before publication. He is also indebted to the Sakkokai Foundation for financial support.

Appendix A

Since $N_\sigma$, the total number of electrons of spin $\sigma$, can be quantum numbers of eigenstates, we write them and their energy eigen-values (including chemical potential) as

$$|a, N_t, N_\sigma\rangle, \quad E(a, N_t, N_\sigma), \quad (A·1)$$

where $a$ represents other quantum numbers. Then from (2·2) we obtain

$$\text{Im } G_t(i, i; E, n_\sigma) = -\frac{\hbar}{\mathcal{Z}} \left( \sum_{a,b} \exp \{-E(a, N_t, N_\sigma)/T\} \right)$$

$$\times |\langle a, N_t, N_\sigma| c_{i\uparrow}|b, N_t+1, N_\uparrow\rangle|^2 \delta(E + E(a, N_t, N_\sigma) - E(b, N_t+1, N_\uparrow))$$

$$+ \sum_{a,b} \exp \{-E(b, N_t, N_\uparrow)/T\} |\langle b, N_t, N_\uparrow| c_{i\downarrow}|a, N_t-1, N_\uparrow\rangle|^2$$

$$\times \delta(E + E(a, N_t-1, N_\uparrow) - E(b, N_t, N_\uparrow)) \quad (A·2)$$
with \(N_e = N_{n_e}\), and
\[
Z = \sum_a \exp \{-E(a, N_t, N_d)/T\}.
\] (A·3)

When \(N_e\) takes equilibrium values, two terms in the r.h.s. of (A·2) are stationary with respect to the variation in \(N_e\); this is the fundamental assumption in using the grand canonical ensemble average instead of the canonical ensemble average. Therefore we can replace \(N_t\) in the second term by \(N_t + 1\). Then we have

\[
\text{Im} G_\tau(i, i; E, n_e) = -\frac{1}{Z} \sum_{a,b} \left[ \exp \{-E(a, N_t, N_d)/T\} + \exp \{-E(b, N_t + 1, N_d)/T\}\right] |\langle a, N_t, N_d|c_{i\tau}^\dagger|b, N_t + 1, N_d\rangle|^2 \\
\times \delta(E + E(a, N_t, N_d) - E(b, N_t + 1, N_d)),
\] (A·4)

from which (2·4) can be derived easily.

On the other hand, if \(N_e\) do not take equilibrium values, the above-mentioned replacement of \(N_t\) by \(N_t + 1\) cannot be allowed. Therefore (2·4) does not hold for arbitrary values of \(N_e\).

**Appendix B**

We write
\[
\text{g}_\epsilon(k, i, j; E) = \langle c_k, -\epsilon|c_i, -\epsilon_{\epsilon, i}; c_j, \epsilon\rangle_E.
\] (B·1)

Then, after doing the approximation stated below (4·19), (4·18) can be written as
\[
g_\epsilon(k, i, j; E) = \frac{1}{F^{-\epsilon}(E)} \sum_l t_{kl} g_\epsilon(l, i, j; E).
\] (B·2)

If we introduce a momentum representation of \(g_\epsilon\):
\[
\bar{g}_\epsilon(p, i, j; E) = \sum_k g_\epsilon(k, i, j; E) \exp \{-i p \cdot R_{kl}\},
\] (B·3)

(B·2) becomes
\[
\bar{g}_\epsilon(p, i, j; E) = \frac{1}{F^{-\epsilon}(E)} \sum_k \sum_l t_{kl} g_\epsilon(l, i, j; E) \exp \{-i p \cdot R_{kl}\} + G_\epsilon^-(i, j; E),
\] (B·4)

where it is to be noted that (B·2) is correct for \(k \neq i\) and that
\[
g_\epsilon(i, i, j; E) = G_\epsilon^-(i, j; E).
\] (B·5)

From (B·4) we obtain
\[
\bar{g}_\epsilon(p, i, j; E) = \frac{1}{F^{-\epsilon}(E)} \sum_k \sum_l t_{kl} g_\epsilon(l, i, j; E) \exp \{-i p \cdot R_{kl}\}
\]
and hence

\[ g_e(p, i, j; E) = \frac{1}{F_{-e}(E)} \left\{ t_p g_e(p, i, j; E) - \frac{1}{N} \sum_p t_p g_e(p, i, j; E) \right\} + G_e^-(i, j; E), \] (B.7)

from which it follows that

\[ g_e(p, i, j; E) = \frac{1}{1 - \frac{t_p}{F_{-e}(E)}} \times \left\{ G_e^-(i, j; E) - \frac{1}{F_{-e}(E)} \frac{1}{N} \sum_p t_p g_e(p, i, j; E) \right\}. \] (B.8)

Multiplying the both sides of that equation with \( t_p \) and summing over \( p \), we easily obtain (4.20), if we note the relation

\[ \sum_k t_{ik} g_e(k, i, j; E) = \frac{1}{N} \sum_p t_p g_e(p, i, j; E). \] (B.9)

References

3) A. Sakurai, Prog. Theor. Phys. 39 (1968), 312.