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Functional-derivative study of the Hubbard model. III. Fully renormalized Green's function

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The functional-derivative method of calculating the Green's function developed earlier for the Hubbard model is generalized and used to obtain a fully renormalized solution. Higher-order functional derivatives operating on the basic Green's functions, G and Γ, are all evaluated explicitly, thus making the solution applicable to the narrow-band region as well as the wide-band region. Correction terms Φ generated from functional derivatives of equal-time Green's functions of the type $\delta^n\langle N\rangle/\delta\epsilon^n$, etc., with $n \geq 2$. It is found that the Φ's are, in fact, renormalization factors involved in the self-energy Σ and that the structure of the Φ's resembles that of Σ and contains the same renormalization factors Φ. The renormalization factors Φ are shown to satisfy a set of equations and can be evaluated self-consistently. In the presence of the Φ's, all difficulties found in the previous results (papers I and II) are removed, and the energy spectrum ω can now be evaluated for all occupations n. The Schwinger relation is the only basic relation used in generating this fully self-consistent Green's function, and the Baym-Kadanoff continuity condition is automatically satisfied.

I. INTRODUCTION

In the first two papers in this series, I[1] and II[2], we have developed a functional-derivative method of solving equations of motion for basic Green's functions and applied it to obtain a nonmagnetic solution of the Hubbard model.[3] The method is neither a perturbation method in the conventional sense nor a decoupling approach as used in the equation-of-motion method.[4] By using an exact relation found by Schwinger,[5] higher-order Green's functions Γ', which appear in the equations of motion for the basic Green's functions G and Γ, are all transformed to functional derivatives of G and Γ with respect to an external field $\delta\epsilon$

$$\Gamma' = F\left(\frac{\delta G}{\delta\epsilon}, \frac{\delta\Gamma}{\delta\epsilon}\right). \tag{1.1}$$

For example,

$$\begin{aligned}\langle\langle C_{R\sigma}(t)C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle &= i\frac{\delta\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle}{\delta\epsilon(RR''\bar\sigma t)}\\ &\quad + \langle C^\dagger_{R\bar\sigma}(t)C_{R''\bar\sigma}(t)\rangle\langle\langle C_{R\sigma}(t)C^\dagger_{R'\sigma}(t')\rangle\rangle,\end{aligned} \tag{1.2}$$

where $C_{R\sigma}$ is the distribution operator of an electron with spin σ at site R and $\bar\sigma$ denotes a spin opposite to σ. Since an infinite hierarchy of equations is replaced by the functional derivatives $\delta G/\delta\epsilon$ and $\delta\Gamma/\delta\epsilon$, and only two basic Green's functions G and Γ enter the two equations, the problem can, in principle, be solved. The basic difficulty associated with the equation-of-motion method is thus formally eliminated.

In fact, we have obtained an exact expression for the self-energy Σ in Paper I and evaluated it under the following two restrictions in Paper II. First, the equal-time Green's functions, $\langle N_{R\sigma}(t)\rangle = \langle C^\dagger_{R\sigma}(t)C_{R\sigma}(t)\rangle$ and $\langle C^\dagger_{R\sigma}(t)C_{R'\sigma}(t)\rangle$ defined by Eq. (2.11) of Paper I, are assumed to be independent of the external field $\delta\epsilon$, that is, $\delta\langle N\rangle/\delta\epsilon = \delta\langle C^\dagger C\rangle/\delta\epsilon = 0$, and, second, a correction term $\Pi(\Delta)$ involving higher-order derivatives is neglected; otherwise, this solution is exact for any values of the hopping matrix elements $\epsilon_{RR'}$ and the interaction energy I. Here Δ is the bandwidth. This solution will be referred to as the step-1 solution. The step-1 solution was improved in Sec. V of Paper II by adding contributions Φ from $\delta\langle N\rangle/\delta\epsilon$ and $\delta\langle C^\dagger C\rangle/\delta\epsilon$ as perturbations. From the calculation in Secs. II and III, it will be found that contributions from $\delta\langle N\rangle/\delta\epsilon$, $\delta\langle C^\dagger C\rangle/\delta\epsilon$, and $\Pi(\Delta)$ are all of order Δ^2/I under expansions in powers of (ϵ/I), and even that part of the step-1 solution linear in ϵ obtained in Paper I is exact in that order, a result never attained before.

Nevertheless, serious defects still remain in those solutions. First, since the term $\Pi(\Delta)$ of order Δ^2/I is neglected, the result cannot be extended to the wide-band region and hence the metal-nonmetal transition cannot be studied. Second, the calculation of the correction terms ϕ developed in Sec. V of Paper II is incomplete, overestimating the value of ϕ greatly. Moreover, the correction terms ϕ are introduced to prevent functions called p, K, and L appearing in the step-1 solution [see Eqs. (4.16) and (5.2) of Paper II] from diverging in the limit of low electron (or hole) concentration, but possible corrections to other equal-time Green's function involved are not fully included. In fact, the parameters x and y involved in ϕ are calculated under the restriction that $\delta\langle N\rangle/\delta\epsilon = \delta\langle C^\dagger C\rangle/\delta\epsilon = 0$ [see the paragraph involving Eq. (5.10) of Paper II]. The result given by Eq. (5.12) of Paper II is then inconsistent, and the value of ϕ so obtained becomes infinitely large in the nearly empty limit because of this inconsistency. Third, poles of the Green's function given by the step-1 solution become complex in the limit where the lower band is nearly or exactly filled. This is in contradiction to the basic mathematical requirement[6] that, except for the discontinuity along the real axis, the Green's function must be analytic in the complex ω plane. Hence properties of the Hubbard model cannot be properly evaluated by the use of the step-1 solution in the limit where the lower band is nearly or exactly filled, even though this is one of the most interesting cases in the Hubbard model.

Contributions from higher-order functional derivatives operating on the basic Green's functions G and Γ can be included easily. Contributions Φ from functional derivatives of all equal-time Green's functions, which include those entering the coefficients x and y in the resulting correction terms Φ, can be calculated in exactly the same manner as the original Φ's themselves are calculated. The divergences of p, K, and L in the results of Sec. V of Paper II are thus eliminated, and the Green's function so obtained is a renormalized one. Because of the inconsistency discussed in the preceding paragraph and in particular, because of the divergence of the correction terms ϕ, however, it is not fully renormalized. A Green's function which is fully renormalized is introduced in Sec. II of this paper; it is obtained by including the contributions from $\delta\langle N\rangle/\delta\epsilon$ and $\delta\langle C^\dagger C\rangle/\delta\epsilon$ everywhere, neglecting only higher-order derivatives $\delta^n\langle N\rangle/\delta\epsilon^n$, etc., with $n \geq 2$.

In Sec. II, we construct the fully renormalized Green's function which is valid both in the narrow-band region and wide-band regions. The analysis developed in Sec. III will suggest that the correction terms Φ involved in the self-energy Σ are, in fact, renormalization factors. The Φ's are generated from equal-time Green's functions in a manner analogous to the way Σ is contructed, and involve renormalization factors which are closely related to the original Φ's. Therefore, the Φ's can be evaluated self-consistently, eliminating *all* divergencies found in the step-1 solution. As far as we are aware of, this is the first time that such renormalization factors are found based solely on first principles.[7] Since the Schwinger relation (1.1) or (1.2) is the only basic relation used in generating the fully renormalized solution and the functional derivatives are all evaluated self-consistently, particle number, momentum, and energy are conserved in the manner discussed by Baym and Kadanoff,[8] ensuring the significance of the renormalization factors found here. Any other method, which is by its definition not completely based on the Schwinger relation, does not necessarily satisfy this relation nor the conservation laws. Hence, it is necessary to adjust approximations in such a way that these laws are properly obeyed. In Sec. IV, we evaluate the energy spectrum of an electron in the narrow-band region and show that the fully renormalized Green's function, having finite correction terms Φ, is indeed analytic everywhere except for the discontinuity along the real axis, and that properties of the Hubbard model can now be calculated for all occupations n without introducing basic difficulties. For simplicity, however, we shall treat only a less than singly occupied atomic orbital or an exactly singly occupied orbital in the narrow-band region so that the lower band is partly or completely filled but the upper band remains empty. The case where the upper band is partly filled may be treated in exactly the same manner by reversing the roles of electrons and holes.

In the following paper, Ref. 9, we shall calculate the ground-state energy, the chemical potential, and the dynamic and thermodynamic stability conditions in the narrow-band region using the various approximate Green's functions available. We find that all previous solutions fail to satisfy these stability conditions for some occupations n while the fully renormalized solution does satisfy them for all occupations n. Our results also suggest that the Landau theory of Fermi liquids[10] does not apply to the Hubbard model and that a gap appears between the chemical potential and the excitation spectrum. The consequences will be analyzed in detail (Ref. 11).

II. FULLY RENORMALIZED GREEN'S FUNCTION

The exact expression for the self-energy Σ found in Eq. (3.21) of I may be rewritten as[12]

$$\Sigma_{RR'\sigma}(tt') = \sum_{n=0}^{\infty} [\bar\lambda_{\bar\sigma}(Rt)\bar B_{\bar\sigma}(Rt)I]^{-n} \times \int_0^{-i\beta} dt_1 \sum_{R_1} \{[\delta(R\sigma t)]^n[\delta(R\sigma t)+\bar\delta(R\bar\sigma t)] \times G_{RR_1\sigma}(tt_1)\} G^{-1}_{R_1R'\sigma}(t_1t'), \tag{2.1}$$

where

$$\delta(R\sigma t) \equiv [\bar{\lambda}_{\bar{\sigma}}(Rt)]^2 \bar{B}_{\bar{\sigma}}(Rt) \sum_{R'' \neq R} \epsilon(RR''\sigma t)\left(i \frac{\delta}{\delta\epsilon(RR''\sigma t^-)} - i \frac{\delta}{\delta\epsilon(RR''\sigma t^+)}\right), \tag{2.2a}$$

$$\bar{\delta}(R\bar{\sigma} t) \equiv F_{\bar{\sigma}}(Rt) \sum_{R'' \neq R} \left[\epsilon(RR''\bar{\sigma} t)\left((w-I)^{-1} i \frac{\delta}{\delta\epsilon(RR''\bar{\sigma} t^-)} - w^{-1} i \frac{\delta}{\delta\epsilon(RR''\bar{\sigma} t^+)}\right) - \epsilon(R''R\bar{\sigma} t)\left((w-I)^{-1} i \frac{\delta}{\delta\epsilon(R''R\bar{\sigma} t^+)} - w^{-1} i \frac{\delta}{\delta\epsilon(R''R\bar{\sigma} t^-)}\right)\right], \tag{2.2b}$$

$$w = i\partial/\partial t, \tag{2.3a}$$

$$\bar{\lambda}_{\bar{\sigma}}(Rt) = [w - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I]^{-1}, \tag{2.3b}$$

$$\bar{F}_{\bar{\sigma}}(Rt) = [\langle \bar{N}_{R\bar{\sigma}} \rangle (w-I)^{-1} + (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) w^{-1}]^{-1}, \tag{2.3c}$$

$$\bar{B}_{\bar{\sigma}}(Rt) = \langle \bar{N}_{R\bar{\sigma}} \rangle (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) + I^{-1} \sum_{R'' \neq R} [\epsilon(RR''\bar{\sigma} t) \langle \bar{C}^\dagger_{R\bar{\sigma}} \bar{C}_{R''\bar{\sigma}} \rangle - \epsilon(R''R\bar{\sigma} t) \langle \bar{C}^\dagger_{R''\bar{\sigma}} \bar{C}_{R\bar{\sigma}} \rangle], \tag{2.3d}$$

and $\langle \bar{N}_{R\sigma} \rangle$ is defined later in Eq. (2.14).

The fully renormalized Green's function is then calculated as follows:

$$2\pi G^{-1}_{k\sigma}(\omega) = \omega - \bar{\Theta}_\sigma(\omega)\epsilon_k - \langle \bar{N}_{R\bar{\sigma}} \rangle I\omega[\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I]^{-1} - \bar{P}_{k\sigma}(\omega) - \bar{\Theta}_\sigma(\omega)\bar{K}_\sigma(\omega)\epsilon_k[\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I - \bar{K}_\sigma(\omega)]^{-1}$$
$$- \{\langle \bar{N}_{R\bar{\sigma}} \rangle (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I^2 \bar{\Theta}_\sigma(\omega)\epsilon_k + \bar{L}_{k\sigma}(\omega)\epsilon_k[\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I]\}$$
$$\times [\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I](\bar{D}'_\sigma)^{-1}[\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I - \bar{K}_\sigma(\omega)]^{-1}, \tag{2.4}$$

where

$$\bar{P}_{k\sigma}(\omega) = \sum_{R'} [(1 - 2\langle \bar{N}_{R\sigma} \rangle)\epsilon_{RR'} \langle \bar{C}^\dagger_{R\bar{\sigma}} \bar{C}_{R'\bar{\sigma}} \rangle + 2\epsilon_{RR'} \langle \bar{C}^\dagger_{R'\sigma} \bar{C}_{R\sigma} \rangle \langle \bar{C}^\dagger_{R\bar{\sigma}} \bar{C}_{R'\bar{\sigma}} \rangle e^{-ik(R-R')}](\bar{D}_{RR'\sigma})^{-1}, \tag{2.5a}$$

$$\bar{K}_\sigma(\omega) = \sum_{R'} [(\langle \bar{N}_{R\bar{\sigma}} \rangle - \langle \bar{N}_{R\sigma} \rangle)(\bar{D}^{(+)}_{RR'\sigma})^{-1} + (1 - \langle \bar{N}_{R\sigma} \rangle - \langle \bar{N}_{R\bar{\sigma}} \rangle)(\bar{D}^{(-)}_{RR'\sigma})^{-1}]\epsilon_{RR'} \langle \bar{C}^\dagger_{R\bar{\sigma}} \bar{C}_{R'\bar{\sigma}} \rangle, \tag{2.5b}$$

$$L_{k\sigma}(\omega) = \sum_{R'} [(\bar{D}^{(+)}_{RR'\sigma})^{-1} + (\bar{D}^{(-)}_{RR'\sigma})^{-1}]\epsilon_{RR'} \langle \bar{C}^\dagger_{R'\sigma} \bar{C}_{R\sigma} \rangle \langle \bar{C}^\dagger_{R\bar{\sigma}} \bar{C}_{R'\bar{\sigma}} \rangle e^{-ik(R-R')}, \tag{2.5c}$$

$$\bar{\Theta}_\sigma(\omega) = [1 + (\bar{\lambda}_{\bar{\sigma}}/I)\Sigma_{RR\sigma}]^{-1}, \tag{2.5d}$$

$$\bar{D}_{RR'\sigma} = (\tfrac{1}{2} - \langle \bar{N}_{R\bar{\sigma}} \rangle)^2 - (\tfrac{1}{2} - \langle \bar{N}_{R\sigma} \rangle)^2 + \langle \bar{C}^\dagger_{R\sigma} \bar{C}_{R'\sigma} \rangle \langle \bar{C}^\dagger_{R'\sigma} \bar{C}_{R\sigma} \rangle, \tag{2.6a}$$

$$\bar{D}^{(\pm)}_{RR'\sigma} = (1 - \bar{g}_{\bar{\sigma}}\bar{\mu}_{\bar{\sigma}})(1 - \bar{\mu}_{\bar{\sigma}})(\bar{\lambda}_{\bar{\sigma}})^{-2}(\bar{g}_{\bar{\sigma}})^{-1} - (\tfrac{1}{2} - \langle \bar{N}_{R\sigma} \rangle)^2 + \langle \bar{C}^\dagger_{R\sigma} \bar{C}_{R'\sigma} \rangle \langle \bar{C}^\dagger_{R'\sigma} \bar{C}_{R\sigma} \rangle \pm (1 - \bar{g}_{\bar{\sigma}})(\bar{\lambda}_{\bar{\sigma}})^{-1}(\bar{g}_{\bar{\sigma}})^{-1}(\tfrac{1}{2} - \langle \bar{N}_{R\sigma} \rangle), \tag{2.6b}$$

$$\bar{D}'_\sigma = [\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I]^2 - \langle \bar{N}_{R\bar{\sigma}} \rangle (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I^2, \tag{2.6c}$$

$$\bar{\mu}_{\bar{\sigma}} = (\omega - I/2)[\omega - (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle) I]^{-1}, \tag{2.7a}$$

$$\bar{g}_{\bar{\sigma}} = [1 - (\bar{\lambda}_{\bar{\sigma}})^2 \langle \bar{N}_{R\bar{\sigma}} \rangle (1 - \langle \bar{N}_{R\bar{\sigma}} \rangle)]^{-1}. \tag{2.7b}$$

The above result is obtained in the following three steps.

Step 1. If we neglect terms with $n \geq 1$, which involve higher-order derivatives on the right-hand side of Eq. (2.1) and which is denoted by $\Pi(\Delta)$ in Papers I and II, and if we assume that equal-time Green's functions $\langle N_{R\sigma}(t) \rangle$ and $\langle C^\dagger_{R\sigma}(t) C_{R'\sigma}(t) \rangle$ are independent of the external field $\delta\epsilon$ (that is, $\delta\langle N \rangle/\delta\epsilon = \delta\langle C^\dagger C \rangle/\delta\epsilon = 0$), Eq. (2.1) can be solved exactly by a power-expansion method developed in Paper II. The result $(G^{(1)})^{-1}_{k\sigma}(\omega)$ expressed by Eq. (4.15) of II may be found in Eqs. (2.4)–(2.7) by removing bars over all letters and by setting $\Theta_\sigma(\omega)$ equal to unity. Here $\langle N_{R\sigma} \rangle = n_\sigma$ and $\langle C^\dagger_{R\sigma} C_{R'\sigma} \rangle$ are the values of equal-time Green's functions $\langle N_{R\sigma}(t) \rangle$ and $\langle C^\dagger_{R\sigma}(t) C_{R'\sigma}(t) \rangle$ in the limit of a vanishing external field.

The step-1 result $G^{(1)}$ contains a number of difficulties. First, the terms with $n \geq 1$, which are neglected in the step-1 calculation, yield corrections of order Δ^2/I and hence the result $G^{(1)}$ is limited to the narrow-band region even though, after the neglect of those higher-order terms with $n \geq 1$, the basic equation is solved by a nonperturbative method and all approximations included thereafter are equally valid in the wide- and narrow-band regions.

Second, in the nonmagnetic case ($n_\sigma = n_{\bar\sigma}$) the denominator $D_{RR'\sigma}$ of $P_{k\sigma}$ becomes equal to $\langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle^2$, making the value of $P_{k\sigma}$ abnormally large. This difficulty appears because $\langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle$, which is given by

$$\langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle = \frac{1}{N_a}\sum_{k i} A^{(i)}_{k\sigma} f(\omega^{(i)}_{k\sigma}) e^{-ik(R-R')}, \qquad (2.8)$$

vanishes in the limit of a nearly empty band ($n_\sigma = n_{\bar\sigma} \approx 0$) regardless of the bandwidth Δ, making the value of $P_{k\sigma}$ infinitely large in this limit. Here $A^{(i)}_{k\sigma}$ is the spectral weight of the ith solution $\omega^{(i)}_{k\sigma}$ of $G_{k\sigma}(\omega)$ and $f(\omega)$ the Fermi function.[13] $\langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle$ also vanishes in the narrow-band limit ($\Delta \approx 0$) of a nearly-half-filled case ($n_\sigma = n_{\bar\sigma} \approx \frac{1}{2}$), although $P_{k\sigma}$ remains finite (and negative) because of the factor $(1-2n_\sigma)$ which also vanishes. Since, in the limit of the half-filled case ($n_\sigma = n_{\bar\sigma} = \frac{1}{2}$), $K + L_k\epsilon_k$ becomes equal to $P_{k\sigma}$ and, even in other cases, shares essentially the same functional form, it also exhibits the difficulties just described. That is, $K + L_k \epsilon_k$ also becomes infinitely large in the nearly empty limit and, although it remains finite, the value is too large in the nearly-half-filled limit.

The third and the most serious difficulty is that the excitation spectrum ω calculated from $(G^{(1)})^{-1} = 0$ becomes complex in the nearly-half-filled case, making $G^{(1)}$ nonanalytic and unphysical as is elaborated in the following. If we regard $P_\sigma(\omega)$, $K_\sigma(\omega)$, and $L_{k\sigma}(\omega)$ to be constants independent of ω, the eigenvalue equation $(G^{(1)})^{-1}(\omega) = 0$ is an equation of fifth degree in ω. We then find that, unless $P_{k\sigma}$ and K_σ are abnormally large (of order I) and unless $n_\sigma = n_{\bar\sigma} \approx \frac{1}{2}$, the lower-band solution $\omega^{(1)}_{k\sigma}$ being proportional to Δ is isolated from all other poles $\omega^{(i)}_{k\sigma}$, $i = 2, 3, \ldots, 5$, involving the large parameter I. The lower-band solution $\omega^{(1)}_{k\sigma}$ can then be expanded unambiguously in powers of ϵ_k/I. The result

$$\tilde\omega^{(1)}_{k\sigma} = \frac{(1-n_{\bar\sigma})^2}{1-2n_{\bar\sigma}}\epsilon_k + (1-n_{\bar\sigma})P_{k\sigma} + O(\epsilon^2/I) \qquad (2.9)$$

is exact up through terms linear in ϵ.

In a nearly-half-filled case ($n_\sigma = n_{\bar\sigma} \approx \frac{1}{2}$), the value of the second-lowest solution $\tilde\omega^{(a)}_\sigma$

$$\tilde\omega^{(a)}_\sigma = \{(1-n_{\bar\sigma}) - [n_{\bar\sigma}(1-n_{\bar\sigma})]^{1/2}\} I + \cdots, \qquad (2.10)$$

becomes small and comparable to $\tilde\omega^{(1)}_{k\sigma}$. Therefore, it is necessary to solve a "quadratic" equation obtained from Eq. (2.4) by neglecting K_σ and $L_{k\sigma}$ of order ϵ^2.

The results are then

$$\omega^{(1)}_{k\sigma},\ \omega^{(a)}_{k\sigma} = \tfrac{1}{2}\big(\tilde\omega^{(1)}_{k\sigma} + \tilde\omega^{(a)}_\sigma + X \pm \{(\tilde\omega^{(a)}_\sigma + X - \tilde\omega^{(1)}_{k\sigma})^2 + 4X[\tilde\omega^{(1)}_{k\sigma} - (1-n_{\bar\sigma})I]\}^{1/2}\big), \qquad (2.11)$$

where X is a parameter of order ϵ_k. As long as $|\tilde\omega^{(a)}_\sigma| \gg |\tilde\omega^{(1)}_{k\sigma}|$, the above expression can be expanded in the form shown in Eq. (2.9). In the nearly-half-filled case, however,

$$|4(1-n_{\bar\sigma})XI| \geq |\tilde\omega^{(a)}_\sigma + X - \tilde\omega^{(1)}_{k\sigma}|^2, \qquad (2.12)$$

and hence the expansion (2.9) becomes invalid. If $\epsilon_k > 0$, in particular, the quantity $\{\cdots\}$ on the right-hand side of Eq. (2.11) becomes negative making $\omega^{(1)}_{k\sigma}$ and $\omega^{(a)}_{k\sigma}$ a paired complex. This is a serious defect in the present approximation because the Green's function should be a well-behaved function except along the real axis and should not have complex poles.[6,13] Therefore, the nearly- or completely-half-filled case cannot be treated under the present approximation, even though this is the most interesting case in the Hubbard model.

Step 2. The contributions from higher-order derivatives involved in Σ can now be evaluated by inserting the results $G^{(1)}$ and $\Sigma^{(1)}$ obtained in step 1. Under the present approximation, only the term $n=1$ involving second derivatives contributes, yielding

$$\Sigma_{RR\sigma}(tt') = \Sigma^{(1)}_{RR\sigma}(tt'), \qquad (2.13a)$$

$$\Sigma_{RR'\sigma}(tt') = \Sigma^{(1)}_{RR'\sigma}(tt') + [\lambda_{\bar\sigma}(Rt)/I]\,\Sigma_{RR\sigma}(tt)(\Delta G)^{-1}_{RR'\sigma}(tt'), \qquad (2.13b)$$

where $(\Delta G)^{-1}$ is a portion of the result G^{-1}, which is proportional to $\epsilon_{RR'} + \delta\epsilon(RR'\sigma t)$. The result $(G^{(2)})^{-1}_{k\sigma}(\omega)$ is again expressed in the form (2.4) except that bars over letters are all removed in Eqs. (2.4)–(2.7). However, $\Theta_\sigma(\omega)$ is now given by Eq. (2.5d); that is,

$$\Theta_\sigma(\omega) = [1 + (\lambda_{\bar\sigma}/I)\Sigma^{(2)}_{RR\sigma}]^{-1}, \qquad (2.5d')$$

and the result can be applied to the wide-band region although it still exhibits the second and third difficulties discussed in step 1.

Step 3. Finally, the contributions Φ from equal-time Green's functions can be included in a fully self-consistent manner by repeated applications of the basic method developed in Sec. V of Paper II to all equal-time Green's functions, which enter $G^{(2)}$ including those involved in the resulting Φ's. The result is then given by Eqs. (2.4)–(2.7), where

$$\langle \bar N_{R\sigma'}\rangle = n_{\sigma'} + \Phi_\sigma(R\sigma';\omega), \qquad (2.14a)$$

$$\langle \bar C^\dagger_{R\sigma'} \bar C_{R'\sigma'}\rangle = \langle C^\dagger_{R\sigma'} C_{R'\sigma'}\rangle + \Phi_\sigma(RR'\sigma';\omega), \qquad (2.14b)$$

and the Φ's are correction terms similar to

$\phi_{RR_1\sigma}(R_1R_2;\omega)$ introduced by Eq. (5.15) of II, and can be obtained by inserting the following changes in Eqs. (5.15), (5.16), and (5.6) of II: (i) $D_{RR'\sigma'}(t')$ in Eq. (5.6) of Paper II is replaced by $\langle \overline{N}_{R\sigma'}\rangle$ or $\langle \overline{C}^\dagger_{R\sigma'}\overline{C}_{R'\sigma'}\rangle$. (ii) All equal-time Green's functions denoted by n_σ and $\langle C^\dagger_{R\sigma}C_{R'\sigma}\rangle$ in Eq. (5.16) of II are replaced by the expressions on the right-hand sides of Eqs. (2.14a) and (2.14b).

The correction terms Φ are now included everywhere in the Green's function G in a fully self-consistent manner. If, in fact, G given by Eq. (2.4) is inserted into the right-hand side of the self-energy expression (2.1), we obtain Σ, which is exactly the same as the original Σ found in Eq. (2.4) except for terms involving second derivatives of equal-time Green's functions,

$$\delta^2\langle N_{R\sigma}(t)\rangle/[\delta\epsilon(RR'\sigma t)\delta\epsilon(R''R'''\sigma' t)],$$

etc. Since the second derivatives are three-particle correlation functions and independent of the current density and the time derivative of the total angular momentum, the conservation laws of number, momentum, and energy are indeed satisfied by the fully renormalized solution (2.4) in the presence of the external field $\delta\epsilon$, proving our assertion in Sec. I.

We now want to calculate the correction terms Φ correctly through terms linear in ϵ. Since the expression for Φ is already linear in ϵ, it is sufficient to calculate $\delta\langle N\rangle/\delta\epsilon$ through terms of order ϵ°. Use of the results found in Eqs. (B1)–(B4) of Paper I yields[14]

$$\Phi_\sigma(R\sigma;\omega)=\overline{\lambda}_{\overline{\sigma}}\langle\overline{N}_{R\sigma}\rangle\varphi^{(1)}_{R\sigma}+\varphi^{(2)}_{R\sigma}+\cdots, \tag{2.15a}$$

$$\Phi_\sigma(R\overline{\sigma};\omega)=\varphi^{(1)}_{R\sigma}+\overline{\lambda}_{\sigma}\langle\overline{N}_{R\overline{\sigma}}\rangle\varphi^{(2)}_{R\sigma}+\cdots, \tag{2.15b}$$

$$\Phi_\sigma(RR'\sigma';\omega)=\overline{\lambda}_{\overline{\sigma}'}\langle\overline{C}^\dagger_{R'\sigma'}\overline{C}_{R\sigma'}\rangle\Phi_\sigma(R\overline{\sigma};\omega)+\cdots, \tag{2.15c}$$

where

$$\varphi^{(1)}_{R\sigma}=\sum_{R_1}\{(\overline{d}^{(1)}_{RR_1\sigma}+\overline{\lambda}_{\overline{\sigma}}\overline{d}^{(2)}_{RR_1\sigma})[\epsilon_{RR_1}\eta_{R_1R\sigma}(\omega)]+(\overline{d}^{(1)}_{RR_1\sigma}-\overline{\lambda}_{\overline{\sigma}}\overline{d}^{(2)}_{RR_1\sigma})[\epsilon_{R_1R}\zeta_{RR_1\sigma}(\omega)]\}(\overline{D}_{RR_1\sigma}\overline{d}_0)^{-1}, \tag{2.16a}$$

$$\varphi^{(2)}_{R\sigma}=\sum_{R1}[2\overline{\lambda}^2_{\overline{\sigma}}\overline{d}^{(2)}_{RR_1\sigma}\epsilon_{RR_1}\langle\overline{C}^\dagger_{R\overline{\sigma}}\overline{C}_{R_1\overline{\sigma}}\rangle\xi_\sigma(\omega)](\overline{D}_{RR_1\sigma}\overline{d}_0)^{-1}, \tag{2.16b}$$

$$\overline{d}_0=1-\overline{\lambda}_\sigma\overline{\lambda}_{\overline{\sigma}}\langle\overline{N}_{R\sigma}\rangle\langle\overline{N}_{R\overline{\sigma}}\rangle. \tag{2.17a}$$

$$\overline{d}^{(1)}_{RR_1\sigma}=\tfrac{1}{2}-\langle\overline{N}_{R\sigma}\rangle+\langle\overline{C}^\dagger_{R_1\sigma}\overline{C}_{R\sigma}\rangle, \tag{2.17b}$$

$$\overline{d}^{(2)}_{RR_1\sigma}=(\tfrac{1}{2}-\omega/I)(\tfrac{1}{2}-\langle\overline{N}_{R\overline{\sigma}}\rangle)+(\tfrac{1}{2}-\langle\overline{N}_{R\sigma}\rangle)^2-\langle\overline{C}^\dagger_{R\sigma}\overline{C}_{R_1\sigma}\rangle\langle\overline{C}^\dagger_{R_1}\overline{C}_{R\sigma}\rangle, \tag{2.17c}$$

and ξ, η, and ζ are the Fourier transforms of $[G(tt_1)G(t_1t)G(tt_1)]$;

$$\xi_\sigma(Z_\nu)=\int_0^{-i\beta}dt\,e^{iZ_\nu(t-t_1)}G_{RR\sigma}(tt_1)G_{RR\sigma}(t_1t)G_{RR\sigma}(tt_1), \tag{2.18a}$$

$$\eta_{RR_1\sigma}(Z_\nu)=\int_0^{-i\beta}dt\,e^{iZ_\nu(t-t_1)}G_{RR\sigma}(tt_1)G_{RR\overline{\sigma}}(t_1t)G_{RR_1\overline{\sigma}}(tt_1), \tag{2.18b}$$

$$\zeta_{R_1R\sigma}(Z_\nu)=\int_0^{-i\beta}dt\,e^{iZ_\nu(t-t_1)}G_{RR\sigma}(tt_1)G_{R_1R\overline{\sigma}}(t_1t)G_{RR\overline{\sigma}}(tt_1). \tag{2.18c}$$

These values, calculated at discrete points $Z_\nu=(\pi\nu/-i\beta)+\mu$ with odd integers ν, can be analytically continued[15] to all ω. For instance, $\eta_{RR_1\sigma}(\omega)$ becomes

$$\eta_{RR_1\sigma}(\omega)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{d\omega_3}{2\pi}\frac{A_{RR\sigma}(\omega_1)A_{RR\overline{\sigma}}(\omega_2)A_{RR_1\overline{\sigma}}(\omega_3)}{\omega-\omega_1+\omega_2-\omega_3}f(\omega_1,\omega_2,\omega_3), \tag{2.19}$$

where

$$f(\omega_1,\omega_2,\omega_3)=\frac{f(\omega_1)[1-f(\omega_2)]f(\omega_3)}{f(\omega_1-\omega_2+\omega_3)}=\frac{[1-f(\omega_1)]f(\omega_2)[1-f(\omega_3)]}{1-f(\omega_1-\omega_2+\omega_3)}. \tag{2.20}$$

The Fourier transforms of $\sum\epsilon_{R_1R}\zeta_{RR_1\sigma}(\omega)$, etc., are then reduced to the form

$$\sum\epsilon_k\zeta_{k\sigma}(\omega)=(2\pi N_a)^{-1}\sum_k\{B^{(1)}(\omega_k)f(\omega_k)+B^{(2)}(\omega_k)[1-f(\omega_k)]\}/(\omega-\omega_k), \tag{2.21}$$

where

$$B^{(j)}(\omega_k) = (2\pi N_a)^{-2}\sum_{k_1 i_1}\sum_{k_2 i_2}\sum_{k_3 i_3} \epsilon_{k_2} A^{(i)}_{k_1\sigma}A^{(i)}_{k_2\sigma}A^{(i)}_{k_3\sigma}\theta^{(j)}\,\delta(\omega_k - \omega_{k_1} + \omega_{k_2} - \omega_{k_3}),$$
$$\Theta^{(1)} = [1 - f(\omega_{k_1})][1 - f(\omega_{k_3})],$$
$$\Theta^{(2)} = f(\omega_{k_1}) f(\omega_{k_3}). \qquad (2.22)$$

III. CALCULATION OF THE RENORMALIZATION FACTORS Φ

In Sec. II, we have shown that, in the absence of the correction terms Φ, the quantities P, K, and L become abnormally large both in the nearly empty limit and in the nearly-half-filled limit, and also the solution ω becomes unphysical in the nearly-half-filled case. We now demonstrate that those two difficulties can be removed by the inclusion of the Φ's and that the Φ's can be regarded as renormalization factors. For simplicity, we shall limit our calculation to the narrow-band region.

Let us first note that the structure of the Φ's given by Eqs. (2.15)–(2.18) resembles the structure of P defined by Eq. (2.5). P is generated in the course of constructing the Green's function and represents a static interaction energy with all electrons of opposite spin $\bar{\sigma}$, while the Φ's result from repeated operations of functional derivatives on the equal-time Green's functions and represents fluctuations in the densities of electrons at atomic sites, which are introduced by the creation or destruction of electron-hole pairs with opposite spin. Both $\bar{P}_\sigma$ and the Φ's have a common denominator $\bar{D}_\sigma$ given by Eq. (2.6a)

$$\bar{D}_\sigma = \langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle^2 + 2\delta[\Phi_\sigma(R\sigma;\omega) - \Phi_\sigma(R\bar{\sigma};\omega)] - \Phi_\sigma(R\sigma;\omega)^2 + \Phi_\sigma(R\bar{\sigma};\omega)^2, \qquad (3.1)$$

where $\delta = \frac{1}{2} - n_\sigma = \frac{1}{2} - n_{\bar{\sigma}}$. Since $\langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle$ is smaller than the Φ's entering on the right-hand side of Eq. (3.1), the value of the denominator $\bar{D}_\sigma$ of the Φ's is determined by the original Φ's, suggesting that the Φ's are in fact the renormalization factors. It is essential to evaluate the Φ's given by Eq. (2.15)–(2.18) self-consistently.

There are two sets of Φ's: $\Phi_\sigma(R\sigma';\omega)$'s entering $G_{k\sigma}(\omega)$ for an electron k with spin σ and $\Phi_{\bar{\sigma}}(R\sigma';\omega)$'s entering $G_{k\bar{\sigma}}(\omega)$ for electron k with opposite spin σ. If the number N of electrons is appreciably smaller than the number N_a of atoms (that is, $N \ll N_a$) and the lower band is only partly filled, we may assume that an electron k with opposite spin $\bar{\sigma}$ behaves in exactly the same manner as the corresponding electron k with spin σ, making $G_{k\bar{\sigma}}(\omega)$ equal to $G_{k\sigma}(\omega)$; that is,

$$\Phi_{\bar{\sigma}}(R\bar{\sigma};\omega) = \Phi_\sigma(R'\sigma;\omega),$$
$$\Phi_{\bar{\sigma}}(R\sigma;\omega) = \Phi_\sigma(R'\bar{\sigma};\omega) \qquad (3.2a)$$

for the majority of sites R and $R'(\neq R)$. If the number N of electrons is comparable to the number N_a of atoms, however, the number of empty sites R into which an added electron can hop becomes small introducing strong correlations between two electrons with opposite spins. We then recognize that the equal-time Green's function $\langle N_{R\sigma'}(t)\rangle$ entering $G_{k\bar{\sigma}}(\omega)$ must be the same as $\langle N_{R\sigma'}(t)\rangle$ entering $G_{k\sigma}(\omega)$ and

$$\Phi_{\bar{\sigma}}(R\sigma;\omega) = \Phi_\sigma(R\sigma;\omega),$$
$$\Phi_{\bar{\sigma}}(R\bar{\sigma};\omega) = \Phi_\sigma(R\bar{\sigma};\omega) \qquad (3.2b)$$

for all R. Two electrons with opposite spin will then travel in time-dependent induced fields created from the common $\langle N_{R\sigma}(t)\rangle$ and $\langle N_{R\bar{\sigma}}(t)\rangle$. If an electron with spin σ is at site R, the induced field around a second electron with spin $\bar{\sigma}$ will be modified in such a way that the second electron $\bar{\sigma}$ is energetically prevented from entering the same site at the same time.

The following calculations will show that, although the two types of solutions just described in Eq. (3.2) are possible for all occupations $n_\sigma = n_{\bar{\sigma}}$, the solution satisfying condition (3.2a) is found to yield the ground state in the partly-filled-lower-band case ($N \ll N_a$), while the solution satisfying condition (3.2b) yields the ground state in the nearly-filled-lower-band case ($N \lesssim N_a$).

The magnitude of $\sum \epsilon_k \eta_{k\sigma}(\omega)$, $\sum \epsilon_k \zeta_{k\sigma}(\omega)$, and $\xi_\sigma(\omega)$ may be estimated by replacing $B^{(i)}(\omega)$ involved on the right-hand side of Eq. (2.21) by average values $B^{(i)}_{\rm av}$. We then find that

$$\sum \epsilon_k \eta_{k\sigma}(\omega) = -[n_\sigma(\tfrac{1}{2} - n_{\bar{\sigma}}) + n_{\bar{\sigma}}(\tfrac{1}{2} - n_\sigma)] \times (1 - n_\sigma)\Delta S_\sigma(\bar{\sigma}) K(\omega),$$
$$\sum \epsilon_k \zeta_{k\sigma}(\omega) = -[(\tfrac{1}{2} - n_\sigma)(\tfrac{1}{2} - n_{\bar{\sigma}}) + n_\sigma n_{\bar{\sigma}}] \times (1 - n_\sigma)\Delta S_\sigma(\bar{\sigma}) K(\omega), \qquad (3.4)$$
$$\xi_\sigma(\omega) = n_{\bar{\sigma}}(\tfrac{1}{2} - n_{\bar{\sigma}})(1 - n_\sigma) K(\omega),$$

where

$$S_\sigma(\bar{\sigma}) = (1 - n_\sigma)^{-1}\langle C^\dagger_{R\sigma} C_{R'\sigma}\rangle,$$
$$K(\omega) = (-1/\Delta)\ \ln|(\omega - \mu)/\Delta|, \qquad (3.5)$$

and R' is a nearest neighbor of R.

The magnitudes of the renormalization factors Φ in the narrow-band region ($\Delta \ll I$) can now be estimated as follows.

(i) In the nearly empty case ($n_\sigma = n_{\bar\sigma} \ll 1$), we have

$$\bar d_0 = 1\,, \quad \bar d^{(1)}_{RR'\sigma} = \bar d^{(2)}_{RR'\sigma} = \tfrac12\,, \quad \bar\lambda_{\bar\sigma} = -1\,,$$

and

$$\begin{aligned}\Phi_\sigma(R\bar\sigma;\omega) &= \mp\Big(-\sum_k \epsilon_k \zeta_{k\sigma}(\omega)\Big)^{1/2}\\ &\approx \mp\tfrac12\,[S_\sigma(\bar\sigma)K(\omega)\Delta]^{1/2}\,,\\ \Phi_\sigma(R\sigma;\omega) &= \mp\tfrac12 n_\sigma [S_\sigma(\bar\sigma)K(\omega)\Delta]^{1/2}\,,\\ \bar P_{k\sigma}(\omega) &\approx \mp 2[\Delta S_\sigma(\bar\sigma)/K(\omega)]^{1/2}\,.\end{aligned} \tag{3.6}$$

In Eq. (4.9) of Sec. IV, we shall find that the energy of an electron in the lower band is given by

$$\omega^{(1)}_{k\sigma} \approx [1 - n_{\bar\sigma} - \Phi_\sigma(R\bar\sigma;\omega)][\epsilon_k + \bar P_{k\sigma}(\omega)] + \cdots\,, \tag{3.7}$$

and hence the solution, which is obtained by taking upper signs in Eq. (3.6) and which satisfies condition (3.2a) for all R and R', yields the ground state with the lowest energy because both $\bar P_{k\sigma}$ and $\bar P_{k\bar\sigma}$ are small but negative, and the Φ's are negligible in Eq. (3.7).

(ii) If the lower band is nearly filled ($n_\sigma = n_{\bar\sigma} \approx \frac13$), we find that

$$\bar d_0 \approx \tfrac34\,, \quad \bar d^{(1)}_{RR'\sigma} \approx \tfrac16\,,$$
$$\bar d^{(2)}_{RR'\sigma} \approx \tfrac19\,, \quad \lambda \approx -\tfrac32\,,$$

and hence

$$\begin{aligned}\bar D_\sigma &= \tfrac13[\Phi_\sigma(R\sigma;\omega) - \Phi_\sigma(R\bar\sigma;\omega)]\\ &= \pm\tfrac19 [S_\sigma(\bar\sigma)K(\omega)\Delta]^{1/2}\,,\\ \Phi_\sigma(R\sigma;\omega) &= \Big(-\tfrac29\sum_k \epsilon_k\zeta_{k\sigma}(\omega) - \tfrac49\Delta S_\sigma(\bar\sigma)\xi_\sigma(\omega)\Big)\Big/\bar D_\sigma\\ &= \pm\tfrac{1}{27}[S_\sigma(\bar\sigma)K(\omega)\Delta]^{1/2}\,,\\ \Phi_\sigma(R\bar\sigma;\omega) &= \Big(\tfrac49\sum_k \epsilon_k\zeta_{k\sigma}(\omega) + \tfrac29\Delta S_\sigma(\bar\sigma)\xi_\sigma(\omega)\Big)\Big/\bar D_\sigma\\ &= \mp\tfrac{8}{27}[S_\sigma(\bar\sigma)K(\omega)\Delta]^{1/2}\,,\\ \bar P_{k\sigma}(\omega) &= \mp 2[S_\sigma(\bar\sigma)\Delta/K(\omega)]^{1/2}\,.\end{aligned} \tag{3.8}$$

We again find that the solution for the ground state is obtained by taking upper signs in Eq. (3.8) and by imposing condition (3.2a).

(iii) In the nearly-half-filled case, where $\delta = \frac12 - n_\sigma = \frac12 - n_{\bar\sigma}$ is of order Δ/I, the Φ's become of order unity. Hence

$$\begin{aligned}\bar d^{(1)}_{RR'\sigma} &= \delta - \Phi_\sigma(R\sigma;\omega) + \cdots\,,\\ \bar d^{(2)}_{RR'\sigma} &= \tfrac12\delta[1 - 4\Phi_\sigma(R\sigma;\omega)] - \tfrac12\Phi_\sigma(R\bar\sigma;\omega)\\ &\quad + \Phi_\sigma(R\sigma;\omega)^2 + \cdots\,,\\ \bar\lambda_{\bar\sigma} &\approx -2[1 - 2\Phi_\sigma(R\bar\sigma;\omega)]^{-1}\,.\end{aligned} \tag{3.9}$$

If we neglect the term involving $\xi_\sigma(\omega)$, we find a simple relation

$$[1 - 2\delta]\Phi_\sigma(R\bar\sigma;\omega) = -[1 + 2\delta - (2\omega/I)]\Phi_\sigma(R\sigma;\omega)\,, \tag{3.10}$$

yielding

$$\begin{aligned}\bar D_\sigma &= \langle C^\dagger_{R\sigma}C_{R'\sigma}\rangle^2 + 4\delta\Phi_\sigma(R\sigma;\omega)[1 + 2\Phi_\sigma(R\sigma;\omega)]\\ &\quad - (4\omega/I)\Phi_\sigma(R\sigma;\omega)^2 + \cdots\,.\end{aligned} \tag{3.11}$$

For small δ, the Φ's and P can then be evaluated as follows:

$$\Phi_\sigma(R\sigma;\omega) \approx -\Phi_\sigma(R\bar\sigma;\omega) \approx \pm\frac18\left(\frac{S_\sigma(\bar\sigma)K(\omega)\Delta}{(2\delta - \omega/I)}\right)^{1/2}\,, \tag{3.12}$$

$$\begin{aligned}\bar P_{k\sigma}(\omega) &\approx -\tfrac14[\delta - \Phi_\sigma(R\sigma;\omega)]S_\sigma(\bar\sigma)\\ &\quad \times\Delta[\delta - (\omega/I)\Phi_\sigma(R\sigma;\omega)]^{-1}[\Phi_\sigma(R\sigma;\omega)]^{-1}\,.\end{aligned} \tag{3.13}$$

As long as δ is greater than $|\Phi_\sigma(R\sigma;\omega)|$ and $|\omega/(2I)|$, the Φ's evaluated from Eq. (3.12) remain a small fraction of $S_\sigma(\bar\sigma)^{1/2}$. A solution not very different from that given by Eq. (3.8) is then obtained by taking the upper sign in Eq. (3.12), yielding negative $\bar P_{k\sigma}$ and negative $\omega^{(1)}_{k\sigma}$. The ground-state solution is, therefore, obtained under condition (3.2a).

If δ is smaller than $|\omega/I|$ and $|\Phi_\sigma(\sigma)|$, both $\bar P_{k\sigma}$ and $\omega^{(1)}_{k\sigma}$ calculated from Eq. (4.9) will become positive and the solution obtained under condition (3.2a) no longer yields a state with the lowest energy. Instead, the ground-state solution is obtained by taking the lower sign in Eq. (3.12) and by assuming condition (3.2b). Since $\bar P_{k\sigma}/2$ and $\omega^{(1)}_{k\sigma}$ are of the same order, the value of $\omega^{(1)}_{k\sigma}$ may be computed from Eq. (3.13). In the limit $\delta \to 0$, we find that

$$\begin{aligned}\omega^{(1)}_{k\sigma} &\approx -[-I\Delta S_\sigma(\bar\sigma)/8\Phi_\sigma(R\sigma;\omega)]^{1/2}\\ &\quad \times[1 - 2\Phi_\sigma(R\bar\sigma;\omega)]\,.\end{aligned} \tag{3.14}$$

By inserting the above result into Eq. (3.12), we obtain

$$\begin{aligned}\Phi_\sigma(R\sigma;\omega) &\approx -\tfrac18[I\Delta S_\sigma(\bar\sigma)K(\omega)^2]^{1/3}\\ &\quad \times\{1 + \tfrac14[I\Delta S_\sigma(\bar\sigma)K(\omega)^2]^{1/3}\}^2\,,\end{aligned} \tag{3.15}$$

$$\begin{aligned}\omega^{(1)}_{k\sigma} &\approx -[I\Delta S_\sigma(\bar\sigma)/K(\omega)]^{1/3}\\ &\quad \times\{1 - \tfrac14[I\Delta S_\sigma(\bar\sigma)K(\omega)^2]^{1/3}\}^2\,,\end{aligned} \tag{3.16a}$$

$$\omega^{(1)}_{k\sigma} \approx -[I\Delta S_\sigma(\bar\sigma)/K(\omega)]^{1/3}\,. \tag{3.16b}$$

IV. EXCITATION SPECTRUM OF THE FULLY RENORMALIZED SOLUTION IN THE NARROW-BAND REGION

We are now ready to calculate the excitation spectrum of an electron added to the system of N electrons in the narrow-band region by using the fully renormalized Green's function. Since $\Delta/I \ll 1$, we may again neglect terms of order Δ^2/I in the inverse Green's function G^{-1} given by Eq. (2.4). This means that terms involving $L_{k\sigma}\epsilon_k$ and $K_\sigma\epsilon_k$ are discarded and the factor

$$\frac{\overline{\Theta}_\sigma(\omega)[\omega-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I]}{[\omega-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I-\overline{K}_\sigma]}$$

involved in the last term on the right-hand side of Eq. (2.4) is replaced by 1. Then $G^{-1}(\omega)$ is reduced to

$$2\pi G^{-1}(\omega)=\frac{(\omega-\overline{\omega}^{(1)}_{k\sigma})(\omega-\overline{\omega}^{(2)}_{k\sigma})}{\omega-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I}-\frac{\langle \overline{N}_{R\bar\sigma}\rangle(1-\langle \overline{N}_{R\bar\sigma}\rangle)I^2\epsilon_k}{(\omega-\overline{\omega}^{(a)}_{k\sigma})(\omega-\overline{\omega}^{(b)}_{k\sigma})}, \quad (4.1)$$

where $\omega^{(1)}_{k\sigma}$ and $\omega^{(2)}_{k\sigma}$ are solutions of

$$[\omega-\epsilon_k-\overline{P}_{k\sigma}(\omega)][\omega-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I]-\langle \overline{N}_{R\bar\sigma}\rangle I\omega=0, \quad (4.2)$$

and may be expanded as

$$\overline{\omega}^{(1)}_{k\sigma}=[1-n_{\bar\sigma}-\Phi_\sigma(\bar\sigma)][\epsilon_k+\overline{P}_{k\sigma}(\omega)]+O(\Delta^2/I),$$

$$\overline{\omega}^{(2)}_{k\sigma}=I+[n_{\bar\sigma}+\Phi_\sigma(\bar\sigma)][\epsilon_k+\overline{P}_{k\sigma}(\omega)]+O(\Delta^2/I), \quad (4.3)$$

while $\overline{\omega}^{(a)}_{k\sigma}$ and $\overline{\omega}^{(b)}_{k\sigma}$ are

$$\overline{\omega}^{(a,b)}_{k\sigma}=\{1-n_{\bar\sigma}-\Phi_\sigma(\bar\sigma)\mp[n_\sigma+\Phi_\sigma(\bar\sigma)]^{1/2}\times[1-n_{\bar\sigma}-\Phi_\sigma(\bar\sigma)]^{1/2}\}I, \quad (4.4)$$

where $\Phi_\sigma(\sigma')$ is shorthand for $\Phi_\sigma(R\sigma';\omega)$ with an appropriate ω. Here again we find that, unless n_σ is nearly equal to $\frac{1}{2}$, the lower-band solution $\omega^{(1)}_{k\sigma}$ being proportional to Δ is isolated from all other solutions $\omega^{(i)}_{k\sigma}$, $i=2,3,\ldots 5$, involving the large parameter I. In the nearly-half-filled case $(n_\sigma, n_{\bar\sigma}\approx\frac{1}{2})$, however, the value of $\overline{\omega}^{(a)}_{k\sigma}$ may become small and comparable to $\overline{\omega}^{(1)}_{k\sigma}$. Therefore, we need to solve the following quadratic equation by regarding $X(\omega)$ as a parameter with an appropriate ω

$$(\omega-\overline{\omega}^{(1)}_{k\sigma})(\omega-\overline{\omega}^{(a)}_{k\sigma})-X(\omega)[\omega-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I]=0, \quad (4.5)$$

where

$$X(\omega)=\frac{\langle \overline{N}_{R\bar\sigma}\rangle(1-\langle \overline{N}_{R\bar\sigma}\rangle)I^2\epsilon_k}{(\omega-\overline{\omega}^{(2)}_{k\sigma})(\omega-\overline{\omega}^{(b)}_{k\sigma})}. \quad (4.6)$$

The result is

$$\omega^{(1)}_{k\sigma}=\tfrac{1}{2}(\overline{\omega}^{(1)}_{k\sigma}+\overline{\omega}^{(a)}_{k\sigma}+X-\{(\overline{\omega}^{(a)}_{k\sigma}+X-\overline{\omega}^{(1)}_{k\sigma})^2+4X[\overline{\omega}^{(1)}_{k\sigma}-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I]\}^{1/2}). \quad (4.7)$$

For $n_\sigma \ll \frac{1}{2}$, the above expression can be expanded as

$$=[1-n_{\bar\sigma}-\Phi_\sigma(\bar\sigma)](\epsilon_k+\overline{P}_{k\sigma})+\frac{[n_{\bar\sigma}(1-n_{\bar\sigma})+a]\epsilon_k}{F_\sigma(\bar\sigma)}+O\left(\frac{\Delta^2}{I}\right), \quad (4.8)$$

where

$$F_\sigma(\bar\sigma)=1-2n_{\bar\sigma}-2\Phi_\sigma(\bar\sigma)-[2(1-n_{\bar\sigma})-2n_{\bar\sigma}(1-2n_{\bar\sigma})-4(1-2n_{\bar\sigma})\Phi_\sigma(\bar\sigma)+4\Phi_\sigma(\bar\sigma)^2](\overline{P}_{k\sigma}/I)+\cdots,$$
$$a=(1-2n_{\bar\sigma})\Phi_\sigma(\bar\sigma)-\Phi_\sigma(\bar\sigma)^2. \quad (4.9)$$

In the absence of the correction term $\Phi_\sigma(\bar\sigma)$, the above expression is reduced to that given by Eq. (2.9) and, hence, it is invalid in the nearly-half-filled case because of the condition (2.12). In the presence of a finite $\Phi_\sigma(\bar\sigma)$, however, the magnitude of

$$(\overline{\omega}^{(a)}_{k\sigma}+X-\overline{\omega}^{(1)}_{k\sigma})^2\approx[\Phi_\sigma(\bar\sigma)I+\overline{P}_{k\sigma}/2+\cdots]^2 \quad (4.10)$$

is of order I^2 and hence remains greater than the magnitude of

$$4X[\overline{\omega}^{(1)}_{k\sigma}-(1-\langle \overline{N}_{R\bar\sigma}\rangle)I]\approx\tfrac{1}{2}\epsilon_k I$$

in the nearly-half-filled limit $(n_\sigma, n_\sigma\approx\frac{1}{2})$. Therefore the condition (2.12) is never satisfied and the expansion (4.8) is valid for all occupations $n_\sigma=n_{\bar\sigma}$, proving that the fully renormalized solution is indeed analytic everywhere in the narrow-band region.

V. CONCLUSIONS

We have eliminated the three difficulties discussed in the Introduction. The fully renormalized solution found in Sec. II, in fact, includes all higher-order functional derivatives operating directly on the basic Green's functions G and Γ and also corrections resulting from functional derivatives of equal-time Green's functions in a fully self-consistent manner, neglecting only higher-order derivatives of equal-time Green's function, $\delta^n\langle N\rangle/\delta\epsilon^n$ etc., with $n \geq 2$. Since the basic structure of the Green's function is obtained by a nonperturbative method developed in Paper II, the result can be applied to the narrow-band region as well as the wide-band region, thus eliminating the first difficulty discussed in Sec. I.

We have also shown that the correction terms Φ generated from equal-time Green's functions are renormalization factors. Since the structure of the Φ's is analogous to that of $\bar{P}_{k\sigma}$ and the Φ's themselves involve renormalization factors which are essentially the same as the original Φ's, the Φ's can be evaluated self-consistently. The resulting Φ's found in Sec. III eliminate all singularities entering the step-1 solution thus eliminating the second difficulty. We note that this is the first time that fully self-consistent renormalization factors are evaluated starting from first principles.

The calculation in Sec. IV shows that the unphysical result found in the nearly-half-filled case is eliminated and the excitation spectrum ω can be evaluated in all occupations $n_\sigma = n_{\bar{\sigma}}$, thus removing the third difficulty.

Since the Schwinger relation (1.1) or (1.2) is the only basic relation used in generating the fully self-consistent Green's function, the conservation laws on the number of electrons, momentum, and energy are automatically satisfied in the manner discussed by Baym and Kadanoff, justifying the calculation of the renormalization factors. This is a notable advantage of the present method not found in any other many-body treatments.

In the following paper, we shall calculate the ground-state energy and chemical potential, and test the stability conditions of the present result.

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

$\lambda_{\bar{\sigma}}(0)$ and $F_{\bar{\sigma}}(0)$ in Papers I and II should then be replaced by $\lambda_{\bar{\sigma}}(Rt)$ and $F_{\bar{\sigma}}(Rt)$, respectively. The $\Delta^{(\pm)}$'s involved in Eq. (3.21) of I are eliminated completely by the repeated use of Eq. (3.8) of I.

[13]$\omega^{(i)}_{k\sigma}$ is the ith pole of the advanced or retarded Green's function, $G^{(A)}(\omega)$ or $G^{(R)}(\omega)$, obtained from the analytic continuations of $G(\omega)$ onto the unphysical sheets and is not a pole of $G(\omega)$ itself. See, for instance, Ref. 6.

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