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Functional-derivative study of the Hubbard model. I. Perturbation method and first-order approximation*

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In order to study the properties of the Hubbard model for narrow bands, a systematic treatment of the equations of motion of the Green's functions appropriate to that model has been developed. Higher-order Green's functions are reduced to functional derivatives of the basic Green's function G and calculated iteratively in a perturbation scheme which takes the Hubbard I solution G_0 as the zeroth-order Green's function. A zeroth-order approximation to the self-energy correction obtained by inserting G_0 into the functional derivatives is compared with various existing solutions. The perturbation scheme is further extended to an infinite order and the self-energy is calculated exactly up to terms linear in the hopping motion ϵ, a result which has not been obtained previously. The self-energy correction in this final result is drastically different from the zeroth-order solution, demonstrating the importance of the infinite-order iterative procedure. Finally, the electron correlations included in the final result are discussed in terms of diagrams.

I. INTRODUCTION

A correct description of the state of d electrons in transition metals has been the subject of considerable discussion in the theory of magnetism.[1] In metals, d electrons are considered itinerant and so contribute to the Fermi surface and to the electric conductivity. To explain the insulating properties observed in many oxides of transition elements, on the other hand, Mott[2] has postulated that d electrons in these materials are normally localized and do not introduce a Fermi surface or a metallic conductivity. As their density increases, however, the d electrons become itinerant, giving rise to metallic behavior.

Hubbard[3,4] has described the insulating and metallic states as well as the metal-nonmetal transition on the basis of a very simple model. In the presence of a strong intra-atomic repulsive interaction I, a narrow band of d electrons splits into two and, if the lower band is filled and the upper band empty with a finite energy gap between the two, the lattice is an insulator. As the density increases, the bandwidth $2D$ increases and the gap decreases and eventually vanishes, yielding a metallic state with two overlapping subbands.

Although the Hubbard treatment has been regarded as one of the most promising approaches to d electrons in transition metals, many puzzling questions on the nature of the solutions are unanswered. For instance, if the lower (or upper) band is partly filled, the lattice would be metallic. According to Herring,[1] however, in Hubbard's solution the ratio between the Fermi-surface volume and the number of electrons deviates from the value predicted for weakly interacting normal electrons and the discrepancy becomes a factor of 2 when the number of electrons N is nearly equal to the number of atoms N_a forming the lattice. This is contradictory to Luttinger's theorem[5] that the Fermi-surface volume is unchanged by electron interactions to all orders of perturbation. One might, of course, argue that the conventional many-body perturbation approach on which Luttinger's theorem is based is not dependable in the narrow-band region where the Hubbard approximation is valid. However, the abnormal behavior of the Fermi-surface volume in the Hubbard solutions persists even when the density of electrons and the bandwidth increase and the lattice becomes metallic with two overlapping subbands.[6] There exists no experimental evidence to support the Hubbard metallic state.

The Hubbard insulating state appears only if the lower band is completely filled and the upper band remains empty. This simple picture has a drawback. Since the maximum number of electrons the lower band can accept N_{max} is not necessarily equal to the number of atoms N_a, the lattice with one electron per atom may not be an insulator, even though this is the most probable case.[1]

To answer the foregoing questions, one needs to obtain a more accurate solution to the Hubbard-model Hamiltonian. The equation-of-motion approach has been successful in many problems involving phase transitions in predicting the correct behavior over wide ranges of temperature while conventional many-body perturbation methods have failed. Nevertheless, the validity of results obtained by this approach is often questioned because the decoupling approximations used in solving the equations are ill justified and there has been no systematic way to improve the approximation. The Hubbard treatment based on decoupling approximations is no exception.

The conventional perturbation method appropriate for metals fails to exhibit the Hubbard splitting of a narrow band.[7] Moreover, perturbation expansions developed in the atomic limit involve numerous complications due to the spin and possibly spatial degeneracy in the unperturbed ground state.[8] In Hubbard's alloy analogy,[4] the narrow-band problem is replaced by an alloy problem which is treated approximately. In fact, Soven's result[9] in the coherent-potential approximation (CPA) for disordered binary alloys is identical to the Hubbard III solution.[10] Unfortunately, systematic improvement of the alloy analogy and of the CPA solution calculated under the single-site approximation is as difficult as systematic improvement of the decoupling approximation in the equation-of-motion approach.

However, the alloy analogy suggests that, in each set of the multiple-scattering processes, an electron with spin σ sees a two-valued potential which is dynamically determined according to whether the site is occupied by another electron with opposite spin $\bar{\sigma}$ at the time the electron σ hops into the site and that it is very important to take this effect into account explicitly. In the Hubbard treatments as well as in the CPA results, this effect is included whenever an electron returns to an original site but, when the electron hops to neighboring sites, the effect is neglected and the dynamical process is replaced by an average static potential. To improve the existing methods by including the dynamical process explicitly at all sites in the lattice, higher-order Green's functions have to be treated in exactly the same manner as the single-particle Green's function G.

The purpose of the present and the following paper[11] is strictly limited to developing a new perturbation technique in such a way that the dynamical correlations mentioned above can be included at each site of the lattice and the equations of motion can be solved systematically. Discussion of the properties of the Hubbard model calculated by this method will be summarized in a third paper.[12] Attention is limited to the nonmagnetic solution at $T = 0\ ^\circ\mathrm{K}$. The method is based on the functional-derivative technique originally proposed by Schwinger[13] which, in the present case, reduces the higher-order Green's functions involved in the equations of motion of basic Green's functions G to functional derivatives of G with respect to an infinitesimal external field describing electronic hopping.[14] Since the number of Green's functions involved is the same as the number of equations, the latter can, in principle, be solved. In practice, approximation schemes are required, and we adopt an iterative approach here. The zeroth-order solution G^0 is given by solving the set of equations after neglecting functional derivatives. The functional derivatives and hence the self-energy correction to G^0 are now computed by using G^0, yielding an improved solution $G^{(1)}$. Use of $G^{(1)}$ in computing the functional derivatives gives a further improved solution $G^{(2)}$ and so on.

Kadanoff and Baym[15] have proved that the iterative approach is equivalent to a conventional perturbation expansion and yields a complete set of diagrams if the equation of motion for the single-particle Green's function $G_{RR'\sigma} \equiv \langle\langle C_{R\sigma}; C^\dagger_{R'\sigma}\rangle\rangle$ is used and if the zeroth-order Green's function is defined as the solution of the equation in the absence of the interaction. In the above expression, $C^\dagger_{R\sigma}$ and $C_{R\sigma}$ are the creation and destruction operators of an electron with spin σ at the atomic site R. For the Hubbard model, we propose instead to use the two equations of motion for the two Green's functions $\langle\langle C_{R\sigma} N^{(\pm)}_{R\bar{\sigma}}; C^\dagger_{R'\sigma}\rangle\rangle \equiv \Gamma^{(\pm)}$, where $N^{(+)}_{R\sigma} = N_{R\sigma} = C^\dagger_{R\sigma} C_{R\sigma}$; $N^{(-)}_{R\sigma} = 1 - N_{R\sigma}$, and spin $\bar{\sigma}$ is opposite to σ.

The main advantage of this method over conventional many-body perturbation methods and the Kadanoff-Baym method is that the Hubbard I solution can be taken as the zeroth-order Green's function G^0, which includes the dynamical correlation at site R explicitly, and in which a narrow band is split into two. Functional derivatives are calculated by using the G^0 and hence, in the resulting higher-order Green's functions, the dynamical correlation are explicitly included at each site where multiple-scattering processes are being calculated. The equations of motion for the basic Green's functions can now be solved systematically up to any order of accuracy, thus fulfilling the main object of this paper.

We shall outline how the functional-derivative technique can be applied to the Hubbard model in Sec. II and derive explicit expressions needed for calculating the functional derivatives and the self-energy corrections in Sec. III. The zeroth-order calculation in Sec. IV illustrates how various types of functional derivatives are calculated, while in Sec. V we repeat the iterative procedure on selected terms infinite times and calculate the inverse Green's function G^{-1} correctly through terms linear in the hopping parameter ϵ, a result which has not previously been obtained. The self-energy correction obtained in the zeroth-order calculation in Sec. IV is modified drastically in this final result, demonstrating the importance of the infinite-order iterative procedure. As we shall discuss in the third paper, this difference will also be critical for maintaining the stability of the Hubbard lattice. Although serious difficulties still remain in the final result, it will no longer be feasible or advisable to improve the accuracy of the self-energy correction in a straightforward manner, through terms quadratic in the hopping parameters for instance. In Paper II, instead, we shall describe a self-consistent method of improving the accuracy so that a more reliable energy spectrum can be calculated.

II. FUNCTIONAL DERIVATIVE APPROACH TO THE HUBBARD MODEL

Let us consider the Hubbard Hamiltonian

$$\mathcal{H} = \sum_{R,R',\sigma} \epsilon_{RR'} C^\dagger_{R\sigma} C_{R'\sigma} + I \sum_R N_{R\sigma} N_{R\bar{\sigma}},$$

$$\epsilon_{RR} = 0 \quad (2.1)$$

in the presence of a small external field;

$$\mathcal{H}' = \sum_{R,R',\sigma} \delta\epsilon(RR'\sigma t) C^\dagger_{R\sigma}(t) C_{R'\sigma}(t);$$

$$\delta\epsilon(RR'\sigma t) = \begin{cases} \delta\epsilon(R'R\sigma t)^*, \\ 0 \quad \text{if } R'=R. \end{cases} \quad (2.2)$$

Here $\epsilon_{RR'}$ is the hopping matrix element, and I is the intra-atomic interaction between two electrons with opposite spins σ and $\bar{\sigma}$ at the same site R.

According to Kadanoff and Baym,[15] the one-particle Green's function is defined in the imaginary time interval $0 \sim -i\beta$ as

$$G_{RR'\sigma}(tt') \equiv \langle\langle C_{R\sigma}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle \equiv \frac{1}{i} \frac{\langle T[S C_{R\sigma}(t) C^\dagger_{R'\sigma}(t')]\rangle}{\langle T[S]\rangle}. \quad (2.3)$$

We introduce also the two-particle Green's functions

$$\Gamma^{(\pm)}_{RR'\sigma}(tt') \equiv \langle\langle C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle \equiv \frac{1}{i} \frac{\langle T[S C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')]\rangle}{\langle T[S]\rangle}, \quad (2.4)$$

where $N^{(+)}_{R\sigma} \equiv N_{R\sigma} = C^\dagger_{R\sigma} C_{R\sigma}$, $N^{(-)}_{R\sigma} \equiv 1 - N_{R\sigma}$, T means imaginary time ordering, and β is the inverse temperature, while the operator S is given by

$$S = \exp\left(-i \int_0^{-i\beta} dt \sum_{R_1,R_2,\sigma} \delta\epsilon(R_1 R_2 \sigma t) \times C^\dagger_{R_1\sigma}(t) C_{R_2\sigma}(t)\right). \quad (2.5)$$

We now want to construct the equations of motion for $\Gamma^{(\pm)}$ and rearrange them in the form

$$\left(i \frac{\partial}{\partial t} + W^{(\pm)}\right) \Gamma^{(\pm)}_{RR'\sigma}(tt') = \langle N^{(\pm)}_{\bar{\sigma}}(t)\rangle \delta_{tt'} \delta_{RR'} \quad (2.6)$$

to make transparent the uniqueness of the formal solutions. This is carried out in the following two steps:

Step 1. Use of the relation

$$i \frac{\partial}{\partial t} C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) = [C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t), \mathcal{H} + \mathcal{H}'] \quad (2.7)$$

yields

$$\left(i \frac{\partial}{\partial t} - I\delta^{(\pm)}\right) \langle\langle C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle - \sum_{R''\neq R} \epsilon(RR''\sigma t) \langle\langle C_{R''\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$\mp \sum_{R''\neq R} [\epsilon(RR''\bar{\sigma}t) \langle\langle C_{R\sigma}(t) C^\dagger_{R\bar{\sigma}}(t) C_{R''\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$- \epsilon(R''R\bar{\sigma}t) \langle\langle C_{R\sigma}(t) C^\dagger_{R''\bar{\sigma}}(t) C_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle] = \langle N^{(\pm)}_{R\bar{\sigma}}(t)\rangle \delta_{RR'} \delta_{tt'}, \quad (2.8)$$

where $\delta^{(+)} = 1$, $\delta^{(-)} = 0$, and

$$\epsilon(RR'\sigma t) = \epsilon_{RR'} + \delta\epsilon(RR'\sigma t). \quad (2.9)$$

Step 2. In Eq. (2.8), the derivative $i(\partial/\partial t)$ has operated on $C_{R\sigma}(t)$ and $N^{(\pm)}_{R\bar{\sigma}}(t)$ involved in $\Gamma^{(\pm)}$ and has modified $\Gamma^{(\pm)}$ to

$$\langle\langle C_{R''\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle, \quad \langle\langle C_{R\sigma}(t) C^\dagger_{R\bar{\sigma}}(t) C_{R''\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle, \quad \text{or} \quad \langle\langle C_{R\sigma}(t) C^\dagger_{R''\bar{\sigma}}(t) C_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle.$$

These changes may be reproduced by using the fact that an infinitesimal change $\delta\epsilon$ in ϵ introduces a change in S and hence changes in $\Gamma^{(\pm)}$:

$$i\delta\Gamma^{(\pm)} = i\delta\langle\langle C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$= \int_0^{-i\beta} dt_1 \sum_{R_1,R_2,\sigma_1} \{\langle\langle C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) [C^\dagger_{R_1\sigma_1}(t_1) C_{R_2\sigma_1}(t_1)] C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$- \langle C^\dagger_{R_1\sigma_1}(t_1) C_{R_2\sigma_1}(t_1)\rangle \langle\langle C_{R\sigma}(t) N^{(\pm)}_{R\bar{\sigma}}(t) C^\dagger_{R'\sigma}(t')\rangle\rangle\} \delta\epsilon(R_1 R_2 \sigma_1 t_1), \quad (2.10)$$

where $\langle C^\dagger_{R_1\sigma_1}(t_1) C_{R_2\sigma_1}(t_1)\rangle$ is shorthand for

$$-\langle T[SC_{R_2\sigma_1}(t_1)C^\dagger_{R_1\sigma_1}(t_1^+)]\rangle/\langle T[S]\rangle = iG_{R_2R_1\sigma_1}(t_1t_1^+)\,, \tag{2.11}$$

and similarly for $\langle N^{(\pm)}_{R\bar\sigma}(t)\rangle$, etc., and is not a simple thermodynamical average.

More explicitly,

$$i\left(\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \langle\langle C_{R''\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,, \tag{2.12}$$

$$i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^-)}\langle\langle C_{R\sigma}(t)N^{(+)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \langle\langle C_{R\sigma}(t)C^\dagger_{R\bar\sigma}(t^-)C_{R''\bar\sigma}(t^-)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$-\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle\langle\langle C_{R\sigma}(t)N^{(+)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,, \tag{2.13}$$

$$i\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^+)}\langle\langle C_{R\sigma}(t)N^{(+)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \langle\langle C^\dagger_{R''\bar\sigma}(t^+)C_{R\bar\sigma}(t^+)C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$-\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle\langle\langle C_{R\sigma}(t)N^{(+)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,, \tag{2.14}$$

$$i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^+)}\langle\langle C_{R\sigma}(t)N^{(-)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \langle\langle C^\dagger_{R\bar\sigma}(t^+)C_{R''\bar\sigma}(t^+)C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$-\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle\langle\langle C_{R\sigma}(t)N^{(-)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,, \tag{2.15}$$

$$i\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^-)}\langle\langle C_{R\sigma}(t)N^{(-)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \langle\langle C_{R\sigma}(t)C^\dagger_{R''\bar\sigma}(t^-)C_{R\bar\sigma}(t^-)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$-\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle\langle\langle C_{R\sigma}(t)N^{(-)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,. \tag{2.16}$$

Note that if t^- is replaced by t^+ in Eqs. (2.13) and (2.16), the first terms on the right-hand sides are replaced by corresponding terms which vanish because $C^\dagger_{R\bar\sigma}(t^+)C_{R''\bar\sigma}(t^+)N_{R\bar\sigma}(t)=0$, etc. The same is true in Eqs. (2.14) and (2.15), and hence the choices of t^+ and t^- in the above equations are unique.

By inserting Eqs. (2.12)–(2.16) into Eq. (2.8), we find the desired equations

$$\Bigg[i\frac{\partial}{\partial t}-I\delta^{(\pm)}-\sum_{R''\neq R}\epsilon(RR''\sigma t)\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\mp\sum_{R''\neq R}\epsilon(RR''\bar\sigma t)\left(\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle+i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^\mp)}\right)$$
$$\pm\sum_{R''\neq R}\epsilon(R''R\bar\sigma t)\left(\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle+i\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^\pm)}\right)\Bigg]\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \langle N^{(\pm)}_{R\bar\sigma}(t)\rangle\delta_{RR'}\delta_{tt'}\,, \tag{2.17}$$

which has the form of Eq. (2.6). The basic idea involved in the foregoing derivation is to replace $i(\partial/\partial t)$ in part by $i(\delta/\delta\epsilon)$ in $W^{(\pm)}$. For instance,

$$\langle\langle C_{R\sigma}(t)C^\dagger_{R\bar\sigma}(t)\left(i\frac{\partial}{\partial t}C_{R\bar\sigma}(t)\right)C^\dagger_{R'\sigma}(t')\rangle\rangle = \sum_{R''}\epsilon(RR''\bar\sigma t)\left(\langle C^\dagger_{R\bar\sigma}C_{R''\bar\sigma}\rangle+i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^-)}\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle. \tag{2.18}$$

It looks as if the two equations for $\Gamma^{(+)}$ and $\Gamma^{(-)}$ given by Eq. (2.17) may be solved independently of each other. If, for instance, functional derivatives $\delta/\delta\epsilon$ involved in Eq. (2.17) are neglected, the equation for $\Gamma^{(+)}$ becomes

$$\left(i\frac{\partial}{\partial t}-I-\sum_{R''\neq R}\left[\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle-\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle\right]\right)\Gamma^{(+)}_{RR'\sigma}(tt') = \langle N^{(+)}_{R\bar\sigma}(t)\rangle\delta_{RR'}\delta_{tt'}\,. \tag{2.19}$$

The approximate solution $\Gamma^{(+)}_{a0}$ obtained from Eq. (2.19) may be used in calculating functional derivatives involved in Eq. (2.17). This would yield an approximate expression for the self-energy correction $\Sigma^{(+)}_{a1}$ introduced later and hence an improved solution $\Gamma^{(+)}_{a1}$; $\Gamma^{(+)}_{a1}$ could then be used to compute an improved $\Gamma^{(+)}_{a2}$ by Eq. (2.17) and so on. However, since the large parentheses in Eq. (2.19) do not involve $\epsilon(RR''\sigma t)$ explicitly, the derivative $\delta\Gamma^{(+)}_{a0}/\delta\epsilon(RR''\sigma t^\pm)$ is small and the hopping motion of electrons with the same spin σ could not be included easily in such an approximation scheme based on $\Gamma^{(\pm)}_{a0}$.

In the following, we shall develop an iterative perturbation method similar to the one just outlined. However, instead of $\Gamma^{(\pm)}_{a0}$ or the Hartree-

Fock solution G_{HF}, the Hubbard I solution will be used as the zeroth order solution G_0. Since the Hubbard I solution includes the hopping motion as well as the dynamical correlation due to the two-valued potential at site R and is correct both in the atomic and free-electron limits in zeroth order, our iterative perturbation method is expected to converge rapidly and to yield reliable results for narrow-band systems. The principle of the calculation is simple. Let us assume that all derivatives $\delta/\delta\epsilon$ in Eq. (2.17) are zero and solve the two equations. In the limit of negligibly small external field $\delta\epsilon = 0$, the solution is equivalent to the Hubbard I solution,

$$2\pi[G_0(k\sigma,\omega)]^{-1}|_{\delta\epsilon\to 0} = \omega - \epsilon_k - \frac{I n_{\bar\sigma}\omega}{\omega - (1-n_{\bar\sigma})I}\,, \qquad (2.20)$$

where ϵ_k is the Fourier transform of $\epsilon_{RR'}$, and $n_{\bar\sigma}$ is the value of $\langle N_{R\bar\sigma}(t)\rangle$ in the limit of $\delta\epsilon = 0$. The G_0 or the corresponding $\Gamma_0^{(\pm)}$ may be used in calculating the derivatives involved in Eq. (2.17), which, in turn, yield improved solutions G_1 and $\Gamma_1^{(\pm)}$ to be used again in calculating the derivatives. By repeating the iterative process, all possible terms in the perturbation series will be generated without any ambiguity.

III. CALCULATION OF SELF-ENERGY CORRECTIONS

The iterative process described in the proceeding section can be carried out more conveniently when derivatives $\delta\Gamma^{(\pm)}/\delta\epsilon$ are transformed to derivatives of the one-electron Green's function $\delta G/\delta\epsilon$ by replacing $\Gamma^{(\pm)}$ by G. The calculation of G can then be performed without using Γ. Derivatives with respect to charge transfers of opposite spin $\bar\sigma$, $\delta\Gamma^{(\pm)}/\delta\epsilon(R_1R_2\bar\sigma t^{\pm})$, can be converted to $\delta G/\delta\epsilon(R_1R_2\bar\sigma t^{\pm})$ immediately by using the property of the projection operators $N^{(\pm)}_{R\bar\sigma}(t)$ as follows:

$$\left(\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle + i\,\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^{\mp})}\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \left(\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle + i\,\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^{\mp})}\right)\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,, \qquad (3.1)$$

$$\left(\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle + i\,\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^{\pm})}\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \left(\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle + i\,\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^{\pm})}\right)\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\,. \qquad (3.2)$$

To convert $\delta\Gamma^{(\pm)}/\delta\epsilon(RR''\sigma t^{\pm})$ to $\delta G/\delta\epsilon(RR''\sigma t^{\pm})$, we need to compare Eq. (2.17) with the equation of motion for G:

$$i\,\frac{\partial}{\partial t}\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle - \sum_{R''\neq R}\epsilon(RR''\sigma t)\langle\langle C_{R''\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle - I\langle\langle C_{R\sigma}(t)N_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle = \delta_{tt'}\delta_{RR'}\,. \qquad (3.3)$$

If one subtracts from Eq. (2.17) the expression in Eq. (3.3) multiplied by $n^{(\pm)}_{\bar\sigma} \equiv \langle N^{(\pm)}_{R\bar\sigma}\rangle$, one obtains

$$\begin{aligned}
&\left(i\,\frac{\partial}{\partial t} - (1-n_{\bar\sigma})I\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle \\
&\quad = \left(i\,\frac{\partial}{\partial t} - I(1-\delta^{(\pm)})\right)n^{(\pm)}_{\bar\sigma}\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle \\
&\qquad + \sum_{R''\neq R}\epsilon(RR''\sigma t)\left[-n^{(\pm)}_{\bar\sigma}\langle\langle C_{R''\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle + \left(i\,\frac{\delta}{\delta\epsilon(RR''\sigma t^{-})} - i\,\frac{\delta}{\delta\epsilon(RR''\sigma t^{+})}\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\right] \\
&\qquad \pm \sum_{R''\neq R}\left[\epsilon(RR''\bar\sigma t)\left(\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle + i\,\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^{\mp})}\right) - \epsilon(R''R\bar\sigma t)\left(\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle + i\,\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^{\pm})}\right)\right] \\
&\qquad \times\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle + [\langle N^{(\pm)}_{R\bar\sigma}(t)\rangle - n^{(\pm)}_{\bar\sigma}]\delta_{RR'}\delta_{tt'}\,,
\end{aligned} \qquad (3.4)$$

where $n_{\bar\sigma} = n^{(+)}_{\bar\sigma}$ and $n^{(-)}_{\bar\sigma}$ are the values of $\langle N^{(\pm)}_{R\bar\sigma}(t)\rangle$ calculated in the limit of $\delta\epsilon = 0$ and hence $\delta n^{(\pm)}_{\bar\sigma}/\delta\epsilon = 0$. Use of Eq. (2.12) and the trivial relation $N^{(\pm)}_{R\bar\sigma}(t) = n^{(\pm)}_{\bar\sigma} + [N^{(\pm)}_{R\bar\sigma}(t) - n^{(\pm)}_{\bar\sigma}]$ yields

$$\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$

$$=n^{(\pm)}_{\bar\sigma}\langle\langle C_{R''\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle+\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\langle\langle C_{R\sigma}(t)[N^{(\pm)}_{R\bar\sigma}(t)-n^{(\pm)}_{\bar\sigma}]C^\dagger_{R'\sigma}(t')\rangle\rangle\ . \quad (3.5)$$

By inserting Eq. (3.5) and Eqs. (2.13)–(2.16) into Eq. (3.4), we obtain

$$\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle=n^{(\pm)}_{\bar\sigma}\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$\pm[w-(1-n_{\bar\sigma})I]^{-1}\{B_{\bar\sigma}(Rt)I\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle+\Delta^{(\pm)}_{RR'\sigma}(tt')\pm[\langle N^{(\pm)}_{R\bar\sigma}(t)\rangle-n^{(\pm)}_{\bar\sigma}]\delta_{RR'}\delta_{tt'}\}\ , \quad (3.6)$$

where

$$w=i\frac{\partial}{\partial t}\ , \quad (3.7)$$

$$\Delta^{(\pm)}_{RR'\sigma}(tt')=\pm\sum_{R''\neq R}\epsilon(RR''\sigma t)\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\langle\langle C_{R\sigma}(t)[N^{(\pm)}_{R\bar\sigma}(t)-n^{(\pm)}_{\bar\sigma}]C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$+\sum_{R''\neq R}\left(\epsilon(RR''\bar\sigma t)\,i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^{\mp})}-\epsilon(R''R\bar\sigma t)\,i\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^{\pm})}\right)\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\ , \quad (3.8)$$

$$B_{\bar\sigma}(Rt)=n_{\bar\sigma}(1-n_{\bar\sigma})+\frac{1}{I}\sum_{R''\neq R}[\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle-\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle]\ . \quad (3.9)$$

By differentiating Eq. (3.6), derivatives $\delta\Gamma^{(\pm)}/\delta\epsilon(RR''\sigma t^{\pm})$ are converted to $\delta G/\delta\epsilon$, $\delta\langle C^\dagger_{R\bar\sigma}C_{R'\bar\sigma}\rangle/\delta\epsilon$, etc., as follows:

$$\frac{\delta\langle\langle C_{R\sigma}(t)[N^{(\pm)}_{R\bar\sigma}(t)-n^{(\pm)}_{\bar\sigma}]C^\dagger_{R'\sigma}(t')\rangle\rangle}{\delta\epsilon(R_1R_2\sigma_1t_1)}=\pm[w-(1-n_{\bar\sigma})I]^{-1}\left(B_{\bar\sigma}(Rt)I\frac{\delta G_{RR'\sigma}(tt')}{\delta\epsilon(R_1R_2\sigma_1t_1)}+\frac{\delta B_{\bar\sigma}(Rt)}{\delta\epsilon(R_1R_2\sigma_1t_1)}IG_{RR'\sigma}(tt')\right.$$
$$\left.+\frac{\delta\Delta^{(\pm)}_{RR'\sigma}(tt')}{\delta\epsilon(R_1R_2\sigma_1t_1)}\pm\frac{\delta\langle N^{(\pm)}_{R\bar\sigma}(t)\rangle}{\delta\epsilon(R_1R_2\sigma_1t_1)}\delta_{RR'}\delta_{tt'}\right)\ . \quad (3.10)$$

Note that $\delta\Delta/\delta\epsilon$ on the right-hand side of Eq. (3.10) still involves $\delta\Gamma/\delta\epsilon$. However, the derivative on the left-hand side $\delta(\Gamma-n_{\bar\sigma}G)/\delta\epsilon$ may be evaluated by neglecting $\delta\Delta/\delta\epsilon$. Use of the result in Eq. (3.8) will yield an approximate value of $\delta\Delta/\delta\epsilon$ and hence an improved $\delta(\Gamma-n_{\bar\sigma}G)/\delta\epsilon$ to be used in Eq. (3.8). By repeating the iterative process, the expression $\delta(\Gamma-n_{\bar\sigma}G)/\delta\epsilon$ can be evaluated correctly. As we shall show in Appendix A, the contribution from $\delta\Delta/\delta\epsilon$ to the self-energy correction Σ is proportional to ϵ^2 or higher order and hence we may neglect it in the following.

We now return to the exact analysis. By using Eqs. (3.1), (3.2), and (3.5), the master equation (2.17) may be rewritten

$$(w-I\delta^{(\pm)})\langle\langle C_{R\sigma}(t)N^{(\pm)}_{R\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle-n^{(\pm)}_{\bar\sigma}\sum_{R''\neq R}\epsilon(RR''\sigma t)\langle\langle C_{R''\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$\mp\sum_{R''\neq R}[\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle-\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle]\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle\mp\Delta^{(\pm)}_{RR'\sigma}(tt')=\langle N^{(\pm)}_{R\bar\sigma}(t)\rangle\delta_{RR'}\delta_{tt'}\ . \quad (3.11)$$

If we insert the formal expressions for $\Gamma^{(+)}$ and $\Gamma^{(-)}$ given in Eq. (3.11) into the trivial relation $G=\Gamma^{(+)}+\Gamma^{(-)}$, we find that

$$F_{\bar\sigma}(Rt)G_{RR'\sigma}(tt')-F_{\bar\sigma}(Rt)[F_{\bar\sigma}(0)]^{-1}\sum_{R''\neq R}\epsilon(RR''\sigma t)G_{R''R'\sigma}(tt')$$
$$-\lambda_{\bar\sigma}(Rt)\sum_{R''\neq R}[\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle-\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle]\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$
$$-F_{\bar\sigma}(Rt)[(w-I)^{-1}\Delta^{(+)}_{RR'\sigma}(tt')-w^{-1}\Delta^{(-)}_{RR'\sigma}(tt')]=\delta_{RR'}\delta_{tt'}\ , \quad (3.12)$$

where

$$F_{\bar\sigma}(Rt)=[(w-I)^{-1}\langle N_{R\bar\sigma}(t)\rangle+w^{-1}\langle 1-N_{R\bar\sigma}(t)\rangle]^{-1}\,, \tag{3.13}$$

$$F_{\bar\sigma}(0)=[(w-I)^{-1}n_{\bar\sigma}+w^{-1}(1-n_{\bar\sigma})]^{-1}\,, \tag{3.14}$$

$$\lambda_{\bar\sigma}(Rt)=F_{\bar\sigma}(Rt)[(w-I)^{-1}-w^{-1}],\quad \lambda_{\bar\sigma}(0)=F_{\bar\sigma}(0)[(w-I)^{-1}-w^{-1}]\,. \tag{3.15}$$

Let us now define the inverse of $G_{RR'\sigma}(tt')$ by

$$\int_0^{-i\beta}dt_1\sum_{R_1}G_{RR_1\sigma}(tt_1)G^{-1}_{R_1R'\sigma}(t_1t')=\delta_{RR'}\delta_{tt'}\,. \tag{3.16}$$

Equation (3.12) is then rewritten

$$\begin{aligned}G^{-1}_{RR'\sigma}(tt')=&F_{\bar\sigma}(Rt)\delta_{RR'}\delta_{tt'}-F_{\bar\sigma}(Rt)[F_{\bar\sigma}(0)]^{-1}\sum_{R''\neq R}\epsilon(RR''\sigma t)\delta_{R''R'}\delta_{tt'}\\&-\lambda_{\bar\sigma}(Rt)\sum_{R''\neq R}[\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle-\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}\\&-F_{\bar\sigma}(Rt)\int_0^{-i\beta}dt_1\sum_{R_1}[(w-I)^{-1}\Delta^{(+)}_{RR_1\sigma}(tt_1)-w^{-1}\Delta^{(-)}_{RR_1\sigma}(tt_1)]G^{-1}_{R_1R'\sigma}(t_1t')\,.\end{aligned} \tag{3.17}$$

Since the unperturbed Green's function G_0 is defined as the solution of Eq. (3.12) with $\Delta^{(\pm)}=0$, the inverse $(G_0)^{-1}$ can be written

$$\begin{aligned}(G_0)^{-1}_{RR'\sigma}(tt')=&F_{\bar\sigma}(Rt)\delta_{RR'}\delta_{tt'}-F_{\bar\sigma}(Rt)[F_{\bar\sigma}(0)]^{-1}\epsilon(RR'\sigma t)\delta_{tt'}\\&-\lambda_{\bar\sigma}(Rt)\sum_{R''\neq R}[\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle-\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}\,,\end{aligned} \tag{3.18}$$

and the self-energy Σ defined by

$$G^{-1}_{RR'\sigma}(tt')=(G_0)^{-1}_{RR'\sigma}(tt')-\Sigma_{RR'\sigma}(tt')\,, \tag{3.19}$$

is thus given by

$$\Sigma_{RR'\sigma}(tt')=F_{\bar\sigma}(Rt)\int_0^{-i\beta}dt_1\sum_{R_1}[(w-I)^{-1}\Delta^{(+)}_{RR_1\sigma}(tt_1)-w^{-1}\Delta^{(-)}_{RR_1\sigma}(tt_1)]G^{-1}_{R_1R'\sigma}(t_1t')\,. \tag{3.20}$$

The above expression for the self-energy Σ may be evaluated by inserting Eqs. (3.8) and (3.10). The result is

$$\begin{aligned}\Sigma_{RR'\sigma}(tt')=\Bigg\{&\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)\sum_{R''\neq R}\epsilon(RR''\sigma t)\int_0^{-i\beta}dt_1\sum_{R_1}B_{\bar\sigma}(Rt)\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)G_{RR_1\sigma}(tt_1)\\&+F_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)\,I^{-1}\sum_{R''\neq R}\epsilon(RR''\sigma t)\int_0^{-i\beta}dt_1\sum_{R_1}\Bigg[(w-I)^{-1}\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\Delta^{(+)}_{RR_1\sigma}(tt_1)\\&\qquad-w^{-1}\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right)\Delta^{(-)}_{RR_1\sigma}(tt_1)\Bigg]\\&+F_{\bar\sigma}(Rt)\int_0^{-i\beta}dt_1\sum_{R_1}\sum_{R''\neq R}\Bigg[\epsilon(RR''\bar\sigma t)\left((w-I)^{-1}i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^-)}-w^{-1}i\frac{\delta}{\delta\epsilon(RR''\bar\sigma t^+)}\right)G_{RR_1\sigma}(tt_1)\\&\qquad-\epsilon(R''R\bar\sigma t)\left((w-I)^{-1}i\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^+)}\right.\\&\qquad\left.-w^{-1}i\frac{\delta}{\delta\epsilon(R''R\bar\sigma t^-)}\right)G_{RR_1\sigma}(tt_1)\Bigg]\Bigg\}G^{-1}_{R_1R'\sigma}(t_1t')\,,\end{aligned} \tag{3.21}$$

where

$$\lambda_{\bar\sigma}(0)=[w-(1-n_{\bar\sigma})I]^{-1}I\,. \tag{3.22}$$

Note that $\delta B/\delta\epsilon$ and $\delta\langle N\rangle/\delta\epsilon$ involved in Eq. (3.10) do not contribute to Σ since

$$\delta\langle N_{R\bar\sigma}(t)\rangle/\delta\epsilon(RR''\sigma t^+)=\delta\langle N_{R\bar\sigma}(t)\rangle/\delta\epsilon(RR''\sigma t^-)\,,\quad \delta B_{\bar\sigma}(Rt)/\delta\epsilon(RR''\sigma t^+)=\delta B_{\bar\sigma}(Rt)/\delta\epsilon(RR''\sigma t^-)\,. \tag{3.23}$$

Since the calculation of $\delta G_0^{-1}/\delta\epsilon$ by using Eq. (3.18) is trivial and easier than the calculation of $\delta G_0/\delta\epsilon$, Eq. (3.21) will become more convenient if the derivatives operating over G are shifted to G^{-1} by the relation

$$\int_0^{-i\beta} dt_3 \sum_{R_3} \frac{\delta G_{RR_3\sigma}(tt_3)}{\delta\epsilon(R_1R_2\sigma_1t_1)}\, G^{-1}_{R_3R'\sigma}(t_3t') = -\int_0^{-i\beta} dt_3 \sum_{R_3} G_{RR_3\sigma}(tt_3)\, \frac{\delta G^{-1}_{R_3R'\sigma}(t_3t')}{\delta\epsilon(R_1R_2\sigma_1t_1)}\,, \tag{3.24}$$

which is obtained by differentiating Eq. (3.16). Equation (3.21) is then written

$$\begin{aligned}\Sigma_{RR'\sigma}(tt') = \int_0^{-i\beta} dt_1 \sum_{R_1}\sum_{R_2\neq R} \Bigg[& \lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)B_{\bar\sigma}(Rt)(-i)G_{RR_1\sigma}(tt_1)\epsilon(RR_2\sigma t)\left(\frac{\delta}{\delta\epsilon(RR_2\sigma t^-)}-\frac{\delta}{\delta\epsilon(RR_2\sigma t^+)}\right)\\ &+(-i)G_{RR_1\sigma}(tt_1)\epsilon(RR_2\bar\sigma t)F_{\bar\sigma}(Rt)\left((w-I)^{-1}\frac{\delta}{\delta\epsilon(RR_2\bar\sigma t^-)}-w^{-1}\frac{\delta}{\delta\epsilon(RR_2\bar\sigma t^+)}\right)\\ &-(-i)G_{RR_1\sigma}(tt_1)\epsilon(R_2R\bar\sigma t)F_{\bar\sigma}(Rt)\left((w-I)^{-1}\frac{\delta}{\delta\epsilon(R_2R\bar\sigma t^+)}-w^{-1}\frac{\delta}{\delta\epsilon(R_2R\bar\sigma t^-)}\right)\Bigg]\\ &\times[(G_0)^{-1}_{R_1R'\sigma}(t_1t')-\Sigma_{R_1R'\sigma}(t_1t')]+\pi[\Delta_{RR'\sigma}(tt')]\,,\end{aligned} \tag{3.25}$$

where

$$\begin{aligned}\pi[\Delta_{RR'\sigma}(tt')] = \int_0^{-i\beta} dt_1 \sum_{R_1}\sum_{R_2\neq R} & \lambda_{\bar\sigma}(0)\epsilon(RR_2\sigma t)F_{\bar\sigma}(Rt)I^{-1}\\ &\times\left\{(w-I)^{-1}\left(i\frac{\delta}{\delta\epsilon(RR_2\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR_2\sigma t^+)}\right)\Delta^{(+)}_{RR_1\sigma}(tt_1)\right.\\ &\left.-w^{-1}\left(i\frac{\delta}{\delta\epsilon(RR_2\sigma t^-)}-i\frac{\delta}{\delta\epsilon(RR_2\sigma t^+)}\right)\Delta^{(-)}_{RR_1\sigma}(tt_1)\right\}G^{-1}_{R_1R'\sigma}(t_1t')\,.\end{aligned} \tag{3.26}$$

Equations (3.25) and (3.18) are the basic equations for generating the self-energy Σ in the present and the following papers. If we insert G_0^{-1} given by Eq. (3.18) into Eq. (3.25) and neglect Σ and $\pi[\Delta_{RR'\sigma}(tt')]$ on the right-hand side of Eq. (3.25), the zeroth-order approximation to the self-energy, say $\Sigma^{(1)}$, is obtained. Use of $\Sigma^{(1)}$ in Eq. (3.25) will generate an improved solution $\Sigma^{(2)}$ and so on. By repeating the iterative process, in principle, an exact expansion of the self-energy will be obtained. As will be discussed in Appendix A, however, the contribution from $\pi[\Delta]$ will be of higher order and will be neglected in the following calculation. We shall calculate the zeroth-order approximate solution $\Sigma^{(1)}$ in Sec. IV and extend it in Sec. V in such a way that the self-energy is given correctly up through terms linear in ϵ.

IV. ZEROTH-ORDER APPROXIMATION TO THE SELF-ENERGY CORRECTION

We shall calculate $\Sigma^{(1)}$, the zeroth-order approximation to the self-energy, by inserting the unperturbed solution G_0^{-1} given by Eq. (3.18) into the working equation (3.25), and by neglecting Σ and $\pi[\Delta]$ on the right-hand side.

Functional derivatives of G_0^{-1} are calculated as

$$\begin{aligned}\frac{\delta(G_0)^{-1}_{R_1R'\sigma}(t_1t')}{\delta\epsilon(R_iR_j\sigma t^\pm)} = &-F_{\bar\sigma}(R_1t_1)[F_{\bar\sigma}(0)]^{-1}\delta_{R_1R_i}\delta_{R'R_j}\delta_{t^\pm t_1}\delta_{t_1t'}\\ &-\lambda_{\bar\sigma}(R_1t_1)\Bigg[\frac{\delta\langle N_{R_1\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\sigma t^\pm)}(G_0)^{-1}_{R_1R'\sigma}(t_1t')\\ &+\sum_{R''\neq R_1}\left(\epsilon(R_1R''\bar\sigma t_1)\frac{\delta\langle C^\dagger_{R_1\bar\sigma}(t_1)C_{R''\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\sigma t^\pm)}-\epsilon(R''R_1\bar\sigma t_1)\frac{\delta\langle C^\dagger_{R''\bar\sigma}(t_1)C_{R_1\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\sigma t^\pm)}\right)\delta_{R_1R'}\delta_{t_1t'}\Bigg]\,,\end{aligned} \tag{4.1}$$

$$\begin{aligned}\frac{\delta(G_0)^{-1}_{R_1R'\sigma}(t_1t')}{\delta\epsilon(R_iR_j\bar\sigma t^\pm)} = &-\lambda_{\bar\sigma}(R_1t_1)\Bigg[\langle C^\dagger_{R_i\bar\sigma}(t^\pm)C_{R_j\bar\sigma}(t^\pm)\rangle(\delta_{R_iR_1}-\delta_{R_jR_1})\delta_{R_1R'}\delta_{t^\pm t_1}\delta_{t_1t'}+\frac{\delta\langle N_{R_1\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t^\pm)}(G_0)^{-1}_{R_1R'\sigma}(t_1t')\\ &+\sum_{R''\neq R_1}\left(\epsilon(R_1R''\bar\sigma t_1)\frac{\delta\langle C^\dagger_{R_1\bar\sigma}(t_1)C_{R''\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t^\pm)}-\epsilon(R''R_1\bar\sigma t_1)\frac{\delta\langle C^\dagger_{R''\bar\sigma}(t_1)C_{R_1\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t^\pm)}\right)\delta_{R_1R'}\delta_{t_1t'}\Bigg]\,.\end{aligned} \tag{4.2}$$

Note that terms involving $\delta\langle N\rangle/\delta\epsilon$ on the right-hand sides of Eqs. (4.1) and (4.2) come from $\delta F_{\bar\sigma}(R_1t_1)/\delta\epsilon$. By inserting the above expression together with $\Sigma=0$ and $\pi[\Delta]=0$ on the right-hand side of Eq. (3.25), we obtain

$$\begin{aligned}\Sigma^{(1)}_{RR'\sigma}(tt') &= \lambda_{\bar\sigma}(Rt)^2B_{\bar\sigma}(Rt)\epsilon(RR'\sigma t)[iG_{RR\sigma}(tt^-)\delta_{t-t'} - iG_{RR\sigma}(tt^+)\delta_{t+t'}]\\ &+\lambda_{\bar\sigma}(Rt)F_{\bar\sigma}(Rt)\Big(\sum_{R''}\epsilon(RR''\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle[(w-I)^{-1}iG_{RR\sigma}(tt^-)-w^{-1}iG_{RR\sigma}(tt^+)]\\ &\qquad+\sum_{R''}\epsilon(R''R\bar\sigma t)\langle C^\dagger_{R''\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle[(w-I)^{-1}iG_{RR\sigma}(tt^+)-w^{-1}iG_{RR\sigma}(tt^-)]\Big)\delta_{RR'}\delta_{tt'}\\ &\qquad-\lambda_{\bar\sigma}(R't)F_{\bar\sigma}(Rt)\{\epsilon(RR'\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R'\bar\sigma}(t)\rangle[(w-I)^{-1}iG_{RR'\sigma}(tt^-)-w^{-1}iG_{RR'\sigma}(tt^+)]\\ &\qquad\qquad+\epsilon(R'R\bar\sigma t)\langle C^\dagger_{R'\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle[(w-I)^{-1}iG_{RR'\sigma}(tt^+)-w^{-1}iG_{RR'\sigma}(tt^-)]\}\delta_{tt'}\\ &+\xi^{(1)}_{RR'\sigma}(tt')+\xi^{(2)}_{RR'\sigma}(tt')\,,\end{aligned}\tag{4.3}$$

where

$$\xi^{(1)}_{RR'\sigma}(tt')=\int_0^{-i\beta}dt_1\sum_{R_1}\sum_{R_2\neq R}\lambda_{\bar\sigma}(R_1t_1)\lambda_{\bar\sigma}(Rt)iG_{RR_1\sigma}(tt_1)\times\left(\epsilon(RR_2\bar\sigma t)\frac{\delta\langle N_{R_1\bar\sigma}(t_1)\rangle}{\delta\epsilon(RR_2\bar\sigma t)}-\epsilon(R_2R\bar\sigma t)\frac{\delta\langle N_{R_1\bar\sigma}(t_1)\rangle}{\delta\epsilon(R_2R\bar\sigma t)}\right)(G_0)^{-1}_{R_1R'\sigma}(t_1t')\,,\tag{4.4}$$

$$\begin{aligned}\xi^{(2)}_{RR'\sigma}(tt')=\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't')iG_{RR'\sigma}(tt')\sum_{R_1\neq R'}\sum_{R_2\neq R}\Bigg(&\epsilon(RR_2\bar\sigma t)\epsilon(R_1R'\bar\sigma t')\frac{\delta\langle C^\dagger_{R'\bar\sigma}(t')C_{R_1\bar\sigma}(t')\rangle}{\delta\epsilon(RR_2\bar\sigma t)}\\ &-\epsilon(RR_2\bar\sigma t)\epsilon(R_1R'\bar\sigma t')\frac{\delta\langle C^\dagger_{R_1\bar\sigma}(t')C_{R'\bar\sigma}(t')\rangle}{\delta\epsilon(RR_2\bar\sigma t)}\\ &-\epsilon(R_2R\bar\sigma t)\epsilon(R'R_1\bar\sigma t')\frac{\delta\langle C^\dagger_{R'\bar\sigma}(t')C_{R_1\bar\sigma}(t')\rangle}{\delta\epsilon(R_2R\bar\sigma t)}\\ &+\epsilon(R_2R\bar\sigma t)\epsilon(R_1R'\bar\sigma t')\frac{\delta\langle C^\dagger_{R_1\bar\sigma}(t')C_{R'\bar\sigma}(t')\rangle}{\delta\epsilon(R_2R\bar\sigma t)}\Bigg)\,.\end{aligned}\tag{4.5}$$

Use of the relations[16]

$$iG_{RR\sigma}(tt^-)=1-\langle N_{R\sigma}(t)\rangle,\quad iG_{RR\sigma}(tt^+)=-\langle N_{R\sigma}(t)\rangle\,,\tag{4.6}$$

reduces Eq. (4.3) to the following form:

$$\begin{aligned}\Sigma^{(1)}_{RR'\sigma}(tt')&=\lambda_{\bar\sigma}(Rt)^2B_{\bar\sigma}(Rt)\epsilon(RR'\sigma t)\delta_{tt'}+\lambda_{\bar\sigma}(Rt)^2\sum_{R''}b^{(+)}(RR''\bar\sigma t)[\tfrac12-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}\\ &+\lambda_{\bar\sigma}(Rt)\mu_{\bar\sigma}(Rt)\sum_{R''}b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'}+\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)b^{(+)}(RR'\bar\sigma t)\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}\\ &+\xi^{(1)}_{RR'\sigma}(tt')+\xi^{(2)}_{RR'\sigma}(tt')\,,\end{aligned}\tag{4.7}$$

where

$$b^{(\pm)}(RR'\bar\sigma t)=\epsilon(RR'\bar\sigma t)\langle C^\dagger_{R\bar\sigma}(t)C_{R'\bar\sigma}(t)\rangle\pm\epsilon(R'R\bar\sigma t)\langle C^\dagger_{R'\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle\,,\tag{4.8}$$

$$\mu_{\bar\sigma}(Rt)=\tfrac12F_{\bar\sigma}(Rt)[(w-I)^{-1}+w^{-1}]\,.\tag{4.9}$$

In the limit of vanishing external field $\delta\epsilon=0$, $F_{\bar\sigma}(Rt)=F_{\bar\sigma}(0)$ and the Fourier transform of the above equation may be written

$$2\pi\Sigma^{(1)}(k\sigma,\omega)=I^2g(k\sigma)/[\omega-(1-n_{\bar\sigma})I]^2+\xi^{(1)}(k\sigma,\omega)+\xi^{(2)}(k\sigma,\omega)\,,\tag{4.10}$$

where

$$g(k\sigma)=n_{\bar\sigma}(1-n_{\bar\sigma})\epsilon_k+(1-2n_\sigma)\frac{1}{N_a}\sum_q\epsilon_qn_{q\bar\sigma}+\frac{2}{N_a^2}\sum_{q_1}\sum_{q_2}\epsilon_{k-q_1+q_2}n_{q_1\bar\sigma}n_{q_2\sigma}\,.\tag{4.11}$$

The resulting Green's function is then

$$2\pi G^{-1}(k\sigma,\omega)=\omega-\epsilon_k-\frac{In_{\bar\sigma}\omega}{\omega-(1-n_{\bar\sigma})I}-\frac{I^2g(k\sigma)}{[\omega-(1-n_{\bar\sigma})I]^2}-\xi^{(1)}(k\sigma,\omega)-\xi^{(2)}(k\sigma,\omega)\,. \tag{4.12}$$

The first term on the right-hand side of Eq. (4.10) is parallel to those obtained by Esterling and Lange[8b] and by Fedro and Wilson[17] except for a factor in the second term and the sign of the third term in Eq. (4.11). However, it is premature to discuss these differences under the present approximation since, when the self-energy expression is calculated exactly through terms linear in ϵ in Sec. V, the structure of the corresponding terms will be altered completely as is shown in Eq. (5.14).

By inspection, we find that $\xi^{(1)}$ and $\xi^{(2)}$ are, at most, of order ϵ and ϵ^2, respectively. They may be evaluated explicitly by using the fact that $\langle N_{R\bar\sigma}(t)\rangle$ and $\langle C^\dagger_{R'\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle$, respectively, are really equivalent to $iG_{RR\bar\sigma}(tt')$ and $iG_{RR'\bar\sigma}(tt')$ by the definition given by Eq. (2.11). Therefore their derivatives are calculated by Eq. (3.24) as follows:

$$\frac{\delta\langle C^\dagger_{R'\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}=i\,\frac{\delta G_{RR'\bar\sigma}(tt^+)}{\delta\epsilon(R_iR_j\bar\sigma t')}$$

$$=-i\int_0^{-i\beta}dt_1\int_0^{-i\beta}dt_2\sum_{R_1}\sum_{R_2}G_{RR_1\bar\sigma}(tt_1)\frac{\delta[(G_0)^{-1}_{R_1R_2\bar\sigma}(t_1t_2)-\Sigma_{R_1R_2\bar\sigma}(t_1t_2)]}{\delta\epsilon(R_iR_j\bar\sigma t')}G_{R_2R'\bar\sigma}(t_2t^+)\,. \tag{4.13}$$

Here we have replaced G^{-1} by $G_0^{-1}-\Sigma$ to indicate explicitly that Eq. (4.13) may be used to calculate the derivative $\delta\langle\;\rangle/\delta\epsilon$ iteratively. Use of Eq. (4.1) will yield an explicit expression for the derivative, which is correct through terms of order ϵ^0 and hence $\xi^{(1)}$ and $\xi^{(2)}$, respectively, will be calculated correctly through terms of order ϵ and ϵ^2. We shall summarize the calculation of $\xi^{(1)}$ in Appendix B. Although $\xi^{(1)}$ is of order ϵ for arbitrary ω, the result in Appendix B shows that the value is reduced to $\sim\epsilon^2$ for ω satisfying the condition $G^{-1}(\omega)=0$ and hence $\xi^{(1)}$ may be neglected in the present paper.

Finally, we shall discuss some aspects of the solution obtained. As we have already suggested, the inverse Green's function calculated in Eq. (4.12) with $\xi^{(1)}=\xi^{(2)}=0$ is not a satisfactory solution but still yields a result which is a great improvement over the Hubbard I result given by Eq. (2.20). Let ω_1 and ω_2 be the Hubbard I roots of $G_0^{-1}(\omega)=0$. The present result may then be rewritten

$$2\pi G^{-1}(k\sigma,\omega)=\frac{(\omega-\omega_1)(\omega-\omega_2)}{\omega-(1-n_{\bar\sigma})I}-\frac{I^2g(k\sigma)}{[\omega-(1-n_{\bar\sigma})I]^2}\,. \tag{4.14}$$

In the limit of narrow bands, the three roots of the cubic equation ω_1', ω_2', and ω_3' are all real and satisfy the relation

$$\omega_1'\approx\omega_1<\omega_3'\approx(1-n_{\bar\sigma})I<\omega_2'\approx\omega_2\,. \tag{4.15}$$

If we neglect the second and third terms in $g(k\sigma)$ given by Eq. (4.11) and assume that $g(k\sigma)\approx n_{\bar\sigma}(1-n_{\bar\sigma})\epsilon_k$, the condition that the resulting cubic equation yields two complex and one real roots is

$$|\epsilon_k|>0.15\,I \text{ for a half-filled lattice } (n_{\bar\sigma}=\tfrac12)\,, \tag{4.16}$$

$$|\epsilon_k|>|1-2n_{\bar\sigma}|I \text{ for } n_{\bar\sigma}<0.4 \text{ or } n_{\bar\sigma}>0.6\,.$$

A similar result is obtained even if the second and third terms in $g(k\sigma)$ are restored. As the bandwidth increases, therefore, Hubbard's split bands disappear and only a single band capable of accepting two electrons per state appears, indicating that an essential mechanism for the metal-nonmetal transition, which is not found in the Hubbard I solution is already included in the present solution.

However, the metal-nonmetal transition cannot be discussed properly using Eq. (4.14) for the following reason. The spectral weights of the solution are given by

$$A(\omega_i')=\frac{[\omega_i'-(1-n_{\bar\sigma})I]^2}{(\omega_i'-\omega_j')(\omega_i'-\omega_k')}\,, \tag{4.17}$$

where ω_i', ω_j', and ω_k', respectively, denote ω_1', ω_2', and ω_3'. In the narrow-band limit, the above result is not different from the Hubbard I result, that is, $A(\omega_1')\approx A(\omega_1)\approx(1-n_{\bar\sigma})>0$, $A(\omega_2')\approx A(\omega_2)\approx n_{\bar\sigma}>0$, and $A(\omega_3')$ is zero within the accuracy of the present calculation. More precisely, $A(\omega_3')$ is negative but its value is of order ϵ^2 and beyond the accuracy of the present calculation. As the bandwidth increases, however, $A(\omega_3')$ remains negative and its magnitude increases. In the limit where the split-band structure is replaced by the single-band structure, $A(\omega_3')$ becomes nearly equal to $-A(\omega_2')$ [or $-A(\omega_1')$], suggesting that the present solution becomes unphysical in the region where the metal-nonmetal transition is to take place.

In Sec. V, we shall iterate the calculation described here an infinite number of times, and obtain a more reliable result.

V. ASYMPTOTIC BEHAVIOR OF THE SELF-ENERGY CORRECTION IN SMALL-HOPPING LIMIT

Although the calculation in Sec. IV is based on the assumption of narrow bands, the result does not correspond to a precise approximation in the hopping parameters ϵ_k. We extend the calculation to determine the self-energy correction at least up to terms linear in ϵ_k correctly. For this purpose, we shall keep calculating higher-order terms until we exhaust all possible terms which are linear in ϵ_k.

Since functional derivatives of $\langle N_{R\sigma}(t)\rangle$ and $\langle C^\dagger_{R\sigma}(t)C_{R'\sigma}(t)\rangle$ yield corrections of order ϵ^2, we shall postpone taking such derivatives until after the self-energy correction is calculated up to terms linear in ϵ_k. For this, we shall introduce the derivative $\delta_0\epsilon$ which operates on $\epsilon(R_iR_j\sigma_it_i)$ only and which yields

$$\delta\langle N_{R\sigma}(t)\rangle/\delta_0\epsilon=\delta\langle C^\dagger_{R\sigma}(t)C_{R'\sigma}(t)\rangle/\delta_0\epsilon=0\,.$$

From the zeroth-order correction $\Sigma^{(1)}$ obtained in Eq. (4.7), we find that

$$-\frac{\delta\Sigma^{(1)}_{R_1R'\sigma}(t_1t')}{\delta_0\epsilon(R_iR_j\sigma t^\pm)}=-\lambda_{\bar\sigma}(R_1t_1)^2B_{\bar\sigma}(R_1t_1)\times\delta_{R_1R_i}\delta_{R't_j}\delta_{t^\pm t_1}\delta_{t_1t'}\,,\tag{5.1}$$

and, by inserting the above result into Eq. (3.25),

$$\Sigma^{(2)}_{RR'\sigma}(tt')=\frac{\lambda_{\bar\sigma}(Rt)}{\lambda_{\bar\sigma}(0)}[\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)B_{\bar\sigma}(Rt)]^2\epsilon(RR'\sigma t)\delta_{tt'}\,.\tag{5.2}$$

The functional derivative $-\delta\Sigma^{(2)}/\delta_0\epsilon(\sigma)$ is exactly the same as that in Eq. (5.1) except for an additional factor $\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)B_{\bar\sigma}(Rt)$ and yields $\Sigma^{(3)}$ which is again the same as that in Eq. (5.2) except for the same additional factor $\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)B_{\bar\sigma}(Rt)$ and so on. We can continue the calculation indefinitely and the series of terms generated in this manner may be summed as follows:

$$\frac{\lambda}{\lambda_0}[(\lambda\lambda_0B)+(\lambda\lambda_0B)^2+(\lambda\lambda_0B)^3+(\;)^4+\cdots]\epsilon(RR'\sigma t)\delta_{tt'}=\frac{\lambda_{\bar\sigma}(Rt)^2B_{\bar\sigma}(Rt)}{1-\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(0)B_{\bar\sigma}(Rt)}\epsilon(RR'\sigma t)\delta_{tt'}\,.\tag{5.3}$$

The derivative of $\Sigma^{(1)}$ with respect to $\delta_0\epsilon(R_iR_j\bar\sigma t^\pm)$ involves the following four terms:

$$\begin{aligned}-\frac{\delta\Sigma^{(1)}_{R_1R'\sigma}(t_1t')}{\delta_0\epsilon(R_iR_j\bar\sigma t^\pm)}=&-\lambda_{\bar\sigma}(R_1t_1)^2\frac{\epsilon(R_1R'\sigma t)}{I}\langle C^\dagger_{R_i\bar\sigma}(t_1)C_{R_j\bar\sigma}(t_1)\rangle(\delta_{R_1R_i}-\delta_{R_1R_j})\delta_{t^\pm t_1}\delta_{t_1t'}\\&-\lambda_{\bar\sigma}(R_1t_1)^2[\tfrac12-\langle N_{R_1\sigma}(t_1)\rangle]\langle C^\dagger_{R_i\bar\sigma}(t_1)C_{R_j\bar\sigma}(t_1)\rangle(\delta_{R_1R_i}+\delta_{R_1R_j})\delta_{R_1R'}\delta_{t^\pm t_1}\delta_{t_1t'}\\&-\lambda_{\bar\sigma}(R_1t_1)\mu_{\bar\sigma}(R_1t_1)\langle C^\dagger_{R_i\bar\sigma}(t_1)C_{R_j\bar\sigma}(t_1)\rangle(\delta_{R_1R_i}-\delta_{R_1R_j})\delta_{R_1R'}\delta_{t^\pm t_1}\delta_{t_1t'}\\&-\lambda_{\bar\sigma}(R_1t_1)\lambda_{\bar\sigma}(R't_1)\langle C^\dagger_{R'\sigma}(t_1)C_{R_1\sigma}(t_1)\rangle\langle C^\dagger_{R_i\bar\sigma}(t_1)C_{R_j\bar\sigma}(t_1)\rangle(\delta_{R_1R_i}\delta_{R'R_j}+\delta_{R_1R_j}\delta_{R'R_i})\delta_{t^\pm t_1}\delta_{t_1t'}\,.\end{aligned}\tag{5.4}$$

Except for an additional factor $\mu_{\bar\sigma}(R_1t_1)$ [Eq. (4.9)], the third term in Eq. (5.4) is the same as the first term in Eq. (4.2) and hence yields terms exactly the same as the second, third, and fourth terms in $\Sigma^{(1)}$ given by Eq. (4.7) except for the additional factor $\mu_{\bar\sigma}$. That is,

$$\begin{aligned}\Sigma^{(2,3)}_{RR'\sigma}(tt')=&\lambda_{\bar\sigma}(Rt)^2\mu_{\bar\sigma}(Rt)\sum_{R''\neq R}b^{(+)}(RR''\bar\sigma t)[\tfrac12-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}+\lambda_{\bar\sigma}(Rt)\mu_{\bar\sigma}(Rt)^2\sum_{R''\neq R}b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'}\\&+\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)\mu_{\bar\sigma}(R't)b^{(+)}(RR'\bar\sigma t)\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}\,.\end{aligned}\tag{5.5}$$

Apart from the same additional factor $\mu_{\bar\sigma}$, the derivative of the above expression $-\delta\Sigma^{(2,3)}/\delta_0\epsilon(\bar\sigma)$ is again the same as $-\delta\Sigma^{(1)}/\delta_0\epsilon(\bar\sigma)$ given by Eq. (5.4). Therefore we can continue the calculation indefinitely and sum the series as before except for the following complication. The second and fourth terms in Eq. (5.4), respectively, yield the following results:

$$\begin{aligned}\Sigma^{(2,2)}_{RR'\sigma}(tt')=&\lambda_{\bar\sigma}(Rt)^3\sum_{R''}b^{(-)}(RR''\bar\sigma t)[\tfrac12-\langle N_{R\sigma}(t)\rangle]^2\delta_{RR'}\delta_{tt'}+\lambda_{\bar\sigma}(Rt)^2\mu_{\bar\sigma}(Rt)\sum_{R''}b^{(+)}(RR''\bar\sigma t)[\tfrac12-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}\\&-\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)^2b^{(-)}(RR'\bar\sigma t)[\tfrac12-\langle N_{R'\sigma}(t)\rangle]\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}\,,\end{aligned}\tag{5.6}$$

$$\Sigma^{(2,4)}_{RR'\sigma}(tt') = \lambda_{\bar\sigma}(Rt)^2\lambda_{\bar\sigma}(R't)b^{(-)}(RR'\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}$$
$$+\lambda_{\bar\sigma}(Rt)\mu_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)b^{(+)}(RR'\bar\sigma t)\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}$$
$$-\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)\sum_{R''}\lambda_{\bar\sigma}(R''t)b^{(-)}(RR''\bar\sigma t)\langle C^\dagger_{R\sigma}(t)C_{R''\sigma}(t)\rangle\langle C^\dagger_{R''\sigma}(t)C_{R\sigma}(t)\rangle\delta_{RR'}\delta_{tt'} . \tag{5.7}$$

Note that, except for the same additional factor $\mu_{\bar\sigma}$, the derivatives of the second terms in $\Sigma^{(2,2)}$ and $\Sigma^{(2,4)}$, respectively, are the same as the second and fourth terms in Eq. (5.4) and hence the calculation may be continued indefinitely. Instead of a simple series similar to that in Eq. (5.3), however, we find that

$$\lambda(R)^2[1+2\mu(R)+3\mu(R)^2+4\mu(R)^3+\cdots]\sum_{R''}b^{(+)}(RR''\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}$$
$$+\lambda(R)\lambda(R')\{1+[\mu(R)+\mu(R')]+[\mu(R)^2+\mu(R)\mu(R')+\mu(R')^2]$$
$$+[\mu(R)^3+\mu(R)^2\mu(R')+\mu(R)\mu(R')^2+\mu(R')^3]+\cdots\}b^{(+)}(RR'\bar\sigma t)\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}$$
$$+\lambda(R)\mu(R)[1+\mu(R)+\mu(R)^2+\cdots]\sum_{R''}b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'}$$
$$=\lambda_{\bar\sigma}(Rt)^2\sum_{R''}b^{(+)}(RR''\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'}/[1-\mu_{\bar\sigma}(Rt)]^2$$
$$+\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)b^{(+)}(RR'\bar\sigma t)\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}/[1-\mu_{\bar\sigma}(Rt)][1-\mu_{\bar\sigma}(R't)]$$
$$+\lambda_{\bar\sigma}(Rt)\mu_{\bar\sigma}(Rt)\sum_{R''}b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'}/[1-\mu_{\bar\sigma}(Rt)] . \tag{5.8}$$

The foregoing expansion generates not only the series in Eq. (5.8) but also series involving terms of types appearing in the first and third places in $\Sigma^{(2,2)}$ and $\Sigma^{(2,4)}$. The sum is

$$\lambda_{\bar\sigma}(Rt)^3[1-\mu_{\bar\sigma}(Rt)]^{-2}\sum_{R''}b^{(-)}(RR''\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]^2\delta_{RR'}\delta_{tt'}$$
$$-\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)^2[1-\mu_{\bar\sigma}(R't)]^{-2}b^{(-)}(RR'\bar\sigma t)[\tfrac{1}{2}-\langle N_{R'\sigma}(t)\rangle]\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}$$
$$+\lambda_{\bar\sigma}(Rt)^2\lambda_{\bar\sigma}(R't)[1-\mu_{\bar\sigma}(Rt)]^{-1}[1-\mu_{\bar\sigma}(R't)]^{-1}b^{(-)}(RR'\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'}$$
$$-\lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)[1-\mu_{\bar\sigma}(R't)]^{-1}\sum_{R''}\lambda_{\bar\sigma}(R''t)[1-\mu_{\bar\sigma}(R''t)]^{-1}b^{(-)}(RR''\bar\sigma t)$$
$$\times\langle C^\dagger_{R\sigma}(t)C_{R''\sigma}(t)\rangle\langle C^\dagger_{R''\sigma}(t)C_{R\sigma}(t)\rangle\delta_{RR'}\delta_{tt'} . \tag{5.9}$$

The sum of the second and third terms in Eq. (5.9) as well as all terms generated from it by differentiation with respect to $\delta_0\epsilon$ will have a factor of the type

$$\lambda_{\bar\sigma}(Rt)[1-\mu_{\bar\sigma}(Rt)]^{-1}[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]-\lambda_{\bar\sigma}(R't)[1-\mu_{\bar\sigma}(R't)]^{-1}[\tfrac{1}{2}-\langle N_{R'\sigma}(t)\rangle] , \tag{5.10}$$

which vanishes in the limit $\delta\epsilon=0$. Therefore, we will not write them explicitly in this section.

The sum of the first and fourth terms in Eq. (5.9) is

$$\lambda_{\bar\sigma}(Rt)\sum_{R''}b^{(-)}(RR''\bar\sigma t)X(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'} , \tag{5.11}$$

where

$$X(RR''\bar\sigma t)=\lambda_{\bar\sigma}(Rt)^2[1-\mu_{\bar\sigma}(Rt)]^{-2}[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]^2-\lambda_{\bar\sigma}(Rt)[1-\mu_{\bar\sigma}(Rt)]^{-1}$$
$$\times\lambda_{\bar\sigma}(R''t)[1-\mu_{\bar\sigma}(R''t)]^{-1}\langle C^\dagger_{R\sigma}(t)C_{R''\sigma}(t)\rangle\langle C^\dagger_{R''\sigma}(t)C_{R\sigma}(t)\rangle . \tag{5.12}$$

The expression in Eq. (5.11) is exactly the same as the third term in $(G_0)^{-1}$ given by Eq. (3.18) except for the factor $X(RR''\bar\sigma t)$ multiplying $\langle C^\dagger_{R\bar\sigma}C_{R''\bar\sigma}\rangle$ and $\langle C^\dagger_{R''\sigma}C_{R\bar\sigma}\rangle$ involved in $(G_0)^{-1}$. Consequently, the series generated from Eq. (5.11) will be summed up in the form shown by Eqs. (5.8) and (5.11) except that $b^{(\pm)}(RR''\bar\sigma t)$'s are replaced by $b^{(\pm)}(RR''\bar\sigma t)X(RR''\bar\sigma t)$. The new expression (5.11) will generate the same series and the same expression (5.11) except for another factor $X(RR''\bar\sigma t)$ added and so on. The sum of all possible terms, which are generated from the second, third and fourth terms in Eq. (5.4) and which do not have a factor of the type shown in Eq. (5.10), is

$$
\begin{aligned}
&\lambda_{\bar\sigma}(Rt)^2 \sum_{R''} [1-\mu_{\bar\sigma}(Rt)]^{-2}[1-X(RR''\bar\sigma t)]^{-1} b^{(+)}(RR''\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'} \\
&\quad + \lambda_{\bar\sigma}(Rt)\lambda_{\bar\sigma}(R't)[1-\mu_{\bar\sigma}(Rt)]^{-1}[1-\mu_{\bar\sigma}(R't)]^{-1}[1-X(RR'\bar\sigma t)]^{-1} b^{(+)}(RR'\bar\sigma t)\langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{tt'} \\
&\quad\quad + \lambda_{\bar\sigma}(Rt) \sum_{R''} \{[1-\mu_{\bar\sigma}(Rt)]^{-1}[1-X(RR''\bar\sigma t)]^{-1}-1\} b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'} \\
&= \sum_{R''\neq R} \{ b^{(+)}(RR''\bar\sigma t)[\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]\delta_{RR'}\delta_{tt'} + [\tfrac{1}{2}-\langle N_{R'\bar\sigma}(t)\rangle][\tfrac{1}{2}-\langle N_{R\bar\sigma}(t)\rangle]^{-1} b^{(+)}(RR'\bar\sigma t) \\
&\qquad \times \langle C^\dagger_{R'\sigma}(t)C_{R\sigma}(t)\rangle\delta_{R''R'}\delta_{tt'} - [\tfrac{1}{2}-\langle N_{R\bar\sigma}(t)\rangle] b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'} \} \\
&\qquad \times \left\{ [\tfrac{1}{2}-\langle N_{R\bar\sigma}(t)\rangle]^2 - [\tfrac{1}{2}-\langle N_{R\sigma}(t)\rangle]^2 + \frac{\tfrac{1}{2}-\langle N_{R\bar\sigma}(t)\rangle}{\tfrac{1}{2}-\langle N_{R''\bar\sigma}(t)\rangle} \langle C^\dagger_{R\sigma}(t)C_{R''\sigma}(t)\rangle\langle C^\dagger_{R''\sigma}(t)C_{R\sigma}(t)\rangle \right\}^{-1} \\
&\quad - \sum_{R''\neq R} I\{w-[1-\langle N_{R\bar\sigma}(t)\rangle]I\}^{-1} b^{(-)}(RR''\bar\sigma t)\delta_{RR'}\delta_{tt'} .
\end{aligned}
\tag{5.13}
$$

In the foregoing calculation, we have not included the series generated by terms of the type shown in the first place in Eq. (5.4) nor functional derivatives of the types $\delta\langle N\rangle/\delta\epsilon$ and $\delta\langle C^\dagger C\rangle/\delta\epsilon$. The contribution from $\pi[\Delta]$ involved in the exact expression for the self-energy correction given by Eq. (3.26) has also been neglected, but otherwise all possible contributions to Σ have been exhausted. By inspection, it is easily found that series generated from terms of the type shown in the first place in Eq. (5.4) are, at most, of order ϵ^2. The contributions from $\delta\langle N\rangle/\delta\epsilon$, $\delta\langle C^\dagger C\rangle/\delta\epsilon$ and $\pi[\Delta]$ are also of order ϵ^2. This implies that the self-energy correction given by the sum of Eq. (5.3) and (5.13) is exact through terms linear in ϵ. In the limit of a small external field $\delta\epsilon=0$, the result is

$$
\begin{aligned}
2\pi\Sigma(k\sigma,\omega) &= \frac{n_{\bar\sigma}(1-n_{\bar\sigma})I^2\epsilon_k}{[\omega-(1-n_{\bar\sigma})I]^2 - n_{\bar\sigma}(1-n_{\bar\sigma})I^2} \\
&\quad + \sum_{R''\neq R} \frac{\epsilon_{RR''}\langle C^\dagger_{R\bar\sigma}C_{R''\bar\sigma}\rangle\{(1-2n_\sigma)+2\langle C^\dagger_{RR''\sigma}C_{R\sigma}\rangle\exp[ik(R-R'')]\}}{(\tfrac{1}{2}-n_{\bar\sigma})^2-(\tfrac{1}{2}-n_\sigma)^2+\langle C^\dagger_{R\sigma}C_{RR''\sigma}\rangle\langle C^\dagger_{R''\sigma}C_{R\sigma}\rangle} .
\end{aligned}
\tag{5.14}
$$

The second term in Eq. (5.14) comes from the second and third terms in Eq. (4.11). Note that the denominator is completely different from that of the original expression in Eq. (4.10) due to the large factor $(1-\mu)^{-2}(1-X)^{-1}$ introduced by the infinite summation. Although the self-energy Σ obtained here is exact through terms linear in ϵ, the solution of $G^{-1}(\omega)=G_0^{-1}(\omega)-\Sigma(\omega)=0$ need not be calculated correctly through terms linear in ϵ, since the equation $G^{-1}(\omega)=0$ is polynomial in ω. Furthermore, the second term in Eq. (5.14) can be abnormally large for a nonmagnetic case where $n_\sigma=n_{\bar\sigma}$ since, in the narrow band limit, $\langle C^\dagger_{R\sigma}C_{R''\sigma}\rangle \times\langle C^\dagger_{R''\sigma}C_{R\sigma}\rangle$ vanishes when the lower band is nearly empty or nearly filled. To remedy these difficulties, the effect of $\delta\langle N\rangle/\delta\epsilon$, etc., has to be included. Terms linear in ϵ will then be added to the denominators in Eq. (5.14) and these terms may become very important, as we shall discuss in Paper II.

VI. DISCUSSION

In Secs. II and III, a systematic treatment of the equations of motion has been developed; higher-order Green's functions, which appear in the equations for basic Green's functions, are reduced to functional derivatives of the basic Green's functions so that they can be calculated, by means of an iterative procedure, rigorously up to any desired accuracy. In principle, the present method is parallel to the perturbation method developed by Kadanoff and Baym.[15] In order to include the strong correlation between two electrons with opposite spins at the same site, however, we have used the two equations of motion for the two basic Green's functions $\Gamma^{(\pm)}$. In the absence of the interaction, $I=0$, these two equations are identical and yield $\Gamma^{(\pm)}=\langle N_{\bar\sigma}^{(\pm)}\rangle G$. In the presence of the interaction I, however, they generate two distinct classes of terms (diagrams). Diagrams generated from the equation for $\Gamma^{(+)}$ will have an electron with spin $\bar\sigma$ at time t at site R, but diagrams generated from the equation for $\Gamma^{(-)}$ will not have an electron with spin $\bar\sigma$ at time t at site R.

We shall now illustrate how the present method works in calculating the electron correlation. Successive hoppings of an electron σ are calculated by the second term on the left-hand side of Eq. (2.8), that is,

$$\phi_1=\sum_{R''\neq R}\epsilon(RR''\sigma t)\langle\langle C_{R''\sigma}(t)N_{R\bar\sigma}^{(\pm)}(t)C_{R'\sigma}^{\dagger}(t')\rangle\rangle . \tag{6.1}$$

Since the Green's functions involved can be reduced to functional derivatives of $\Gamma^{(\pm)}$ as illustrated by Eqs. (2.12) and (3.5), ϕ_1 may be rewritten

$$\phi_1=n_{\bar\sigma}^{(\pm)}\sum_{R''\neq R}\epsilon(RR''\sigma t)\langle\langle C_{R''\sigma}(t)C_{R'\sigma}^{\dagger}(t')\rangle\rangle + \sum_{R''\neq R}\epsilon(RR''\sigma t)\left(i\frac{\delta}{\delta\epsilon(RR''\sigma t^{-})}-i\frac{\delta}{\delta\epsilon(RR''\sigma t^{+})}\right) \times\langle\langle C_{R\sigma}(t)[N_{R\bar\sigma}^{(\pm)}(t)-n_{\bar\sigma}^{(\pm)}]C_{R'\sigma}^{\dagger}(t')\rangle\rangle . \tag{6.2}$$

The original expression for ϕ_1 given by Eq. (6.1) describes a simultaneous motion of two electrons σ and $\bar\sigma$; the electron σ hops from site R' to R'', while the other electron $\bar\sigma$ (or hole $\bar\sigma$) remains at site R as is illustrated by diagram (a) in Fig. 1. In Secs. IV and V, the value of ϕ_1 has been calculated by using Eq. (6.2). In the first term in Eq. (6.2), the electron $N_{R\bar\sigma}$ is replaced by the average field $n_{\bar\sigma}$ created by all electrons with opposite spin $\bar\sigma$ as is shown by Fig. 1, diagram (b). This term is also included in Hubbard I, and introduces the splitting of a narrow band. The second term in Eq. (6.2) is to correct the error created by the replacement of the electron $N_{R\bar\sigma}$ by the average potential $n_{\bar\sigma}$, and yields the series leading to the result in Eq. (5.3). As is shown in Fig. 1, diagram (c), however, the motion of the first electron has been neglected completely in this series. To improve this result, therefore, we need to include more detailed motion of the electron σ. This will be the subject of Paper II.

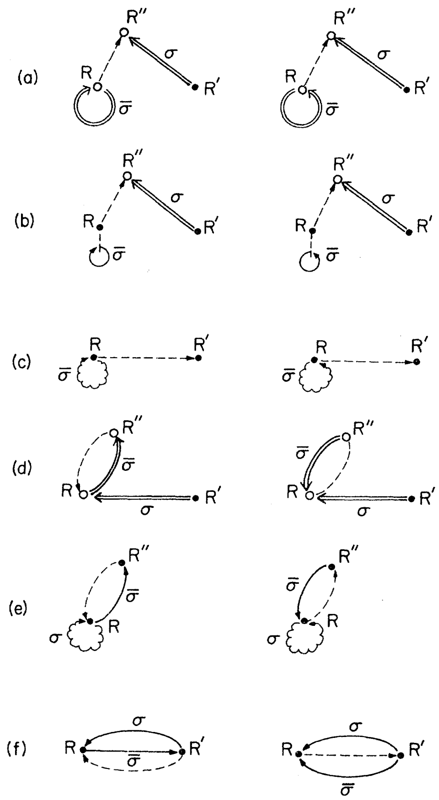

FIG. 1. Diagrams for ϕ_1 and ϕ_2. A double-line $R'\Rightarrow R$ represents the Green's function $\langle\langle C_{R\sigma}(t)C_{R'\sigma}^{\dagger}(t')\rangle\rangle$, a single-line $R'\rightarrow R$ is the equal-time Green's function $\langle C_{R'\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle$, and a dotted line $R'\dashrightarrow R$ denotes $\epsilon_{RR'}$. A counterclockwise loop represents $N_{R\sigma}(t)$ or n_σ, while a clockwise loop $1-N_{R\sigma}(t)$ or $1-n_\sigma$ Diagram (a) describes ϕ_1 given by Eq. (6.1), (b) and (c), respectively, represent the first and second terms in Eq. (6.2), while (d) illustrates ϕ_2 given by Eq. (6.3), and (e) and (f), respectively, describe the first and second terms in Eq. (6.4).

The effect of the motion of electrons with opposite spin $\bar\sigma$ is described by the third term on the left-hand side of Eq. (2.8), that is,

$$\phi_2=\pm\sum_{R''\neq R}[\epsilon(RR''\bar\sigma t)\langle\langle C_{R\sigma}(t)C_{R\bar\sigma}^{\dagger}(t)C_{R''\bar\sigma}(t)C_{R'\sigma}^{\dagger}(t')\rangle\rangle-\epsilon(R''R\bar\sigma t)\langle\langle C_{R\sigma}(t)C_{R''\bar\sigma}^{\dagger}(t)C_{R\bar\sigma}(t)C_{R'\sigma}^{\dagger}(t')\rangle\rangle] . \tag{6.3}$$

Use of Eqs. (2.13)–(2.16), and (3.1), and (3.2) in the above expression yields

$$\phi_2 = \pm \sum_{R''\neq R} \left[\epsilon(RR''\bar{\sigma}t)\langle C^\dagger_{R\bar{\sigma}}(t)C_{R''\bar{\sigma}}(t)\rangle - \epsilon(R''R\bar{\sigma}t)\langle C^\dagger_{R''\bar{\sigma}}(t)C_{R\bar{\sigma}}(t)\rangle\right]\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle$$

$$\pm \sum_{R''\neq R}\left(\epsilon(RR''\bar{\sigma}t)i\,\frac{\delta}{\delta\epsilon(RR''\bar{\sigma}t^{\mp})} - \epsilon(R''R\bar{\sigma}t)\,i\,\frac{\delta}{\delta\epsilon(R''R\bar{\sigma}t^{\pm})}\right)\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle . \quad (6.4)$$

The original expression for ϕ_2 given by Eq. (6.3) describes a simultaneous motion of two electrons σ and $\bar{\sigma}$; the electron σ hops from site R' to R while the other electron $\bar{\sigma}$ moves from R to R'' (or R'' to R). These two processes are described by Fig. 1, diagram (d). In Secs. IV and V, we have calculated their value by using Eq. (6.4). In the first term in Eq. (6.4), the motion of the two electrons are decoupled and the electron σ cannot distinguish the two processes illustrated in Fig. 1, diagram (d). Therefore the value of the first term in Eq. (6.4) vanishes in the limit of small external field $\delta\epsilon = 0$. The nonvanishing contribution calculated from the second term in Eq. (6.4) is given by the first two terms in Eq. (5.13). The series leading to the first term in Eq. (5.13) gives the correlation between the electron σ at site R {represented by $[\frac{1}{2} - \langle N_{R\sigma}(t)\rangle]$} and the second electron $\bar{\sigma}$ which fluctuates between sites R and R''. The series leading to the second term in Eq. (5.13) gives the motion of the electron σ from R' to R, but the motion of the other electron $\bar{\sigma}$ is limited to between R and R', and it can not go to an arbitrary atom R'' in the lattice.

The foregoing discussion will be helpful not only for improving the result obtained in this paper but also for comparing it with other results. In Hubbard I, all diagrams in Fig 1 except (b) are neglected. The result in Eq. (5.3) obtained from ϕ_1 should be compared with Eqs. (37)–(40) of Hubbard III which includes only the scattering correlation, and also the CPA result obtained by Soven by freezing the motion of electrons with opposite spin $\bar{\sigma}$. In fact, Eqs. (37)–(40) of Hubbard III may be rewritten

$$G^{-1}_{k\sigma}(\omega) = \frac{\omega(\omega - I)}{\omega - (1-n_{\bar{\sigma}})I} - \epsilon_k - \frac{n_{\bar{\sigma}}(1-n_{\bar{\sigma}})I^2\Omega_\sigma}{[\omega-(1-n_{\bar{\sigma}})I]^2 - [\omega-(1-n_{\bar{\sigma}})I]\Omega_\sigma}, \quad (6.5)$$

where

$$\Omega_\sigma = F_\sigma - [2\pi G_{RR\sigma}(\omega)]^{-1}. \quad (6.6)$$

If one replaces $G_{RR\sigma}(\omega)$ by $G_{k\sigma}(\omega)$, Ω becomes equal to ϵ_k and the third term in Eq. (6.5) becomes equal to our first term in Eq. (4.11) through terms linear in ϵ_k, it is also parallel to our first term in Eq. (5.14) if $[\omega-(1-n_{\bar{\sigma}})I]\Omega_\sigma$ is replaced by $n_{\bar{\sigma}}(1-n_{\bar{\sigma}})I^2$. Since $G_{RR\sigma}(\omega)$ is not equal to $G_{k\sigma}(\omega)$ but is given by a k-independent quantity $N^{-1}\sum_{k'}G_{k'\sigma}(\omega)$, and since Hubbard III has neglected the correlation function $\langle N_{R'\bar{\sigma}}(N_{R\bar{\sigma}} - n_{\bar{\sigma}})\rangle$, it is difficult to make a more precise comparison between the present results and the Hubbard III result. It is not surprising that the Hubbard III result becomes equivalent to Soven's result obtained by freezing the motion of electrons $\bar{\sigma}$, since $\langle N_{R'\bar{\sigma}}(N_{R\bar{\sigma}} - n_{\bar{\sigma}})\rangle = 0$. Note that our first term in Eq. (4.11) is exactly the same as the corresponding term obtained by Esterling and Lange[8b] and Fedro and Wilson,[17] showing that the results by these authors correspond to our zeroth-order result and are not correct through linear in terms ϵ.

The resonance broadening correction in Hubbard III should correspond to Fig. 1, diagram (d). However, the motion of an electron $\bar{\sigma}$ is decoupled from that of an electron σ and replaced by an average field in Eq. (47) of Hubbard III and therefore the dynamical correlations between two electrons σ and $\bar{\sigma}$ given by ϕ_2 are not included. In fact, the results given by Eqs. (51) and (52) of Hubbard III has no resemblance to our result given by the second term in Eq. (5.14), and, instead, it resembles the first term in Eq. (5.14). As we have discussed before, our second and third terms in Eq. (4.11) have a factor and a sign different from the corresponding results by Esterling and Lange and by Fedro and Wilson, but these differences are unimportant. After the term is calculated correctly through terms linear in ϵ, the form is modified drastically as is shown in the second term in Eq. (5.14). Note that there is the difference by a factor $(1-2n_{\bar{\sigma}})$ between the results of Esterling and Lange and of Fedro and Wilson. This difference is also the same order of magnitude as the difference between our preliminary result in Eq. (4.11) and their results, illustrating that their results are obtained under arbitrary approximations. The calculation in Paper III will indeed show the instability of their results.

APPENDIX A: CALCULATION OF $\pi[\Delta]$

The expression for $\pi[\Delta]$ given by Eq. (3.26) can be calculated by inserting Eqs. (3.8) and (3.10);

$$\pi[\Delta_{RR'\sigma}(tt')] = \int_0^{-i\beta} dt_1 \sum_{R_1} \sum_{R_2 \neq R} \lambda_{\bar\sigma}(0)\epsilon(RR_2\sigma t)I^{-1}\Big[\lambda_{\bar\sigma}(Rt) \sum_{R_3 \neq R} \lambda_{\bar\sigma}(0)B_{\bar\sigma}(Rt)\epsilon(RR_3\sigma t)$$

$$\times\left(i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{--})} - i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{++})}\right)\left(i\frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(RR_3\sigma t^{-})} - \frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(RR_3\sigma t^{+})}\right)$$

$$+F_{\bar\sigma}(Rt)(w-I)^{-1}\sum_{R_3\neq R}\left(i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{--})} - i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{++})}\right)$$

$$\times\left(\epsilon(RR_3\bar\sigma t)i\frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(RR_3\bar\sigma t^{-})} - \epsilon(R_3R\bar\sigma t)i\frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(R_3R\bar\sigma t^{+})}\right)$$

$$-F_{\bar\sigma}(Rt)w^{-1}\sum_{R_3\neq R}\left(i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{--})} - i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{++})}\right)$$

$$\times\left(\epsilon(RR_3\bar\sigma t)i\frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(RR_3\bar\sigma t^{+})} - \epsilon(R_3R\bar\sigma t)i\frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(R_3R\bar\sigma t^{-})}\right)$$

$$+F_{\bar\sigma}(Rt)\sum_{R_3\neq R}\lambda_{\bar\sigma}(0)\epsilon(RR_3\bar\sigma t)I^{-1}\left(i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{--})} - i\frac{\delta}{\delta\epsilon(RR_2\sigma t^{++})}\right)$$

$$\times\left(i\frac{\delta}{\delta\epsilon(RR_3\sigma t^{-})} - i\frac{\delta}{\delta\epsilon(RR_3\sigma t^{+})}\right)[(w-I)^{-1}\Delta^{(+)}_{RR_1\sigma}(tt_1) - w^{-1}\Delta^{(-)}_{RR_1\sigma}(tt_1)]\Big]G^{-1}_{R_1R'\sigma}(t_1t'), \quad \text{(A1)}$$

where t^{++} and t^{--}, respectively, denote time arguments infinitesimally larger or smaller than t^+ and t^-. Second derivatives of G can be evaluated by the following relation:

$$\int_0^{-i\beta} dt_1 \sum_{R_1}\left(\frac{\delta}{\delta\epsilon(R_iR_j\sigma_i t_i)}\frac{\delta G_{RR_1\sigma}(tt_1)}{\delta\epsilon(R_kR_l\sigma_k t_k)}\right)G^{-1}_{R_1R'\sigma}(t_1t')$$

$$= \int_0^{-i\beta} dt_1 \int_0^{-i\beta} dt_2 \int_0^{-i\beta} dt_3 \sum_{R_1}\sum_{R_2}\sum_{R_3}\left(G_{RR_3\sigma}(tt_3)\frac{\delta G^{-1}_{R_3R_2\sigma}(t_3t_2)}{\delta\epsilon(R_iR_j\sigma_i t_i)}G_{R_2R_1\sigma}(t_2t_1)\frac{\delta G^{-1}_{R_1R'\sigma}(t_1t')}{\delta\epsilon(R_kR_l\sigma_k t_k)}\right.$$

$$\left. + G_{RR_3\sigma}(tt_3)\frac{\delta G^{-1}_{R_3R_2\sigma}(t_3t_2)}{\delta\epsilon(R_kR_l\sigma_k t_k)}G_{R_2R_1\sigma}(t_2t_1)\frac{\delta G^{-1}_{R_1R'\sigma}(t_1t')}{\delta\epsilon(R_iR_j\sigma_i t_i)}\right)$$

$$-\int_0^{-i\beta} dt_1 \sum_{R_1} G_{RR_1\sigma}(tt_1)\frac{\delta}{\delta\epsilon(R_iR_j\sigma_i t_i)}\frac{\delta}{\delta\epsilon(R_kR_l\sigma_k t_k)}G^{-1}_{R_1R'\sigma}(t_1t'), \quad \text{(A2)}$$

which is obtained from Eq. (3.24) by differentiation. The last term in Eq. (A1) still involves $\delta\Delta^{(\pm)}/\delta\epsilon$ but it can be evaluated again by inserting the expression for $\Delta^{(\pm)}$. By repeating the above treatment, the correction term π can be calculated up to any order.

The value of π calculated from Eqs. (A1) and (A2) by neglecting the term involving $\Delta^{(\pm)}$ is proportional to ϵ^2. The term involving third derivatives yield a value proportional to ϵ^3 and so on, showing that the contribution from π is of higher order and may be neglected in the present paper.

APPENDIX B: CALCULATION OF $\xi^{(1)}$

We want to calculate the correction term $\xi^{(1)}$ introduced in Eqs. (4.3) and (4.4) correctly through terms linear in ϵ. Since the expression in Eq. (4.4) is linear in ϵ, it is sufficient to calculate $\delta\langle N\rangle/\delta\epsilon(\bar\sigma)$ through terms of order ϵ^0. This can be carried out by inserting Eq. (4.1) into Eq. (4.13). The result is

$$\frac{\delta\langle C^\dagger_{R'\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')} = iF_\sigma(R_it')[F_\sigma(0)]^{-1}G_{RR_i\bar\sigma}(tt')G_{R_jR'\bar\sigma}(t't^+)$$
$$+i\int_0^{-i\beta}dt_1\int_0^{-i\beta}dt_2\sum_{R_1}\sum_{R_2}\lambda_\sigma(R_1t_1)\frac{\delta\langle N_{R_1\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\sigma t')}G_{RR_1\bar\sigma}(tt_1)(G_0)^{-1}_{R_1R_2\bar\sigma}(t_1t_2)G_{R_2R'\bar\sigma}(t_2t^+)$$
$$+i\int_0^{-i\beta}dt_1\sum_{R_1}\sum_{R_2\neq R_1}\lambda_\sigma(R_1t_1)G_{RR_1\bar\sigma}(tt_1)G_{R_1R'\bar\sigma}(t_1t^+)$$
$$\times\left(\epsilon(R_1R_2\sigma t_1)\frac{\delta\langle C^\dagger_{R_1\sigma}(t_1)C_{R_2\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}-\epsilon(R_2R_1\sigma t_1)\frac{\delta\langle C^\dagger_{R_2\sigma}(t_1)C_{R_1\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}\right)$$
$$+i\int_0^{-i\beta}dt_1\int_0^{-i\beta}dt_2\sum_{R_1}\sum_{R_2}G_{RR_1\bar\sigma}(tt_1)\frac{\delta\Sigma_{R_1R_2\bar\sigma}(t_1t_2)}{\delta\epsilon(R_iR_j\bar\sigma t')}G_{R_2R'\bar\sigma}(t_2t^+). \tag{B1}$$

By inserting the trivial identity $(G_0)^{-1}=G^{-1}+\Sigma$ into the second term on the right-hand side of Eq. (B1), the double integral may be reduced to

$$i\lambda_\sigma(R't^+)\frac{\delta\langle N_{R'\sigma}(t^+)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}G_{RR'\bar\sigma}(tt^+)+i\int_0^{-i\beta}dt_1\int_0^{-i\beta}dt_2\sum_{R_1}\sum_{R_2}\lambda_\sigma(R_1t_1)\frac{\delta\langle N_{R_1\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}$$
$$\times G_{RR_1\bar\sigma}(tt_1)\Sigma_{R_1R_2\bar\sigma}(t_1t_2)G_{R_2R'\bar\sigma}(t_2t^+)\,. \tag{B2}$$

In case $R=R'$, therefore, Eq. (B1) is rewritten

$$\frac{\delta\langle N_{R\bar\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}=iF_\sigma(R_it')[F_\sigma(0)]^{-1}G_{RR_i\bar\sigma}(tt')G_{R_jR\bar\sigma}(t't^+)+i\lambda_\sigma(R\ t^+)\frac{\delta\langle N_{R\sigma}(t^+)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}G_{RR\bar\sigma}(tt^+)$$
$$+i\int_0^{-i\beta}dt_1\sum_{R_1}\sum_{R_2\neq R_1}\lambda_\sigma(R_1t_1)G_{RR_1\bar\sigma}(tt_1)G_{R_1R\bar\sigma}(t_1t^+)$$
$$\times\left(\epsilon(R_1R_2\sigma t_1)\frac{\delta\langle C^\dagger_{R_1\sigma}(t_1)C_{R_2\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}-\epsilon(R_2R_1\sigma t_1)\frac{\delta\langle C^\dagger_{R_2\sigma}(t_1)C_{R_1\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}\right)$$
$$+i\int_0^{-i\beta}dt_1\int_0^{-i\beta}dt_2\sum_{R_1}\sum_{R_2}G_{RR_1\bar\sigma}(tt_1)\left(\frac{\delta\Sigma_{R_1R_2\bar\sigma}(t_1t_2)}{\delta\epsilon(R_iR_j\bar\sigma t')}\right.$$
$$\left.+\lambda_\sigma(R_1t_1)\frac{\delta\langle N_{R_1\sigma}(t_1)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}\Sigma_{R_1R_2\bar\sigma}(t_1t_2)\right)G_{R_2R\bar\sigma}(t_2t^+). \tag{B3}$$

Since Σ is at least linear in ϵ, $\delta\langle N\rangle/\delta\epsilon$ is given by

$$\frac{\delta\langle N_{R\bar\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}=iF_\sigma(R_it')[F_\sigma(0)]^{-1}G_{RR_i\bar\sigma}(tt')G_{R_jR\bar\sigma}(t't^+)+i\lambda_\sigma(R\,t^+)\frac{\delta\langle N_{R\sigma}(t^+)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}G_{RR\bar\sigma}(tt^+)+O(\epsilon). \tag{B3$'$}$$

Similarly,

$$\frac{\delta\langle N_{R\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}=\lambda_{\bar\sigma}(R_it')\langle C^\dagger_{R_i\bar\sigma}C_{R_j\bar\sigma}\rangle iG_{RR_i\sigma}(tt')G_{R_iR\sigma}(t't)-\lambda_{\bar\sigma}(R_jt')\langle C^\dagger_{R_i\bar\sigma}C_{R_j\bar\sigma}\rangle iG_{RR_j\sigma}(tt')G_{R_jR\sigma}(t't)$$
$$+i\lambda_{\bar\sigma}(Rt^+)\frac{\delta\langle N_{R\bar\sigma}(t^+)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}G_{RR\sigma}(tt^+)+O(\epsilon) \tag{B3$''$}$$

By inserting Eq. (B3″) into Eq. (B3′), we find that

$$\frac{\delta\langle N_{R\bar\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\bar\sigma t')}=\sum\Lambda(ij;ab)iG_{RR_a\sigma'}(tt')G_{R_bR\sigma'}(t't)+O(\epsilon), \tag{B4}$$

where

$$\Lambda(ij;ij)=F_\sigma(R_it')[F_\sigma(0)]^{-1}\delta_{\sigma'\bar\sigma}/[1+\lambda^2G_{RR\sigma}(tt^+)G_{RR\bar\sigma}(tt^+)]\,,$$
$$\Lambda(ij;ii)=-\Lambda(ij;jj)=\lambda^2\langle C^\dagger_{R_i\bar\sigma}C_{R_j\bar\sigma}\rangle iG_{RR\bar\sigma}(tt^+)\delta_{\sigma'\sigma}/[1+\lambda^2G_{RR\sigma}(tt^+)G_{RR\bar\sigma}(tt^+)]\,, \tag{B4$'$}$$
$$\Lambda(ij;ab)=0,\quad\text{otherwise},$$

which is exact up to zeroth-order terms in ϵ. By inserting the above result into Eq. (4.4), $\xi^{(1)}$ is calculated exactly up to terms linear in ϵ as follows:

$$\xi^{(1)}_{RR'\sigma}(tt')=\int_0^{-i\beta}dt_1\sum_{R_1}\sum_{R_2\neq R}\sum_{\Lambda}\lambda_{\bar\sigma}(R_1t_1)\lambda_{\bar\sigma}(Rt)$$
$$\times[\Lambda(02;ab)\epsilon(RR_2\bar\sigma t)iG_{RR_1\sigma}(tt_1)iG_{R_1R_a\sigma'}(t_1t)G_{R_bR_1\sigma'}(tt_1)(G_0)^{-1}_{R_1R'\sigma}(t_1t')$$
$$-\Lambda(20;ab)\epsilon(R_2R\bar\sigma t)iG_{RR_1\sigma}(tt_1)iG_{R_1R_a\sigma'}(t_1t)G_{R_bR_1\sigma'}(tt_1)(G_0)^{-1}_{R_1R'\sigma}(t_1t')]\,. \qquad \text{(B5)}$$

The derivative $\delta\langle C^\dagger_{R'\bar\sigma}(t)C_{R\bar\sigma}(t)\rangle/\delta\epsilon$ may be calculated by inserting Eq. (B4) into Eqs. (B1) and (B2). Use of the result and an approximate result for Σ in Eq. (B3) will yield improved $\delta\langle N\rangle/\delta\epsilon$ and $\xi^{(1)}$ and so on. However, since the improvement on $\xi^{(1)}$ are of order ϵ^2 and beyond the accuracy we are aiming at in the present paper, we shall not calculate them.

Let us now decompose $G_{RR'\sigma}(tt')$ in terms of the spectral function $A_{RR'\sigma}(\omega)$ as follows[18]:

$$G_{RR'\sigma}(tt')=\begin{cases}\displaystyle\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\,e^{-i\omega(t-t')}A_{RR'\sigma}(\omega)[1-f(\omega)] & \text{for } it>it',\\ \displaystyle\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}e^{-i\omega(t-t')}A_{RR'\sigma}(\omega)f(\omega) & \text{for } it<it',\end{cases} \qquad \text{(B6)}$$

where $A(\omega)$ is given by the discontinuity of $G(\omega)$ across the real axis

$$A(\omega)=i\lim_{\eta\to 0}[G(\omega+i\eta)-G(\omega-i\eta)] \qquad \text{(B7)}$$

and $f(\omega)$ is the Fermi function. In the limit of $\delta\epsilon\to 0$, the Fourier transform of Eq. (B5) is calculated as

$$\xi^{(1)}_{RR'\sigma}(\omega)=-[\omega-(1-n_{\bar\sigma})I]^{-2}I^2\sum_{R_1}\sum_{R_2}\sum_{\Lambda}\int\int\int\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{d\omega_3}{2\pi}(A_{RR_1\sigma}(\omega_1)[1-f(\omega_1)](G_0)^{-1}_{R_1R'\sigma}(\omega)$$
$$\times\{\epsilon_{RR_2}\Lambda(02;ab)A_{R_bR_1\sigma'}(\omega_2)[1-f(\omega_2)]A_{R_1R_a\sigma'}(\omega_3)f(\omega_3)$$
$$-\epsilon_{R_2R}\Lambda(20;ab)A_{R_1R_a\sigma'}(\omega_2)f(\omega_2)A_{R_bR_1\sigma'}(\omega_3)[1-f(\omega_3)]\}[e^{\beta(\mu-\omega_1+\omega_2-\omega_3)}+1]/(\omega-\omega_1+\omega_2-\omega_3)$$
$$+A_{RR_1\sigma}(\omega_1)f(\omega_1)(G_0)^{-1}_{R_1R'\sigma}(\omega)\{\epsilon_{RR_2}\Lambda(02;ab)A_{R_bR_1\sigma'}(\omega_2)f(\omega_2)A_{R_1R_a\sigma'}(\omega_3)[1-f(\omega_3)]$$
$$-\epsilon_{R_2R}\Lambda(20;ab)A_{R_1R_a\sigma'}(\omega_2)[1-f(\omega_2)]A_{R_bR_1\sigma'}(\omega_3)f(\omega_3)\}[1+e^{-\beta(\mu-\omega_1+\omega_2-\omega_3)}]/(\omega-\omega_1+\omega_2-\omega_3)).\qquad \text{(B8)}$$

As usual, the Fourier transformations leading to Eqs. (4.11) and (B8) are carried out for complex frequencies $Z_\nu=(\pi\nu/-i\beta)+\mu$ with odd integer ν and then the resulting expressions for $G(Z_\nu)$ and $\xi(Z_\nu)$ are analytically continued to $G(\omega)$ and $\xi(\omega)$ with real frequencies ω.

In order to understand the collision processes involved in Eq. (B8), it is more convenient to Fourier transform it to k space. The result is

$$\xi^{(1)}(k\sigma,\omega)=-[\omega-(1-n_{\bar\sigma})I]^{-2}I^2\int\int\int\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{d\omega_3}{2\pi}\frac{1}{N^2}\sum_{k'}\sum_{q}(A_{q\sigma}(\omega_1)[1-f(\omega_1)]G_0^{-1}(k\sigma;\omega)$$
$$\times\{\epsilon_{k'}L_{k',k-q}(02;ab)[1-f(\omega_2)]f(\omega_3)$$
$$-\epsilon_{k'}L_{k',k-q}(20;ab)[1-f(\omega_3)]f(\omega_2)\}[e^{\beta(\mu-\omega_1+\omega_2-\omega_3)}+1]/(\omega-\omega_1+\omega_2-\omega_3)$$
$$+A_{q\sigma}(\omega_1)f(\omega_1)G_0^{-1}(k\sigma;\omega)\{\epsilon_{k'}L_{k',k-q}(02;ab)f(\omega_2)[1-f(\omega_3)]$$
$$-\epsilon_{k'}L_{k',k-q}(20;ab)f(\omega_3)[1-f(\omega_2)]\}[1+e^{-\beta(\mu-\omega_1+\omega_2-\omega_3)}]/(\omega-\omega_1+\omega_2-\omega_3))\,, \qquad \text{(B9)}$$

where

$$L_{k'k-q}(02;ab)=\sum_{R_1}\sum_{R_2}\Lambda(02;ab)A_{R_1R_a\sigma'}(\omega_2)A_{R_bR_1\sigma'}(\omega_3)e^{-ik'(R-R_2)}e^{-i(k-q)(R-R_1)}\,. \qquad \text{(B10)}$$

We want to evaluate the value of $\xi^{(1)}(k\sigma,\omega)$ for ω satisfying $G^{-1}(\omega)=G_0^{-1}(\omega)-\Sigma(\omega)=0$. Therefore, we may replace $G_0^{-1}(k\sigma,\omega)$ in Eq. (B9) by $\Sigma(k\sigma,\omega)+G^{-1}(k\sigma,\omega)$ and set $G^{-1}(k\sigma,\omega)=0$. Since $\Sigma(k\sigma,\omega)$ is of order ϵ, the value of $\xi^{(1)}(k\sigma,\omega)$ calculated in this manner is of order ϵ^2.

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$$iG_{RR\sigma}(tt^-)\delta(t^-t')+iG_{RR\sigma}(tt^+)\delta(t^+t')=iG_{RR\sigma}(tt'),$$

which is incorrect. The correct value of the expression on the left-hand side of the above equation should be calculated as follows:

$$\begin{aligned}&iG_{RR\sigma}(tt^-)\delta(t^-t')+iG_{RR\sigma}(tt^+)\delta(t^+t')\\&=[1-\langle N_{R\sigma}(t)\rangle]\delta(tt')+[-\langle N_{R\sigma}(t)\rangle]\delta(tt')\\&=[1-2\langle N_{R\sigma}(t)\rangle]\delta_{tt'},\end{aligned}$$

and it is not equal to $iG_{RR\sigma}(tt')$. Therefore, the energy of an electron added to the lattice should not be different from the energy of the same electron removed from the lattice as suggested in Ref. 14.

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