Functional-derivative study of the Hubbard model. II. Self-consistent equation and its complete solution*

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We develop a self-consistent method to solve the basic equation for the self-energy correction of the Hubbard model obtained in the preceding paper. The term $\pi[\Delta]$ involving second functional derivatives is neglected and the quantities $\langle N_{R\sigma}(t) \rangle$ and $\langle C_{R\sigma}^{\dagger}(t) C_{R'\sigma}(t) \rangle$ are initially assumed to be independent of the external fields $\epsilon(\sigma)$ and $\epsilon(\bar{\sigma})$. Under these restrictions, the complete self-energy correction is shown to be expanded in powers of $\epsilon(\sigma)$ and $\epsilon(\bar{\sigma})$ in the form $\sum_{RR'\sigma}(tt') = \xi_0(RR'\bar{\sigma}t)\delta_{tt'} + \sum_{n=0}\sum_{R''}\sum_{R'''}\sum_{k'''}(RR'',R''')\epsilon(R''R'''')\epsilon(T''',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T'',T'')\epsilon(T',T'')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T'')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T',T'')\epsilon(T',T',T'',T')\epsilon(T',T',T'')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T',T'')\epsilon(T',T',T'')\epsilon(T',T'',T')\epsilon(T',T'',T')\epsilon(T',T',T'')\epsilon(T',T',T'')\epsilon(T',T',T'')\epsilon(T',T',T'')\epsilon(T',T',T'')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T')\epsilon(T',T',T',T')\epsilon(T',T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T',T')\epsilon(T',T')\epsilon(T',T',T')\epsilon(T',T',T')\epsilon(T'$

I. INTRODUCTION

In the preceding paper,¹ we have developed a new perturbation method which can be applied to systems involving strongly interacting electrons such as the Hubbard model. Higher-order Green's functions appearing in the equations of motion for the basic Green's functions G are reduced to functional derivatives of G with respect to a small external field and calculated iteratively.^{2,3} The zeroth-order solution G_0 used in evaluating initial values of the derivatives $\delta G/\delta \epsilon$ is calculated by solving the original set of equations under neglect of $\delta G/\delta \epsilon$. Since G_0 corresponds to the Hubbard I solution⁴ in the presence of the external field and includes the intra-atomic correlation energy exactly in the atomic limit, it is expected that the perturbation series converges rapidly in the strongly interacting limit, where a conventional perturbation expansion based on the Hartree-Fock solution fails.

The method was formulated for the Hubbard model and the self-energy correction was calculated correctly through terms linear in ϵ in Paper I. In the absence of a comparable systematic method to calculate higher-order Green's functions, such a result has never been obtained for the Hubbard model previously. Unfortunately, the result in Paper I still contains some unsatisfactory aspects, suggesting the need of calculating nonlinear corrections. First of all, since the excitation spectrum ω_i is a solution of a polynomial equation in ω , $G_0^{-1}(\omega_i) - \Sigma(\omega_i) = 0$, ω_i may not be calculated correctly even though the self-energy $\Sigma(\omega)$ is determined exactly through terms linear in ϵ . Secondly, one of the denominators of the self-energy correction Σ obtained in Eq. (5.14) of I appears to become abnormally small, thus overestimating the value of Σ . Although corrections $\phi(\epsilon)$ to the denominators are of higher order in ϵ , the value of $\phi(\epsilon)$ can exceed the values of the original denominators obtained in Eq. (5.14) of I, thus modifying the result drastically.

However, it is no longer practical to continue the iterative perturbation expansion. Instead, it is easier to solve the basic Eq. (3.25) of I directly. As will be shown in Sec. II, the results in Paper I are, indeed solutions of the basic equation under certain conditions. In Sec. III, we shall develop a method to calculate a complete solution of the basic equation under the following restrictions and reproduce the result obtained in Paper I. The restrictions imposed on the basic equation are that $\pi[\Delta]$ is neglected and that derivatives $\delta \epsilon$ are replaced by $\delta_0 \epsilon$'s which operate on $\epsilon(\sigma)$ and $\epsilon(\overline{\sigma})$ only and which yield $\delta \langle N \rangle / \delta_0 \epsilon = 0$ and $\delta \langle C^{\dagger} C \rangle / \delta_0 \epsilon = 0$. Under the above conditions, the basic equation can be solved exactly and the complete solution involving infinite powers in ϵ is now written in a closed analytic form as is shown in Sec. IV. In Sec. V, changes introduced by including the effect of $\delta \langle N \rangle /$ $\delta \epsilon$ and $\delta \langle C^{\dagger} C \rangle / \delta \epsilon$ will be calculated. As is discussed in the end of Sec. V, this will eliminate the remaining difficulty in Paper I that one of the terms involved in the self-energy correction may become abnormally large.

II. SELF-CONSISTENCY REQUIREMENT

Let us first show that the solution obtained in Paper I satisfies, under certain conditions, the basic Eq. (3.25) of I, that is,

$$\begin{split} \Sigma_{RR'\sigma}(tt') &= \int_{0}^{-i\beta} dt_{1} \sum_{R_{1}} \sum_{R_{2} \neq R} \left[\lambda_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(0) B_{\overline{\sigma}}(Rt) (-i) G_{RR_{1}\sigma}(tt_{1}) \epsilon (RR_{2}\sigma t) \left(\frac{\delta}{\delta \epsilon (RR_{2}\sigma t^{-})} - \frac{\delta}{\delta \epsilon (RR_{2}\sigma t^{+})} \right) \right. \\ &+ (-i) G_{RR_{1}\sigma}(tt_{1}) \epsilon (RR_{2}\overline{\sigma} t) F_{\overline{\sigma}}(Rt) \left((w-I)^{-1} \frac{\delta}{\delta \epsilon (RR_{2}\overline{\sigma} t^{-})} - w^{-1} \frac{\delta}{\delta \epsilon (RR_{2}\overline{\sigma} t^{+})} \right) \\ &- (-i) G_{RR_{1}\sigma}(tt_{1}) \epsilon (R_{2}R\overline{\sigma} t) F_{\overline{\sigma}}(Rt) \left((w-I)^{-1} \frac{\delta}{\delta \epsilon (R_{2}R\overline{\sigma} t^{+})} - w^{-1} \frac{\delta}{\delta \epsilon (R_{2}R\overline{\sigma} t^{+})} \right) \right] \\ &\times \left[(G_{0})_{R_{1}R'\sigma}^{-1}(t_{1}t') - \Sigma_{R_{1}R'\sigma}(t_{1}t') \right] + \pi \left[\Delta_{RR'\sigma}(tt') \right], \end{split}$$

where

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

$$B_{\overline{\sigma}}(Rt) = n_{\overline{\sigma}}(1 - n_{\overline{\sigma}}) + I^{-1} \sum_{R'' \neq R} b^{(-)}(RR''\overline{\sigma}t), \qquad (2.2)$$

$$b^{(\pm)}(RR''\overline{\sigma}t) = \epsilon (RR''\overline{\sigma}t) \langle C_{R\overline{\sigma}}^{+}(t) C_{R''\overline{\sigma}}(t) \rangle \pm \epsilon (R''R\overline{\sigma}t) \langle C_{R\overline{\sigma}}^{+}(t) C_{R\overline{\sigma}}(t) \rangle,$$

and $w \equiv i\partial/\partial t$; $\lambda_{\overline{\sigma}}(0)$ and $F_{\overline{\sigma}}(0)$ are obtained from $\lambda_{\overline{\sigma}}(Rt)$ and $F_{\overline{\sigma}}(Rt)$ by replacing $\langle N_{R\overline{\sigma}}(t) \rangle$ by $n_{\overline{\sigma}}$, while $\pi[\Delta]$ defined by Eq. (3.26) of I will not be considered in the following. The unperturbed Green's function G_0 is given by Eq. (3.18) of I,

$$(G_{0})_{RR'\sigma}^{-1}(tt') = F_{\overline{\sigma}}(Rt) \,\delta_{RR'} \delta_{tt'} - F_{\overline{\sigma}}(Rt) [F_{\overline{\sigma}}(0)]^{-1} \epsilon (RR'\sigma t) \,\delta_{tt'} \\ - \lambda_{\overline{\sigma}}(Rt) \sum_{R''\neq R} \left[\epsilon (RR''\overline{\sigma}t) \langle C_{R\overline{\sigma}}^{+}(t) C_{R''\overline{\sigma}}(t) \rangle - \epsilon (R''R\overline{\sigma}t) \langle C_{R''\overline{\sigma}}^{+}(t) C_{R\overline{\sigma}}(t) \rangle \right] \delta_{RR'} \delta_{tt'}.$$

$$(2.3)$$

Note that in Eqs. (2.1)-(2.3), and from here on, the presence of the operator $\partial/\partial t$ in quantities of the form $g(t) \delta_{tt}$, is indicated only through the t dependence of g(t).

Since we have neglected the $\delta\epsilon$ dependence of $\langle N \rangle$ and $\langle C^{\dagger}C \rangle$ in Paper I, let us replace $\delta\epsilon$ in Eq. (2.1) by $\delta_{0}\epsilon$ which operates on $\epsilon(RR'\sigma t)$ only and which yields $\delta\langle N \rangle / \delta_{0}\epsilon = 0$ and $\delta\langle C^{\dagger}C \rangle / \delta_{0}\epsilon = 0$. If we also assume the absence of any external field operating on electrons with opposite spin $\overline{\sigma}$, that is, $\delta_{0}\epsilon(RR'\overline{\sigma}t) = 0$ for all R and R', the result obtained in Eq. (5.3) of I,

$$\Sigma_{RR'\sigma}(tt';\sigma) = [\lambda_{\overline{\sigma}}(Rt)/\lambda_{\overline{\sigma}}(0)] \{ [\lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)B_{\overline{\sigma}}(Rt)] + [\lambda\lambda(0)B]^2 + [\cdots]^3 + \cdots \} \in (RR'\sigma t) \delta_{tt},$$

$$= \frac{\lambda_{\overline{\sigma}}^2(Rt)B_{\overline{\sigma}}(Rt)}{1 - \lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)B_{\overline{\sigma}}(Rt)} \in (RR'\sigma t) \delta_{tt},$$
(2.4)

is an exact solution of the basic Eq. (2.1). In fact, $\delta G_0^{-1}/\delta_0 \epsilon(\sigma)$ yields the first term in Eq. (4.7) of I:

$$\delta G_0^{-1} / \delta \epsilon(\sigma) \to \lambda_{\overline{\sigma}}^2(Rt) B_{\overline{\sigma}}(Rt) \epsilon(RR'\sigma t) \delta_{tt'}, \qquad (2.5)$$

while $-\delta \Sigma_{\sigma}(\sigma)/\delta_{0}\epsilon(\sigma)$ yields

$$-\delta\Sigma_{\sigma}(\sigma)/\delta\epsilon(\sigma) \rightarrow \left\{ \left[\lambda_{\overline{\sigma}}^{3}(Rt)\lambda_{\overline{\sigma}}(0)B_{\overline{\sigma}}^{2}(Rt)\right]/\left[1-\lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)B_{\overline{\sigma}}(Rt)\right]\right\}\epsilon(RR'\sigma t)\delta_{tt}'.$$
(2.6)

The sum of the above two expressions is equal to the original $\Sigma_{\sigma}(\sigma)$ given by Eq. (2.4), showing that $\Sigma_{\sigma}(\sigma)$ is, indeed, an exact solution of Eq. (2.1) in the limit of $\delta_0 \epsilon(\overline{\sigma}) = 0$. This conclusion is, of course, evident from the way the series for $\Sigma_{\sigma}(\sigma)$ shown in Eq. (2.4) is generated; $\delta G_0^{-1}/\delta_0 \epsilon$ yields the first term $[\lambda/\lambda(0)][\lambda\lambda(0)B]\epsilon\delta$; the functional derivative of the first term, in turn, yields the second term $[\lambda/\lambda(0)][\lambda\lambda(0)B]^2\epsilon\delta$ and so on. Thus $\delta(G_0^{-1}-\Sigma)/\delta_0\epsilon$ reproduces $\Sigma_{\sigma}(\sigma)$ exactly. We note that the order of magnitude of the first, second, ... terms are the same as the zeroth, first, ... terms, and once the Hubbard correction (the zeroth order term) is taken into account, the whole series $[\lambda/\lambda(0)]\{[\lambda\lambda(0)B]^2 + \cdots\}\delta\epsilon$ has to be included. Otherwise, the Hubbard-type solution cannot be a self-consistent solution of the basic equation (2.1). As we shall discuss in the following paper, the Hubbard I solution as well as solutions of the type shown in Sec. IV of I, are not self-consistent solutions of Eq. (2.1) and are, in fact, unstable.

The same calculation may be applied to the case where $\epsilon(RR'\sigma t) = 0$ for all R and R', and it can be proved

that the result $\Sigma_{\sigma}(\overline{\sigma})$ obtained in Eq. (5.13) of I by successive applications of $\delta \Sigma_{\sigma} / \delta_0 \epsilon(\overline{\sigma})$ is a self-consistent solution of the basic Eq. (2.1). More explicitly, $\Sigma_{\sigma}(\overline{\sigma})$ consists of the following four terms:

$$\Sigma_{\sigma}^{(1)}(\overline{\sigma}) = \sum_{R''} \frac{\lambda_{\overline{\sigma}}(Rt)^2 b^{(+)}(RR''\overline{\sigma}t) \left[\frac{1}{2} - \langle N_{R\sigma}(t) \rangle \right]}{[1 - \mu_{\overline{\sigma}}(Rt)]^2 [1 - X(RR''\overline{\sigma}t)]} \delta_{RR'} \delta_{tt'}, \qquad (2.7)$$

$$\Sigma_{\sigma}^{(2)}(\overline{\sigma}) = \frac{\lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(R't)b^{(+)}(RR'\overline{\sigma}t)\langle C_{R'\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle}{[1-\mu_{\overline{\sigma}}(Rt)][1-\mu_{\overline{\sigma}}(R't)][1-X(RR'\overline{\sigma}t)]}\delta_{tt'}, \qquad (2.8)$$

$$\Sigma_{\sigma}^{(3)}(\overline{\sigma}) = \sum_{R''} \left(\frac{1}{\left[1 - \mu_{\overline{\sigma}}(Rt)\right] \left[1 - X(RR''\overline{\sigma}t)\right]} - 1 \right) \lambda_{\overline{\sigma}}(Rt) b^{(-)}(RR''\overline{\sigma}t) \delta_{RR'} \delta_{tt'}, \qquad (2.9)$$

and $\Sigma_{\sigma}^{(4)}(\overline{\sigma})$ which involves $\delta_{0}\epsilon$ -independent factors of the type shown in Eq. (5.10) of I and which vanishes in the limit of $\delta_{0}\epsilon=0$. Here

$$X(RR''\overline{\sigma}t) = \lambda_{\overline{\sigma}}(Rt)^{2} [1 - \mu_{\overline{\sigma}}(Rt)]^{-2} [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle]^{2} - \lambda_{\overline{\sigma}}(Rt) [1 - \mu_{\overline{\sigma}}(Rt)]^{-1} \lambda_{\overline{\sigma}}(R''t) [1 - \mu_{\overline{\sigma}}(R''t)]^{-1} \langle C_{R\sigma}^{\dagger}(t) C_{R''\sigma}(t) \rangle \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle , \qquad (2.10)$$

and

$$\mu_{\overline{\sigma}}(Rt) = \langle w - \frac{1}{2}I \rangle \{ w - [1 - \langle N_{R\overline{\sigma}}(t) \rangle]I \}^{-1}.$$

$$\delta [G_0^{-1} - \Sigma_0^{(3)}(\overline{\sigma})] / \delta_0 \epsilon(\overline{\sigma}) \text{ yields}$$

$$\sum_{R''} \frac{\lambda_{\overline{\sigma}}(Rt)^2 b^{(+)}(RR''\overline{\sigma}t)}{[1 - \mu_{\overline{\sigma}}(Rt)][1 - X(RR''\overline{\sigma}t)]} [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle]\delta_{RR'} \delta_{tt'} + \sum_{PR''} \frac{\lambda_{\overline{\sigma}}(Rt) \mu_{\overline{\sigma}}(Rt) \mu_{\overline{\sigma}}(Rt) b^{(-)}(RR''\overline{\sigma}t)}{[1 - \mu_{\overline{\sigma}}(Rt)][1 - X(RR''\overline{\sigma}t)]} \delta_{RR'} \delta_{tt'} + \frac{\lambda_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(R't) b^{(+)}(RR''\overline{\sigma}t)}{[1 - \mu_{\overline{\sigma}}(Rt)][1 - X(RR''\overline{\sigma}t)]} \langle C_{R'\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle \delta_{tt'},$$
(2.11)

while $\delta \Sigma_{\sigma}^{(1)}(\vec{\sigma}) / \delta_0 \epsilon(\vec{\sigma})$ and $\delta \Sigma_{\sigma}^{(2)}(\vec{\sigma}) / \delta_0 \epsilon(\vec{\sigma})$ yield

$$\sum_{\mathbf{R}''} \frac{\lambda_{\overline{\sigma}}(Rt)^2 \mu_{\overline{\sigma}}(Rt) b^{(+)}(RR''\overline{\sigma}t)}{[1 - \mu_{\overline{\sigma}}(Rt)]^2 [1 - X(RR''\overline{\sigma}t)]} [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle] \delta_{RR'} \delta_{tt'} + \cdots$$
(2.12)

and

$$\sum_{R''} \frac{\lambda_{\overline{\sigma}}(Rt) \,\mu_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(R't) b^{(+)}(RR'\overline{\sigma}t)}{[1 - \mu_{\overline{\sigma}}(Rt)][1 - \mu_{\overline{\sigma}}(R't)][1 - X(RR'\overline{\sigma}t)]} \langle C_{R'\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle \delta_{tt'} + \cdots, \qquad (2.13)$$

respectively. In the above expressions, we have omitted terms involving $b^{(-)}$ since we are primarily interested in nonvanishing terms in the limit of $\delta \epsilon = 0$. The sum of the above three expressions, indeed, yields $\Sigma_{\sigma}^{(1)}(\overline{\sigma}) + \Sigma_{\sigma}^{(2)}(\overline{\sigma})$. If terms involving $b^{(-)}$ are explicitly included, we will also find $\Sigma_{\sigma}^{(3)}(\overline{\sigma}) + \Sigma_{\sigma}^{(4)}(\overline{\sigma})$, confirming that the solution $\Sigma_{\sigma}(\overline{\sigma})$ obtained in Paper I is a self-consistent solution of the basic equation (2.1) in the limit of $\delta_0 \epsilon(\sigma) = 0$.

The above result is, again, evident from the way the series for $\Sigma_{\sigma}(\bar{\sigma})$ is generated successively in Paper I. If the first-order solution consisting of the second and third terms in Eq. (4.11) of I is included, the entire series leading to $\Sigma_{\sigma}(\bar{\sigma})$ given by Eqs. (2.7) and (2.8) has to be added. Since solutions of the type given by Sec. IV of I do not satisfy the basic Eq. (2.1) and, by including one more term, the values of Σ change drastically, it is meaningless to discuss the accuracy of these solutions.

If we include $\delta_0 \epsilon(\sigma)$ and $\delta_0 \epsilon(\overline{\sigma})$ simultaneously, the result $\Sigma_{\sigma}(\sigma) + \Sigma_{\sigma}(\overline{\sigma})$ given by Eqs. (2.4) and (2.7)-(2.9) is no longer a self-consistent solution because the factor $\lambda^2 B_{\overline{\sigma}} (1 - \lambda^2 B_{\overline{\sigma}})^{-1}$ involved in $\Sigma_{\sigma}(\sigma)$ is a function of $\epsilon(\overline{\sigma})$ and introduces a new series.

III. METHOD AND THE FIRST-ORDER SOLUTION

In Sec. II, we have shown that, if $\delta_0 \epsilon(\overline{\sigma}) = 0$ or $\delta_0 \epsilon(\sigma) = 0$, an exact solution of the basic equation (2.1) is linear in $\epsilon(RR'\sigma t)$ or $\epsilon(RR''\overline{\sigma}t)$ and $\epsilon(R''R\overline{\sigma}t)$ and that the general expression for the self-energy Σ_{σ} is written

$$a_0 \epsilon (RR'\sigma t) \text{ or } \sum_{R''} \left[a_{RR''}^{(+)} b^{(+)} (RR''\bar{\sigma}t) + a_{RR''}^{(-)} b^{(-)} (RR''\bar{\sigma}t) \right],$$
 (3.1)

where $b^{(\pm)}$ is defined by Eq. (2.2). Here, the parameters a_0 and $a^{(\pm)}$ may be determined in such a way

that Eq. (2.1) is satisfied. If $\delta_0 \epsilon(\sigma)$ and $\delta_0 \epsilon(\overline{\sigma})$ are included simultaneously, however, higher-order powers in $\epsilon(\overline{\sigma})$ will appear in Σ because $B_{\overline{\sigma}}(Rt)$ involved in Eq. (2.1) has terms linear in $\epsilon(\overline{\sigma})$. If, for instance, $\Sigma_{\sigma} = a_0 \epsilon(RR'\sigma t) \delta_{tt}$, is inserted into the right-hand side of Eq. (2.1), we obtain

$$a_{0}\lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)\left(n_{\overline{\sigma}}(1-n_{\overline{\sigma}})+I^{-1}\sum_{R''}b^{(-)}(RR''\overline{\sigma}t)\right)\epsilon(RR'\sigma t)\,\delta_{tt},\,\,(3.2)$$

thus finding quadratic terms $b^{(-)}\epsilon$. $\Sigma_{\sigma} = \sum_{R''} b^{(-)}(RR''\overline{\sigma}t) \epsilon(RR'\sigma t) \delta_{tt'}$, in turn, yields

$$\sum_{R''} \lambda_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(0) \left(n_{\overline{\sigma}} | (1 - n_{\overline{\sigma}}) + I^{-1} \sum_{R''} b^{(-)}(RR''\overline{\sigma}t) \right) b^{(-)}(RR''\overline{\sigma}t^{\pm}) \epsilon(RR'\sigma t) \delta_{tt},$$

$$+ \lambda_{\overline{\sigma}}(Rt) \sum_{R''} b^{(+)}(RR''\overline{\sigma}t) \left[\frac{1}{2} - \langle N_{R\sigma}(t) \rangle \right] \epsilon(RR'\overline{\sigma}t^{\pm}) \delta_{tt}, + \mu_{\overline{\sigma}}(Rt) \sum_{R''} b^{(-)}(RR''\overline{\sigma}t) \epsilon(RR'\sigma t^{\pm}) \delta_{tt},$$

$$+ \lambda_{\overline{\sigma}}(Rt) \sum_{R''} b^{(+)}(RR''\overline{\sigma}t) \langle C_{R''\sigma}(t) C_{R\sigma}(t) \rangle \epsilon(R''R'\sigma t^{\pm}) \delta_{tt}, \qquad (3.3)$$

showing the appearance of cubic terms $b^{(-)}(t)b^{(-)}(t^{\pm})\epsilon(t)$, and so on. Here $b^{(-)}(t^{\pm})$ denotes the expression

$$iG_{RR\sigma}(tt^{-})b^{(-)}(RR''\overline{\sigma}t^{-}) - iG_{RR\sigma}(tt^{+})b^{(-)}(RR''\overline{\sigma}t^{+}), \qquad (3.4)$$

and hence the derivative $\delta[b^{(-)}(t)b^{(-)}(t^{\pm})\epsilon(t)]/\delta\epsilon(\overline{\sigma}t)$ operates on $b^{(-)}(t)$ but not on $b^{(-)}(t^{\pm})$.

A general expression for Σ_σ obtained by successive application of the iterative procedure may then be written

$$\Sigma_{RR'\sigma}(tt') = \xi_0(RR'\overline{\sigma}t)\,\delta_{tt'} + \sum_{n=0}^{\infty}\sum_{R''}\sum_{R''}\,\xi^{(n)}(RR';R''R'''\overline{\sigma}t)\,\epsilon(R''R'''\sigma t)\,\delta_{tt'}\,,\tag{3.5}$$

where ξ_0 is the sum of terms linear in $\epsilon(\overline{\sigma})$, while $\xi^{(n)}$ is the sum of terms of *n*th degree in $\epsilon(\overline{\sigma})$. It is obvious that higher powers in $\epsilon(\sigma)$ do not appear. If we insert the above expression on the right-hand side of Eq. (2.1), $\epsilon(R''R'''\sigma t)$ in Σ_{σ} will be replaced by $\epsilon(RR'''\sigma t)$ whenever terms involving $\epsilon(RR''\sigma t)\delta/\delta\epsilon(\sigma)$ operate on Σ_{σ} . When terms involving $\epsilon(\overline{\sigma})\delta/\delta\epsilon(\overline{\sigma})$ operate on Σ_{σ} , however, $\epsilon(R''R'''\sigma t)$ in Σ_{σ} will be replaced by $\epsilon(R_1R''\sigma t)$ if R'' = R and, otherwise, it will remain unchanged. In either case, the index R''will never be replaced and therefore, terms involving $\epsilon(R''R'''\sigma t)$ with $R''' \neq R'$ are decoupled completely from those proportional to $\epsilon(R''R'\sigma t)$ in Eq. (2.1). Since terms generated from G_0^{-1} do not involve $\epsilon(R''R'''\sigma t)$ with $R''' \neq R'$, the solution we are looking for is obtained by inserting $\xi^{(n)}(RR';R''R'''\overline{\sigma}t) = 0$ for $R''' \neq R'$. Equation (3.5) is then reduced to

$$\Sigma_{RR'\sigma}(tt') = \xi_0(RR'\overline{\sigma}t)\,\delta_{tt'} + \sum_{n=0}^{\infty} \xi^{(n)}(RR'\overline{\sigma}t)\,\epsilon(RR'\sigma t)\,\delta_{tt'} + \sum_{n=1}^{\infty} \sum_{R''\neq R} \eta^{(n)}(RR';R''\overline{\sigma}t)\,\epsilon(R''R'\sigma t)\,\delta_{tt'}, \qquad (3.6)$$

where $\eta^{(0)} = 0$, and $\xi^{(n)}$ and $\eta^{(n)}$ consist of terms in the *n*th degree in $\epsilon(\overline{\sigma})$ having the form

$$b^{(\pm)}(t) b^{(\pm)}(t^{\pm}) b^{(\pm)}(t^{2\pm}) \cdots b^{(\pm)}(t^{(n-1)\pm})$$
(3.7)

where

$$t^{(n-1)+} > \cdots > t^{2+} > t^{+} > t^{-} > t^{2-} > \cdots > t^{(n-1)-}$$
(3.8)

If we insert the expressions in Eqs. (2.3) and (3.6) into the right-hand side of Eq. (2.1), we obtain

 $\Sigma_{RR'\sigma}(tt') = \lambda_{\overline{\sigma}}(Rt)^2 B_{\overline{\sigma}}(Rt) \,\epsilon (RR'\sigma t) \,\delta_{tt'} + \Delta \left[G_0^{-1}\right]_{RR'\sigma}(tt') + \Delta \xi_0(RR'\overline{\sigma}t) \,\delta_{tt'},$

$$+\lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)B_{\overline{\sigma}}(Rt)\sum_{n=0}^{\infty}\xi^{(n)}(RR'\overline{\sigma}t)\epsilon(RR'\sigma t)\delta_{tt},$$

$$+\sum_{n=1}^{\infty}\left(\Delta\xi^{(n)}(RR'\overline{\sigma}t)+\sum_{R''}\Delta\eta^{(n)}(RR'R'';R\overline{\sigma}t)\right)\epsilon(RR'\sigma t)\delta_{tt},$$

$$+\sum_{n=1}^{\infty}\sum_{R''}\left[\Delta\xi^{(n)}(RR';R''\overline{\sigma}t)+\Delta\eta^{(n)}(RR';R''\overline{\sigma}t)\right]\epsilon(R''R'\sigma t)\delta_{tt},$$
(3.9)

where ΔG_0^{-1} and $\Delta \xi_0$ as well as

$$\Delta \xi^{(n)} \left(RR'\overline{\sigma}t \right) \epsilon \left(RR'\sigma t \right) + \sum_{R''} \Delta \xi^{(n)} \left(RR'; R''\overline{\sigma}t \right) \epsilon \left(R''R'\sigma t \right)$$

and

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$$\Delta \eta^{(n)} \left(RR'R''; R\overline{\sigma}t \right) \in \left(RR'\sigma t \right) + \Delta \eta^{(n)} \left(RR'; R''\overline{\sigma}t \right) \in \left(R''R'\sigma t \right)$$
(3.10)

are obtained by inserting G_0^{-1} , ξ_0 , $\xi^{(n)}$, and $\eta^{(n)}$, respectively, into the right-hand side of Eq. (2.1) in the absence of the first term involving $\epsilon(\sigma) \delta/\delta\epsilon(\sigma)$. It is again obvious that $\Delta\xi^{(n)}$ and $\Delta\eta^{(n)}$ consist of terms having the structure shown by Eq. (3.7). The expressions for Eq. (3.10) are obtained by using exactly the same reasoning as that used in deriving Eq. (3.6). The term involving $\epsilon(\sigma) \delta/\delta\epsilon(\sigma)$ in Σ_{σ} has generated the first and fourth terms in Eq. (3.9).

The original Σ_{σ} shown in Eq. (3.6) becomes an exact solution of the basic Eq. (2.1), if the expression on the right-hand side of Eq. (3.9) is equal to the original Σ_{σ} . This condition may be separated into three parts. The part not involving $\epsilon(\sigma)$ is

$$\xi_0(RR\,'\overline{\sigma}t)\,\delta_{tt'}=\Delta\,[G_0^{-1}]_{RR'\sigma}(tt')+\Delta\,\xi_0(RR\,'\overline{\sigma}t)\,\delta_{tt'}\,.$$
(3.11)

The part proportional to $\epsilon (RR'\sigma t)$ is

$$\sum_{n} \xi^{(n)} \left(RR'\overline{\sigma}t \right) = \frac{\lambda_{\overline{\sigma}}(Rt)^2 B_{\overline{\sigma}}(Rt)}{1 - \lambda_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(0) B_{\overline{\sigma}}(Rt)} + \frac{1}{1 - \lambda_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(0) B_{\overline{\sigma}}(Rt)} \sum_{n} \left(\Delta \xi^{(n)} \left(RR'\overline{\sigma}t \right) + \sum_{R''} \Delta \eta^{(n)} \left(RR'R''; R\overline{\sigma}t \right) \right),$$
(3.12)

while the part proportional to $\epsilon(R''R'\sigma t)$ is

$$\sum_{n} \eta^{(n)} \left(RR'; R''\overline{\sigma}t \right) = \sum_{n} \left[\Delta \xi^{(n)} \left(RR'; R''\overline{\sigma}t \right) + \Delta \eta^{(n)} \left(RR'; R''\overline{\sigma}t \right) \right].$$
(3.13)

Although Eqs. (3.12) and (3.13) involve all powers in $\epsilon(\overline{\sigma})$, the equalities should, in fact, remain valid for each power. Hence Eq. (3.13) is rewritten

$$\eta^{(n)} \left(RR'; R''\bar{\sigma}t \right) = \Delta \xi^{(n)} \left(RR'; R''\bar{\sigma}t \right) + \Delta \eta^{(n)} \left(RR'; R''\bar{\sigma}t \right).$$
(3.14)

To obtain a corresponding equality for $\xi^{(n)}$, we need to use the following expansion:

$$\left[1 - \lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)B_{\overline{\sigma}}(Rt)\right]^{-1} = f + \phi f^{2} + \phi^{2}f^{3} + \phi^{3}f^{4} + \cdots, \qquad (3.15)$$

where

$$f = \frac{1}{1 - \lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0) n_{\overline{\sigma}}(1 - n_{\overline{\sigma}})}, \quad \phi = \lambda_{\overline{\sigma}}(Rt)\lambda_{\overline{\sigma}}(0)I^{-1}\sum_{R''} b^{(-)}(RR''\overline{\sigma}t).$$
(3.16)

Equation (3.12) is then written

$$\xi^{(0)} \left(RR' \overline{\sigma}t \right) = \lambda \lambda_0^{-1} \left(-1 + f \right), \quad \xi^{(1)} \left(RR' \overline{\sigma}t \right) = \lambda \lambda_0^{-1} f^2 \phi + f \left(\Delta \xi^{(1)} + \sum \Delta \eta^{(1)} \right),$$

$$\xi^{(2)} \left(RR' \overline{\sigma}t \right) = \lambda \lambda_0^{-1} f^3 \phi^2 + f^2 \phi \left(\Delta \xi^{(1)} + \sum \Delta \eta^{(1)} \right) + f \left(\Delta \xi^{(2)} + \sum \Delta \eta^{(2)} \right),$$

$$\xi^{(3)} \left(RR' \overline{\sigma}t \right) = \lambda \lambda_0^{-1} f^4 \phi^3 + f^3 \phi^2 \left(\Delta \xi^{(1)} + \sum \Delta \eta^{(1)} \right) + f^2 \phi \left(\Delta \xi^{(2)} + \sum \Delta \eta^{(2)} \right) + f \left(\Delta \xi^{(3)} + \sum \Delta \eta^{(3)} \right), \quad \text{etc.}$$
(3.17)

In the above expression, $\Delta \xi^{(n)}$ and $\sum \Delta \eta^{(n)}$ represent $\Delta \xi^{(n)}(RR'\overline{\sigma}t)$ and $\sum_{R''} \Delta \eta^{(n)}(RR'R'';R\overline{\sigma}t)$, respectively.

Equations (3.11), (3.14), and (3.17) are now the basic equations for the complete self-energy correction Σ_{σ} . The first equation in Eq. (3.17) yields the result given by Eq. (2.4). In the following, we shall show that Eq. (3.11) yields the result given by Eqs. (2.7)-(2.9). Although the most general expression for $\xi_0(RR'\overline{\sigma}t)$ is

$$\xi_0(RR'\bar{\sigma}t) = \sum_{R''} \sum_{R''} a_{RR',R''R''} \in (R''R''''\bar{\sigma}t), \qquad (3.18)$$

the coefficients $a_{RR',R''R'''}$ satisfying Eq. (3.11) vanish unless R'' = R or R''' = R, because the result $\Delta \xi_0$ obtained by inserting $\Sigma_{\sigma} = \xi_0$ on the right-hand side of Eq. (2.1) does not contain terms proportional to $\epsilon(R''R'''\bar{\sigma}t)$ unless R'' = R or R''' = R. Hence ξ_0 can be expanded in terms of $\epsilon(RR''\bar{\sigma}t)$ and $\epsilon(R''R\bar{\sigma}t)$, or, equivalently, in terms of $b^{(+)}(RR''\bar{\sigma}t)$ and $b^{(-)}(RR''\bar{\sigma}t)$ as follows:

$$\xi_{0}(RR'\overline{\sigma}t) = \sum_{R''} x_{RR''}(R') b^{(+)}(RR''\overline{\sigma}t) + \sum_{R''} y_{RR''}(R') b^{(-)}(RR''\overline{\sigma}t) .$$
(3.19)

 $\Delta\xi_0$ is then calculated to be

$$\Delta \xi_{0}(RR'\overline{\sigma}t) = \sum_{R''} x_{RR''}(R') \{\lambda_{\overline{\sigma}}(Rt) b^{(-)}(RR''\overline{\sigma}t) [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle] + \mu_{\overline{\sigma}}(Rt) b^{(+)}(RR''\overline{\sigma}t) \}$$
$$- \sum_{R''} x_{R''R}(R') \lambda_{\overline{\sigma}}(Rt) b^{(-)}(RR''\overline{\sigma}t) \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle$$
$$+ \sum_{R''} y_{RR''}(R') \{\lambda_{\overline{\sigma}}(Rt) b^{(+)}(RR''\overline{\sigma}t) [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle] + \mu_{\overline{\sigma}}(Rt) b^{(-)}(RR''\overline{\sigma}t) \}$$
$$+ \sum_{R''} y_{R''R}(R') \lambda_{\overline{\sigma}}(Rt) b^{(+)}(RR''\overline{\sigma}t) \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle , \qquad (3.20)$$

while $\Delta [G_0^{-1}]_{RR'\sigma}(tt')$ has been calculated in Eq. (4.7) of I as follows:

$$\Delta \left[G_{0}^{-1} \right]_{RR'\sigma} (tt') = \lambda_{\overline{\sigma}} (Rt)^{2} \sum_{R''} b^{(+)} (RR''\overline{\sigma}t) \left[\frac{1}{2} - \langle N_{R\sigma}(t) \rangle \right] \delta_{RR'} \delta_{tt'} + \lambda_{\overline{\sigma}} (Rt) \mu_{\overline{\sigma}} (Rt) \sum_{R''} b^{(-)} (RR''\overline{\sigma}t) \delta_{RR'} \delta_{tt'} + \lambda_{\overline{\sigma}} (Rt) \lambda_{\overline{\sigma}} (Rt) \lambda_{\overline{\sigma}} (R't) b^{(+)} (RR''\overline{\sigma}t) \langle C_{R'\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle \delta_{tt'}.$$

$$(3.21)$$

Equation (3.11) is satisfied if the coefficients of $b^{(+)}(RR''\bar{\sigma}t)$ and $b^{(-)}(RR''\bar{\sigma}t)$ vanish. This yields that

$$\begin{bmatrix} \mathbf{1} - \mu_{\overline{\sigma}}(Rt) \end{bmatrix} x_{RR''}(R') = \lambda_{\overline{\sigma}}^{2}(Rt) \begin{bmatrix} \frac{1}{2} - \langle N_{R\sigma}(t) \rangle \end{bmatrix} \delta_{RR'} + \lambda_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(R't) \langle C_{R'\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle \delta_{R''R'} + y_{RR''}(R') \lambda_{\overline{\sigma}}(Rt) \begin{bmatrix} \frac{1}{2} - \langle N_{R\sigma}(t) \rangle \end{bmatrix} + y_{R''R}(R') \lambda_{\overline{\sigma}}(Rt) \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle , \qquad (3.22)$$
$$\begin{bmatrix} \mathbf{1} - \mu_{\overline{\sigma}}(Rt) \end{bmatrix} y_{RR''}(R') = \lambda_{\overline{\sigma}}(Rt) \mu_{\overline{\sigma}}(Rt) \delta_{RR'} + x_{RR''}(R') \lambda_{\overline{\sigma}}(Rt) \begin{bmatrix} \frac{1}{2} - \langle N_{R\sigma}(t) \rangle \end{bmatrix} - x_{R''R}(R') \lambda_{\overline{\sigma}}(Rt) \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle . \qquad (3.22)$$

The above equations together with those for $x_{R''R}(R')$ and $y_{R''R}(R')$ can be solved exactly, and, in the limit of a small external field $\delta \epsilon = 0$ where $\lambda(R''t) = \lambda(Rt)$, etc., the results are

$$\begin{aligned} x_{RR''}(R') &= \lambda^{2} \left(\frac{1}{2} - n_{\sigma} \right) D_{RR''}^{-1} \delta_{RR'} + \lambda^{2} \langle C_{R'\sigma}^{\dagger} C_{R\sigma} \rangle \overline{D}_{RR''}^{-1} \delta_{R''R'} , \\ y_{RR''}(R') &= \lambda \left[\mu (1 - \mu) + \lambda^{2} \left(\frac{1}{2} - n_{\sigma} \right) - \lambda^{2} \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle \right] \overline{D}_{RR''}^{-1} \delta_{RR'} , \end{aligned}$$
(3.23)

and $y_{RR'}(R') = 0$. Here

$$\overline{D}_{RR''} = (1-\mu)^2 - \lambda^2 \left(\frac{1}{2} - n_{\sigma}\right)^2 + \lambda^2 \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle .$$
(3.24)

In the present limit, Eqs. (3.19) and (3.23) are exactly the same as the result obtained in Paper I and shown in Eqs. (2.7)-(2.9), confirming that the result in Paper I is exact through terms linear in ϵ . Note that, if needed, the exact solution in the presence of the external field $\delta\epsilon$ can also be obtained from Eq. (3.22), while the result in Paper I does not include terms of the type shown in Eq. (5.10) of I. As mentioned before, they vanish in the limit of $\delta\epsilon = 0$.

IV. COMPLETE SOLUTION OF THE RESTRICTED EQUATION

Let us now calculate the nonlinear corrections by solving Eqs. (3.14) and (3.17) and show that the results can be factorized in powers of ϵ and hence the exact solution can be obtained in a closed analytic form. Before discussing the factorization, we shall calculate the lowest nonlinear corrections involved in the expression in Eq. (3.6), that is, quadratic terms in ϵ . Since they are bilinear in $\delta\epsilon(\sigma)$ and $\delta\epsilon(\bar{\sigma})$, $\xi^{(1)}$ and $\eta^{(1)}$ should be expanded as

$$\xi^{(1)}(RR'\overline{\sigma}t) = \sum_{R''} \left[x_{RR''}^{(1)}(R') b^{(+)}(RR''\overline{\sigma}t) + y_{RR''}^{(1)}(R') b^{(-)}(RR''\overline{\sigma}t) \right],$$

$$\eta^{(1)}(RR'; R''\overline{\sigma}t) = z_{RR''}^{(1)}(R') b^{(+)}(RR''\overline{\sigma}t) + v_{RR''}^{(1)}(R') b^{(-)}(RR''\overline{\sigma}t).$$
(4.1)

Here again, more general terms $b^{(\pm)}(R''R'''\overline{\sigma}t)$ do not appear. $\Delta\xi^{(1)}$ and $\Delta\eta^{(1)}$ are then given by

$$\Delta \xi^{(1)}(RR'\overline{\sigma}t) = \sum_{R''} x_{RR''}^{(1)}(R') \left\{ \lambda(Rt) b^{(-)}(RR''\overline{\sigma}t) \left[\frac{1}{2} - \langle N_{R\sigma}(t) \rangle \right] + \mu(Rt) b^{(+)}(RR''\overline{\sigma}t) \right\}$$

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$$+ \sum_{R''} y_{RR''}^{(1)}(R') \{ \lambda(Rt) b^{(+)}(RR''\overline{\sigma}t) [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle] + \mu(Rt) b^{(-)}(RR''\overline{\sigma}t) \},\$$

$$\Delta \xi^{(1)}(RR'; R''\overline{\sigma}t) = -x_{R''R}^{(1)}(R')\lambda(Rt)b^{(-)}(RR''\overline{\sigma}t)\langle C_{R''\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle + y_{R''R}^{(1)}(R')\lambda(Rt)b^{(+)}(RR''\overline{\sigma}t)\langle C_{R''\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle ,$$

$$\Delta \eta^{(1)}(RR'; R''\overline{\sigma}t) = z_{RR''}^{(1)}(R')\{\lambda(Rt)b^{(-)}(RR''\overline{\sigma}t)[\frac{1}{2} - \langle N_{R\sigma}(t)\rangle] + \mu(Rt)b^{(+)}(RR''\overline{\sigma}t)\} + v_{RR''}^{(1)}(R')\{\lambda(Rt)b^{(+)}(RR''\overline{\sigma}t)[\frac{1}{2} - \langle N_{R\sigma}(t)\rangle] + \mu(Rt)b^{(-)}(RR''\overline{\sigma}t)\},$$

$$(4.2)$$

$$\begin{split} \Delta \eta^{(1)} \left(RR'R''; R\overline{\sigma}t \right) &= -z_{R''R}^{(1)}(R') \lambda(Rt) \, b^{(-)} \left(RR''\overline{\sigma}t \right) \left\langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \right\rangle \\ &+ v_{R''R}^{(1)}(R') \lambda(Rt) \, b^{(+)} \left(RR''\overline{\sigma}t \right) \left\langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \right\rangle , \end{split}$$

By inserting Eqs. (4.1) and (4.2) into Eq. (3.14) and also into the second equation in Eq. (3.17), and by setting the coefficients of $b^{(-)}$ and $b^{(+)}$ zero, we find that

$$\begin{split} \left[1-f\mu\left(Rt\right)\right] x_{RR''}^{(1)}\left(R'\right) \\ &= f\lambda(Rt) \left[\frac{1}{2} - \langle N_{R\sigma}(t)\rangle\right] y_{RR''}^{(1)}\left(R'\right) \\ &+ f\lambda(Rt) \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t)\rangle v_{R''R}^{(1)}(R') \,, \end{split}$$

$$\begin{split} \left[1 - f\mu(Rt)\right] y_{RR''}^{(1)}(R') \\ &= \left[\lambda(Rt)^2 / I\right] f^2 + f\lambda(Rt) \left[\frac{1}{2} - \langle N_{R\sigma}(t) \rangle\right] x_{RR''}^{(1)}(R') \\ &- f\lambda(Rt) \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle z_{R''R}^{(1)}(R'), \end{split}$$
(4.3)

 $[1 - \mu(Rt)] z_{RR''}^{(1)}(R')$

$$\begin{aligned} &= \lambda(Rt) \left\langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \right\rangle y_{R''R}^{(1)}(R') \\ &+ \lambda(Rt) \left[\frac{1}{2} - \left\langle N_{R\sigma}(t) \right\rangle \right] v_{RR''}^{(1)}(R') , \end{aligned}$$

$$\begin{split} \left[1-\mu(Rt)\right] v^{(1)}_{RR''}(R') \\ &= -\lambda(Rt) \left\langle C^{\dagger}_{R''\sigma}(t) C_{R\sigma}(t) \right\rangle x^{(1)}_{R''R}(R') \\ &+ \lambda(Rt) \left[\frac{1}{2} - \left\langle N_{R\sigma}(t) \right\rangle \right] z^{(1)}_{RR''}(R') \,. \end{split}$$

It is obvious that the solutions x, y, z, and v of the above equations are independent of the index R' and, in the limit of $\delta \epsilon = 0$, they are given by

$$\begin{split} & \chi_{RR''}^{(1)} \pm y_{RR''}^{(1)} = \frac{\lambda^3 f^2 I^{-1} \left[\left[\frac{1}{2} - n_{\sigma} \right) \mp \left(\frac{1}{2} - n_{\overline{\sigma}} \right) \right]}{D'_{RR''} \pm (1 - f) \lambda \left(\frac{1}{2} - n_{\sigma} \right)} , \\ & z_{RR''}^{(1)} \pm v_{RR''}^{(1)} = \frac{\lambda^3 f^2 I^{-1} \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle}{D'_{RR''} \mp (1 - f) \lambda \left(\frac{1}{2} - n_{\sigma} \right)} , \end{split}$$
(4.4)

where

$$D'_{RR''} \equiv (1 - f\mu) (1 - \mu) - f\lambda^2 (\frac{1}{2} - n_{\sigma})^2 + f\lambda^2 \langle C^{\dagger}_{R''\sigma} C_{R\sigma} \rangle \langle C^{\dagger}_{R\sigma} C_{R''\sigma} \rangle .$$
(4.5)

If f=1, $D'_{RR''}$ becomes equal to $\overline{D}_{RR''}$ given by Eq. (3.24) and, except for the factor λ/I , $x^{(1)}_{RR''}$ and $Z^{(1)}_{RR''}$ are equal to $x_{RR''}(R')$ and $x_{RR'}(R')$ given by Eq. (3.23), showing that, except for the factor

 $\lambda I^{-1} \epsilon(\sigma)$, the second-order correction is essentially the same as the first-order correction. However, since $f \neq 1$, the ω Fourier transform of the denominator $D'_{RR''} \pm (1-f)\lambda(\frac{1}{2}-n_{\sigma})$ remains a function of ω and is not reduced to the unfortunate form shown in the second term in Eq. (5.14) of I.

Higher-order corrections are given by Eqs. (3.14) and (3.17). By comparing the expressions for $\xi^{(n)}$ and $\xi^{(n-1)}$ given by Eq. (3.17), we find that

$$\xi^{(n)} (RR'\overline{\sigma}t) = f\phi(R\overline{\sigma}t) \xi^{(n-1)} (RR'\overline{\sigma}t) + f\left(\Delta\xi^{(n)} (RR'\overline{\sigma}t) + \sum_{R''} \Delta\eta^{(n)} (RR'R''; R\overline{\sigma}t)\right).$$

$$(4.6)$$

Here the first term on the right-hand side of Eq. (4.6) is equivalent to

$$\lim_{t^{\pm} \to t} \left[f\phi(R\overline{\sigma}t) \xi^{(n-1)}(RR'\overline{\sigma}t^{\pm}) + f\phi(R\overline{\sigma}t^{\pm}) \xi^{(n-1)}(RR'\sigma t) \right], \qquad (4.7)$$

when the expression for $\xi^{(n)}$ is inserted into the right-hand side of the basic equation (2.1). Since $\phi(R\overline{\sigma}t^{\pm})=0$ in the limit of $\delta\epsilon=0$, Eq. (4.6) is, in fact, equivalent to

$$\xi^{(n)} (RR'\overline{\sigma}t) = f\phi(R\overline{\sigma}t) \,\xi^{(n-1)} (RR'\overline{\sigma}t^{\pm}) + f\left(\Delta\xi^{(n)} (RR'\overline{\sigma}t) + \sum_{R''} \Delta\eta^{(n)} (RR'R''; R\overline{\sigma}t)\right).$$
Let us now assume that (4.8)

Let us now assume that

$$\xi^{(n)}(RR'\overline{\sigma}t) = \xi'(RR'\overline{\sigma}t)\,\xi^{(n-1)}(RR'\overline{\sigma}t^{\pm})\,,$$

 $\eta^{(n)}\left(RR\,'\,;R\,''\overline{\sigma}t\right)=\eta'\left(RR\,'\,;R\,''\overline{\sigma}t\right)\,\xi^{(n-1)}\left(RR\,'\overline{\sigma}t^{\pm}\right)\,.$

Then Eq. (4.8) is

$$\left[\xi'(RR'\overline{\sigma}t)-f\phi(R\overline{\sigma}t)\right]$$

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$$f\left(\Delta\xi'(RR'\overline{\sigma}t) + \sum_{R''}\Delta\eta'(RR'R'';R\overline{\sigma}t)\right)\right] \times \xi^{(n-1)}(RR'\overline{\sigma}t^{\pm}) = 0, \quad (4.10)$$

while Eq. (3.14) is reduced to

 $[\eta'(RR'; R''\overline{\sigma}t) - \Delta\xi'(RR'; R''\overline{\sigma}t) - \Delta\eta'(RR'; R''\overline{\sigma}t)]\xi^{(n-1)}(RR'\overline{\sigma}t^{\pm}) = 0.$ (4.11)

Since $\xi^{(n-1)} \neq 0$, the equations for ξ' and η' are the same as those for $\xi^{(1)}$ and $\eta^{(1)}$ given by Eqs. (3.14) and (3.17) except that the first term in Eq. (3.17), $\lambda \lambda_0^{-1} f^2 \phi$, is replaced by $f \phi$. Therefore ξ' and η' for any *n* are calculated as

$$= \sum_{R''} \left[x'_{RR''} b^{(+)} (RR'' \overline{\sigma} t) + y'_{RR''} b^{(-)} (RR'' \overline{\sigma} t) \right],$$
(4.12)

 $\eta'(RR'; R''\overline{\sigma}t) = \eta'(R; R''\overline{\sigma}t)$

 $\xi'(RR'\overline{\sigma}t) = \xi'(R\overline{\sigma}t)$

$$= z'_{RR''} b^{(+)} (RR''\overline{\sigma}t) + v'_{RR''} b^{(-)} (RR'''\overline{\sigma}t) + v'_{RR'''} b^{(-)} (RR'''$$

where, in the limit of $\delta \epsilon = 0$, x', y', z', and v' are given by

$$\begin{aligned} x'_{RR''} &\pm y'_{RR''} = \frac{\lambda^3 f I^{-1} \left[\left(\frac{1}{2} - n_{\sigma} \right) \mp \left(\frac{1}{2} - n_{\overline{\sigma}} \right) \right]}{D'_{RR''} \pm (1 - f) \lambda \left(\frac{1}{2} - n_{\sigma} \right)} , \\ z'_{RR''} &\pm v'_{RR''} = \frac{\lambda^3 f I^{-1} \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle}{D'_{RR''} \mp (1 - f) \lambda \left(\frac{1}{2} - n_{\sigma} \right)} . \end{aligned}$$
(4.13)

The self-energy corrections given by Eq. (3.6) can now be summed as follows:

$$\begin{split} \Sigma_{RR'\sigma}(tt') &= \xi_0(RR'\overline{\sigma}t)\,\delta_{tt}, \\ &+ \left(\frac{\lambda_{\overline{\sigma}}(Rt)^2 n_{\overline{\sigma}}(1-n_{\overline{\sigma}})}{1-\lambda_{\overline{\sigma}}(Rt)\,\lambda_{\overline{\sigma}}(0)\,n_{\overline{\sigma}}(1-n_{\overline{\sigma}})} \right. \\ &+ \frac{\xi^{(1)}(R\overline{\sigma}t)}{1-\xi'(R\overline{\sigma}t)} \right) \epsilon (RR'\sigma t)\,\delta_{tt}, \\ &+ \sum_{R''} \frac{\eta^{(1)}(R;R''\overline{\sigma}t)\,\epsilon (R''R'\sigma t)\,\delta_{tt'}}{1-\xi'(R\overline{\sigma}t)}, \end{split}$$

which is valid in the limit of $\delta \epsilon = 0$ because of the use of Eq. (4.8). In the limit of $\delta \epsilon = 0$, the above expression for the self-energy correction may be written in a more familiar form by using the relations $b^{(+)}(RR''\bar{\sigma}t) = 2\epsilon_{RR''} \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle$ and $b^{(-)}(RR''\bar{\sigma}t) = 0$ as well as Eqs. (3.23), (4.4), and (4.13). The result is

$$\Sigma_{RR'\sigma}(tt') = \sum_{R''} \frac{\left[(1 - 2n_{\sigma}) \,\delta_{RR'} + 2 \langle C_{R'\sigma}^{\dagger} C_{R\sigma} \rangle \,\delta_{R''R'} \right] \epsilon_{RR''} \langle C_{R\overline{\sigma}}^{\dagger} C_{R''\overline{\sigma}} \rangle}{(\frac{1}{2} - n_{\overline{\sigma}})^2 - (\frac{1}{2} - n_{\sigma})^2 + \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \,\langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle} \delta_{tt'} + \left[\left(\left[n_{\overline{\sigma}} (1 - n_{\overline{\sigma}}) I^2 + K_R \right] \epsilon_{RR'} + f \sum_{R''} L_{RR''} \epsilon_{R''R'} \right) / \left\{ \left[w - (1 - n_{\overline{\sigma}}) I \right]^2 - n_{\overline{\sigma}} (1 - n_{\overline{\sigma}}) I^2 - K_R \right\} \right] \delta_{tt'},$$

$$(4.15)$$

where

$$K_{R} = \sum_{R''} \frac{\lambda I \left[D'_{RR''} + (1-f) \lambda \left(\frac{1}{2} - n_{\overline{\sigma}}\right) \right] (1-2n_{\sigma}) \epsilon_{RR''} \langle C_{R\overline{\sigma}}^{\dagger} C_{R''\overline{\sigma}} \rangle}{(D'_{RR''})^{2} - (1-f)^{2} \lambda^{2} \left(\frac{1}{2} - n_{\sigma}\right)^{2}},$$

$$L_{RR''} = \langle \lambda I D'_{RR''} 2 \epsilon_{RR''} \langle C_{R\overline{\sigma}}^{\dagger} C_{R''\overline{\sigma}} \rangle \langle C_{R''\overline{\sigma}}^{\dagger} C_{R\sigma} \rangle / \left[(D'_{RR''})^{2} - (1-f)^{2} \lambda^{2} \left(\frac{1}{2} - n_{\sigma}\right)^{2} \right].$$
(4.16)

If $K_R = L_{RR''} = 0$, the above expression is exactly the same as the self-energy correction calculated in Paper I and given by Eq. (5.14) of I. Note that the first term in Eq. (4.15) remains abnormally large in the present calculation for a half-filled band in the split-band limit, suggesting that the complete solution of the restricted equation is still unsatisfactory, and that the effect of $\delta \langle N \rangle / \delta \epsilon$, etc., should be included in the calculation. This will be the subject of Sec. V.

V. EFFECTS OF $\delta \langle N \rangle / \delta \epsilon$ AND $\delta \langle C^{\dagger} C \rangle / \delta \epsilon$

We now wish to extend our calculation by including the $\delta\epsilon$ dependence of $\langle N \rangle$ and $\langle C^{\dagger}C \rangle$. Since it is no longer feasible to carry out a complete calculation, we shall illustrate how the complete solution of the restricted equation obtained in Sec. IV is modified by including the effect of $\delta \langle N \rangle / \delta\epsilon$ and $\delta \langle C^{\dagger}C \rangle / \delta \epsilon$, but by neglecting higher-order derivatives $\delta^n \langle N \rangle / \delta \epsilon^n$, etc., with $n \ge 2$.

Let us first calculate the contributions to $\xi_0(RR'\overline{\sigma}t)\delta_{tt'}$ obtained in Eqs. (3.19) and (3.23). In the presence of the external field, the parameters x and y are not given by Eq. (3.23) but should be calculated from Eq. (3.22). However, the part of $\xi_0(RR'\overline{\sigma}t)\delta_{tt'}$ which does not vanish in the limit of $\delta \epsilon = 0$ may be written

$$\overline{\xi}_{0}(RR'\overline{\sigma}t)\,\delta_{tt'} = \sum_{R''} \frac{p_{RR''\sigma}(t)\,\delta_{RR'}}{D_{RR''\sigma}(t)}\,\delta_{tt'} + \frac{q_{RR'\sigma}(t)}{D_{RR'\sigma}(t)}\,\delta_{tt'}, \qquad (5.1)$$

where

$$p_{RR''\sigma}(t) = \left[\frac{1}{2} - \langle N_{R\sigma}(t) \rangle\right] b^{(+)} (RR''\overline{\sigma}t) ,$$
$$q_{RR'\sigma}(t) = \langle C_{R'\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle b^{(+)} (RR'\overline{\sigma}t) ,$$

the factor
$$\lambda_{\sigma}^{=2}$$

Let $\delta\langle N \rangle$ and $\delta\langle C^{\dagger}C \rangle$ be the changes in values of $\langle N \rangle$ and $\langle C^{\dagger}C \rangle$ introduced by an external field $\delta\epsilon$, that is, $\delta\langle N \rangle = \langle N_{R\sigma}(t) \rangle - n_{\sigma}$, etc. The quantities p, q, and D will then be modified as $p + \delta p$, $q + \delta q$, and $D + \delta D$, and the resulting change in $\overline{\xi}_0$ may be expanded in powers of D^{-1} as follows:

Note that D defined above and used in the following is different from \overline{D} defined by Eq. (3.24) by

$$\overline{\xi}_{0}(RR'\overline{\sigma}t) = \sum \frac{p}{D} \left(1 + \frac{\delta p}{p}\right) \left(1 - \frac{\delta D}{D} + \frac{(\delta D)^{2}}{D^{2}} - \cdots\right) + \frac{q}{D} \left(1 + \frac{\delta q}{q}\right) \left(1 - \frac{\delta D}{D} + \frac{(\delta D)^{2}}{D^{2}} - \cdots\right).$$
(5.3)

In order to find the contribution from δD to the self-energy correction, let us insert the quantities

$$\sum \left(\frac{p}{D^2}\right) \delta D \,\delta_{tt'} = \sum_{R''} \left(\frac{p_{RR''\sigma}(t)}{[D_{RR''\sigma}(t)]^2}\right) \sum \frac{\delta D_{RR''\sigma}(t)}{\delta \epsilon (R_i R_j \overline{\sigma} t_i)} \delta \epsilon (R_i R_j \overline{\sigma} t_i) \,\delta_{RR'} \delta_{tt'}, \tag{5.4}$$

and

$$\left(\frac{q}{D^2}\right)\delta D\,\delta_{tt'} = \left(\frac{q_{RR'\sigma}(t)}{[D_{RR'\sigma}(t)]^2}\right)\sum \frac{\delta D_{RR'\sigma}(t)}{\delta\epsilon(R_iR_j\overline{\sigma}t_i)}\delta\epsilon(R_iR_j\overline{\sigma}t_i)\,\delta_{tt'},$$

into the right-hand side of Eq. (2.1). The results are

$$\sum_{R''} \frac{p_{R'R''\sigma}}{(D_{R'R''\sigma})^2} \zeta_{RR'\sigma}^{(-)}(R'R'';tt',t') \quad \text{and} \quad \sum_{R''} \frac{q_{R''R'\sigma}}{(D_{R''R'\sigma})^2} \zeta_{RR''\sigma}^{(-)}(R''R';tt',t'),$$
(5.5)

where

$$\begin{aligned} \zeta_{RR''\sigma}^{(\pm)}(R_1R_2;tt_1,t') &= \lambda_{\overline{\sigma}}(Rt) \, iG_{RR''\sigma}(tt_1) \sum_{R_3} b^{(\pm)}[RR_3\overline{\sigma}t;D_{R_1R_2\sigma}(t')] \,, \\ b^{(\pm)}[RR_3\overline{\sigma}t;D_{R_1R_2\sigma}(t')] &= \epsilon (RR_3\overline{\sigma}t) \, \frac{\delta D_{R_1R_2\sigma}(t')}{\delta\epsilon(RR_3\overline{\sigma}t)} \pm \epsilon (R_3R\overline{\sigma}t) \, \frac{\delta D_{R_1R_2\sigma}(t')}{\delta\epsilon(R_3R\overline{\sigma}t)} \,, \end{aligned}$$

$$(5.6)$$

and

$$\frac{\delta D_{RR'\sigma}(t)}{\delta\epsilon(R_iR_j\overline{\sigma}t_i)} = -\left[1 - 2\langle N_{R\overline{\sigma}}(t)\rangle\right] \frac{\delta\langle N_{R\overline{\sigma}}(t)\rangle}{\delta\epsilon(R_iR_j\overline{\sigma}t_i)} + \left[1 - 2\langle N_{R\sigma}(t)\rangle\right] \frac{\delta\langle N_{R\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\overline{\sigma}t_i)} + \langle C_{R\sigma}^{\dagger}(t)C_{R'\sigma}(t)\rangle \frac{\delta\langle C_{R'\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\overline{\sigma}t_i)} + \langle C_{R'\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle \frac{\delta\langle C_{R\sigma}(t)C_{R'\sigma}(t)\rangle}{\delta\epsilon(R_iR_j\overline{\sigma}t_i)} .$$
(5.7)

The corresponding contribution from $(\delta D)^2$ is obtained by inserting derivatives

$$\sum \frac{2!}{2!} \frac{p}{D^3} \zeta^{(-)} \sum \frac{\delta D}{\delta \epsilon} \delta \epsilon \text{ and } \frac{2!}{2!} \frac{q}{D^3} \zeta^{(-)} \sum \frac{\delta D}{\delta \epsilon} \delta \epsilon$$

of the first-order result obtained in Eq. (5.5) into the right-hand side of Eq. (2.1). The results are

$$\sum_{R''} \frac{p_{R'R''\sigma}}{(D_{R'R''\sigma})^3} \int_0^{-i\beta} dt_1 \sum_{R_1} \zeta_{RR_1\sigma}^{(-)}(R'R'';tt_1,t') \zeta_{R_1R'\sigma}^{(-)}(R'R'';tt',t')$$
(5.8)

and

$$\sum_{R''} \frac{q_{R''R'\sigma}}{D_{R''R'\sigma}} \int_0^{-i\beta} dt_1 \sum_{R_1} \zeta_{RR_1\sigma}^{(-)}(R''R';tt_1,t') \zeta_{R_1R''\sigma}^{(-)}(R''R';tt',t'),$$

and so on. By repeating the above calculation, the series on the right-hand side of Eq. (5.3) may be replaced by the following Taylor series: $\overline{\xi}_0(RR'\overline{\sigma}t)\,\delta_{tt'}+\Delta\overline{\xi}_0(RR'\overline{\sigma}tt')$

$$=\sum_{R''} \frac{p_{R'R''\sigma}(t')}{D_{R'R''\sigma}(t')} \left(\delta_{RR'} \delta_{tt'} - \frac{1}{D_{R'R''\sigma}} \xi_{RR'\sigma}^{(-)}(R'R'';tt',t') + \frac{1}{(D_{R'R''\sigma})^2} \int_{0}^{-i\beta} dt_1 \sum_{R_1} \xi_{RR_1\sigma}^{(-)}(R'R'';tt_1,t') \xi_{R_1R'\sigma}^{(-)}(R'R'';t_1t',t') - \frac{1}{(D_{R'R''\sigma})^3} \int_{0}^{-i\beta} dt_1 \int_{0}^{-i\beta} dt_2 \sum_{R_1} \sum_{R_2} \xi_{RR_1\sigma}^{(-)}(tt_1,t') \xi_{R_1R_2\sigma}^{(-)}(t_1t_2;t') \xi_{R_2R'\sigma}^{(-)}(t_2t',t') + \cdots \right) + \sum_{R''} \frac{q_{R''R'\sigma}(t')}{D_{R''R'\sigma}(t')} \left(\delta_{RR''} \delta_{tt'} - \frac{1}{D_{R''R''\sigma}} \xi_{RR''\sigma}^{(-)}(R''R';tt',t') + \frac{1}{(D_{R''R''\sigma})^2} \int_{0}^{-i\beta} dt_1 \sum_{R_1} \xi_{RR_1\sigma}^{(-)}(R''R';tt_1,t') \xi_{R_1R''\sigma}^{(-)}(R''R';t_1t',t') + \frac{1}{(D_{R''R''\sigma})^2} \int_{0}^{-i\beta} dt_1 \sum_{R_1} \xi_{RR_1\sigma}^{(-)}(R''R';tt_1,t') \xi_{R_1R''\sigma}^{(-)}(R''R';t_1t',t') - \frac{1}{(D_{R''R''\sigma})^3} \int_{0}^{-i\beta} dt_1 \int_{0}^{-i\beta} dt_2 \sum_{R_1} \sum_{R_2} \xi_{RR_1\sigma}^{(-)}(tt_1,t') \xi_{R_1R_2\sigma}^{(-)}(t_1t_2,t') \xi_{R_2R'''\sigma}^{(-)}(t_2t',t') + \cdots \right).$$
(5.9)

The above series corresponds to the series in Eq. (3.15). In the presence of $\delta \langle N \rangle / \delta \epsilon$ and $\delta \langle C^{\dagger} C \rangle / \delta \epsilon$, $\overline{\xi}_0$ is expanded as shown in Eq. (5.3) and hence the result $\Delta \overline{\xi}_0$ obtained by inserting $\overline{\xi}_0$ on the right-hand side of the basic equation iteratively includes, among many terms, those shown in Eq. (5.9). Since p as well as $\zeta^{(-)}$ is linear in $\epsilon(\overline{\sigma})$, the result $\Delta \overline{\xi}_0$ is no longer linear in $\epsilon(\overline{\sigma})$. Note that these terms with higher powers of $\epsilon(\bar{\sigma})$ do not involve $\varepsilon(\sigma)$ and hence they are a new type of terms not included in the original series introduced in Eq. (3.6). However, the series in Eq. (5.9) is not a self-consistent solution of the basic equation. If, for instance, $(p/D^2) \zeta^{(-)}$ is inserted into the right-hand side of Eq. (2.1), the derivatives involved operate on $\epsilon(\overline{\sigma})$ in $\zeta^{(-)}$ [but not $\epsilon(R'R''\overline{\sigma}t')$ in $p_{R'R''\overline{\sigma}}(t')$], yielding terms of the type $(p/D^2)[\lambda i G\sum (xb^{(+)}+yb^{(-)})]$. Let us assume that $\delta \langle N \rangle / \delta \epsilon$, etc., are small so that $(\delta \langle N \rangle / \delta \epsilon)^2$, etc., as well as $\delta^2 D / \delta \epsilon^2$ can be neglected. For the moment, let us also neglect δq . Then the most general expression ψ_0 for the $\epsilon(\sigma)$ -independent part of the self-energy correction is obtained from $\overline{\xi}_0 \delta_{tt}$, $+\Delta \overline{\xi}_0$ in Eq. (5.9) by replacing $\zeta^{(-)}$ by

$$\phi_{RR''\sigma}(R_1R_2;tt_1,t') = \lambda_{\overline{\sigma}}(Rt) iG_{RR''\sigma}(tt_1)$$

$$\times \sum_{R_3} \gamma \left[RR_3\overline{\sigma}t; D_{R_1R_2\sigma}(t')\right],$$
(5.10)

$$\begin{split} &\gamma \left[RR_{3}\overline{\sigma}t;D(t')\right] = x_{RR_{3}}b^{(+)} \left[RR_{3}\overline{\sigma}t;D(t')\right] \\ &+ y_{RR_{3}}b^{(-)} \left[RR_{3}\overline{\sigma}t;D(t')\right]. \end{split}$$

Here the parameters x and y should be determined in such a way that the *n*th-order term $\psi_0^{(n)}$ satisfies

$$\psi_{0}^{(n)}\left(RR\,'\overline{\sigma}tt'\right) = \Delta\overline{\xi}_{0}^{(n)}\left(RR\,'\overline{\sigma}tt'\right) + \Delta\psi_{0}^{(n)}\left(RR\,'\overline{\sigma}tt'\right),$$
(5.11)

where $\psi_0^{(n)}$ and $\Delta \overline{\xi}_0^{(n)}$, respectively, are the *n*thorder parts of ψ_0 and $\Delta \overline{\xi}_0$, which consist of terms in the *n*th power of ϕ and $\zeta^{(-)}$, while $\Delta \psi_0^{(n)}$ is the result obtained by inserting $\psi_0^{(n)}$ into the right-hand side of Eq. (2.1). The above equation corresponds to Eqs. (3.11) and (3.14), and makes $\psi_0^{(n)}$ a selfconsistent solution. Since derivatives in Eq. (2.1) operate on the leading terms $\zeta^{(-)}(tt_1, t')$ and $\phi(tt_1, t')$ and do not operate on the subsequent terms $\zeta^{(-)}(t_1t_2, t'), \phi(t_1t_2, t')$, etc., in the *n*-order products involved in $\Delta \overline{\xi}_0^{(n)}$ and $\psi_0^{(n)}$, the parameters x and y obtained by solving Eq. (5.11) are, again, independent of *n* and given by

$$\begin{aligned} x_{RR''} &= \lambda \left(\frac{1}{2} - n_{\sigma} + \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle \right) D_{RR''}^{-1} , \\ y_{RR''} &= \left[\mu \left(1 - \mu \right) + \lambda^2 \left(\frac{1}{2} - n_{\sigma} \right)^2 \right. \\ &\left. - \lambda^2 \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \left\langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle \right] D_{RR''}^{-1} , \end{aligned}$$
(5.12)

in the limit of $\delta \epsilon = 0$.

The self-consistent solution $\psi(RR'\overline{\sigma}tt')$ satisfying the basic Eq. (2.1) is now generated from Eq. (5.9) by replacing $\zeta^{(-)}$ by ϕ with x and y given by Eq. (5.12). Unfortunately, the resulting series ψ cannot be summed exactly into a simple analytic form. To demonstrate the net effect of $\delta \langle N \rangle / \delta \epsilon$, etc., however, let us assume that $\zeta_{RR''\sigma}^{(\pm)}(R_1R_2;tt_1,t')$ defined by Eq. (5.6) is independent of t' and the Fourier transform of $\psi(RR'\overline{\sigma}tt')$ may be calculated by replacing $\phi_{R_1R_2\sigma}(R'R'',tt_1,t')$ [or $\zeta_{R_1R_2\sigma}^{(-)}(R'R'',tt_1,t_1)$] by $\phi_{R_1R_2\sigma}(R'R'',tt_1,t_1)$ [or $\zeta_{R_1R_2\sigma}^{(-)}(R'R'',tt_1,t_1)$]. The resulting series may then be summed as follows:

$$\begin{split} \psi(RR'\bar{\sigma}\omega) &= \int_{0}^{-i\beta} dt \, e^{ix_{v}(t-t')} \psi_{(RR'\bar{\sigma}tt')} \\ &= \sum_{R''} \frac{p_{R'R''\sigma}}{D_{R'R''\sigma}} \bigg[\delta_{RR'} - \bigg(\frac{1}{D_{R'R''\sigma}} \bigg) \phi_{RR'\sigma}(R'R'';\omega) + \bigg(\frac{1}{D_{R'R''\sigma}} \bigg)^{2} \sum_{R_{1}} \phi_{RR_{1}\sigma}(R'R'';\omega) \phi_{R_{1}R'\sigma}(R'R'';\omega) \\ &- \bigg(\frac{1}{D_{R'R''\sigma}} \bigg)^{3} \sum_{R_{1}} \sum_{R_{2}} \phi_{RR_{1}\sigma}(R'R'';\omega) \phi_{R_{1}R_{2}\sigma}(R'R'';\omega) \phi_{R_{2}R'\sigma}(R'R'';\omega) + \cdots \bigg] \\ &+ \sum_{R''} \frac{q_{R''R'\sigma}}{D_{R''R'\sigma}} \bigg[\delta_{RR''} - \bigg(\frac{1}{D_{R''R'\sigma}} \bigg) \phi_{RR''\sigma}(R''R';\omega) + \bigg(\frac{1}{D_{R''R'\sigma}} \bigg)^{2} \sum_{R_{1}} \phi_{RR_{1}\sigma}(R''R';\omega) \phi_{R_{1}R''\sigma}(R''R';\omega) \\ &- \bigg(\frac{1}{D_{R''R'\sigma}} \bigg)^{3} \sum_{R_{1}} \sum_{R_{2}} \phi_{RR_{1}\sigma}(R''R';\omega) \phi_{R_{1}R_{2}\sigma}(R''R';\omega) \phi_{R_{2}R''\sigma}(R''R';\omega) \phi_{R_{1}R''\sigma}(R''R';\omega) \\ &- \bigg(\frac{1}{D_{R''R''\sigma}} \bigg)^{3} \sum_{R_{1}} \sum_{R_{2}} \phi_{RR_{1}\sigma}(R''R';\omega) \phi_{R_{1}R_{2}\sigma}(R''R';\omega) \phi_{R_{2}R'''\sigma}(R''R';\omega) + \cdots \bigg] \\ &= \sum_{R''} \frac{p_{R'R''\sigma}}{D_{R'R''\sigma}} \bigg(\delta_{RR'} - \frac{\varphi_{RR'\sigma}(R'R'';\omega)}{D_{R''R''\sigma} + \varphi_{RR\sigma}(R'R'';\omega)} \bigg) + \sum_{R''} \frac{q_{R''R'\sigma}}{D_{R''R'\sigma}} \bigg(\delta_{RR''} - \frac{\varphi_{RR''\sigma}(R''R';\omega)}{D_{R''R''\sigma} + \varphi_{RR''}(R''R'';\omega)} \bigg) \bigg) + \sum_{R''} \frac{q_{R''R''\sigma}}{D_{R''R''\sigma}} \bigg(\delta_{RR''} - \frac{\varphi_{RR''\sigma}(R''R'';\omega)}{D_{R''R''\sigma} + \varphi_{RR''}(R''R'';\omega)} \bigg) \bigg) \bigg) \bigg\}$$
(5.13)

where, as usual, $\psi(RR'\bar{\sigma}\omega)$ evaluated at $\omega = z_{\nu} = (\pi\nu/-i\beta) + \mu$ with odd integers ν may be continued to an analytic function $\psi(\omega)$ for all ω . Here the notations used are

$$\varphi_{RR_{1}\sigma}(R'R'';\omega) = \phi_{RR_{1}\sigma}(R'R'';\omega) + \sum_{R_{2} \neq R}' \frac{\phi_{RR_{2}\sigma}(R'R'';\omega)\varphi_{R_{2}R_{1}\sigma}(R'R'';\omega)}{D_{R'R''\sigma} + \varphi_{R_{2}R_{2}\sigma}(R'R'';\omega)},$$
(5.14)

$$\phi_{RR_{1}\sigma}(R_{1}R_{2};\omega) = \int_{0}^{-i\beta} dt \, e^{iz_{\nu}(t-t_{1})} \phi_{RR_{1}\sigma}(R_{1}R_{2};tt_{1},t_{1}) ,$$

$$\phi_{RR_{1}\sigma}(R_{1}R_{2};tt_{1},t_{1}) = \lambda_{\overline{\sigma}}(Rt) \, iG_{RR_{1}\sigma}(tt_{1}) \sum_{R''} \gamma \left[RR''\overline{\sigma}t; D_{R_{1}R_{2}\sigma}(t_{1}) \right] ,$$
(5.15)

$$\gamma \left[RR \,^{\prime\prime} \overline{\sigma}t; D(t_{1}) \right] = \frac{\lambda \left(\frac{1}{2} - n_{\sigma} + \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle \right)}{\left(\frac{1}{2} - n_{\sigma}\right)^{2} - \left(\frac{1}{2} - n_{\sigma}\right)^{2} + \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle} b^{(+)} \left[RR \,^{\prime\prime} \overline{\sigma}t; D(t_{1}) \right] + \frac{\mu (1 - \mu) + \lambda^{2} \left(\frac{1}{2} - n_{\sigma}\right)^{2} - \lambda^{2} \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle}{\left(\frac{1}{2} - n_{\sigma}\right)^{2} - \left(\frac{1}{2} - n_{\sigma}\right)^{2} + \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle} b^{(-)} \left[RR \,^{\prime\prime} \overline{\sigma}t; D(t_{1}) \right].$$

$$(5.16)$$

The above expression is obtained by summing all possible closed loops based on site R such as

$$\phi_{RR\sigma}$$
, $\sum_{R_1 \neq R}' \phi_{RR_1\sigma} \phi_{R_1R\sigma}$, $\sum_{R_1}' \sum_{R_2}'' \phi_{RR_1\sigma} \phi_{R_1R_2\sigma} \phi_{R_2R\sigma}$, etc.,

which appear in the series for ψ shown in Eq. (5.13). Since the same function ϕ appears in the denominators of ψ , the self-energy correction ψ obtained in Eq. (5.13) is given in the form of infinite fractions. The approximation used in Eq. (5.13) involves the following replacement:

$$\int_{0}^{-i\beta} dt \int_{0}^{-i\beta} dt_{1} e^{iz_{v}(t-t')} \left(\cdots G(tt_{1}) \frac{\delta \langle N_{R\sigma}(t') \rangle}{\delta \epsilon(t)} \right) \left(\cdots G(t_{1}t') \frac{\delta \langle N_{R\sigma}(t') \rangle}{\delta \epsilon(t_{1})} \right) + \int_{0}^{-i\beta} dt \int_{0}^{-i\beta} dt_{1} e^{iz_{v}(t-t')} \left(\cdots G(tt_{1}) \frac{\delta \langle N_{R\sigma}(t_{1}) \rangle}{\delta \epsilon(t)} \right) \left(\cdots G(t_{1}t') \frac{\delta \langle N_{R\sigma}(t') \rangle}{\delta \epsilon(t_{1})} \right).$$
(5.17)

Since the main contribution to the Fourier integral comes from the narrow time interval where $t \sim t_1 \sim t'$ and also since the leading terms $\phi_{RR'\sigma}(R'R'';\omega)$ and $\phi_{RR''\sigma}(R'R';\omega)$ in the series for ψ have been calculated exactly, the above approximation may

not be unreasonable for our purpose.

In the foregoing calculation, the contributions from δp and δq are neglected, but these contributions may be included similarly. The result is to make the following replacement in the last expres-

sion in Eq. (5.13):

$$p_{R'R''\sigma} - p_{R'R''\sigma} + \phi_{RR'\sigma}^{(p)}(R'R'';\omega),$$

$$q_{R''R'\sigma} - q_{R''R'\sigma} + \phi_{RR''\sigma}^{(q)}(R''R';\omega).$$
(5.18)

Here $\phi^{(p)}$ and $\phi^{(q)}$ are the same as ϕ defined by Eqs. (5.15) and (5.16), except that $b^{(\pm)}[D]$'s involved are replaced by $b^{(\pm)}[p]$ and $b^{(\pm)}[q]$, respectively, where

$$\begin{split} b^{(\pm)}[RR_3\overline{\sigma}t;q_{R_1R_2\sigma}(t_1)] = &\epsilon(RR_3\overline{\sigma}t)\frac{\delta q_{R_1R_2\sigma}(t_1)}{\delta_N\epsilon(RR_3\overline{\sigma}t)} \\ &\pm &\epsilon(R_3R\overline{\sigma}t)\frac{\delta q_{R_1R_2\sigma}(t_1)}{\delta_N\epsilon(R_3R\overline{\sigma}t)} , \end{split}$$

(5.19)

and $\delta_N \epsilon(\overline{\sigma})$ is to operate only on $\langle N_{R'\sigma'}(t_1) \rangle$ and $\langle C_{R'\sigma'}^{\dagger}(t_1) C_{R''\sigma'}(t_1) \rangle$ and not to operate on $\epsilon(\overline{\sigma})$ involved, that is,

$$\frac{\delta q_{RR'\sigma}(t)}{\delta_{N}\epsilon(R_{i}R_{j}\overline{\sigma}t_{i})} = \frac{\delta q_{RR'\sigma}(t)}{\delta\epsilon(R_{i}R_{j}\overline{\sigma}t_{i})} - \frac{\delta q_{RR'\sigma}(t)}{\delta_{0}\epsilon(R_{i}R_{j}\overline{\sigma}t_{i})}$$

$$= b^{(+)}(RR'\overline{\sigma}t) \frac{\delta \langle C_{R'\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle}{\delta\epsilon(R_{i}R_{j}\overline{\sigma}t_{i})}$$

$$+ \langle C_{R'\sigma}^{\dagger}(t)C_{R\sigma}(t)\rangle \left(\epsilon(RR'\overline{\sigma}t) \frac{\delta \langle C_{R'\overline{\sigma}}^{\dagger}(t)C_{R'\overline{\sigma}}(t)\rangle}{\delta\epsilon(R_{i}R_{j}\overline{\sigma}t_{i})} + \epsilon(R'R\overline{\sigma}t) \frac{\delta \langle C_{R'\sigma}^{\dagger}(t)C_{R\overline{\sigma}}(t)\rangle}{\delta\epsilon(R_{i}R_{j}\overline{\sigma}t_{i})}\right). (5.20)$$

The expression for $b^{(\pm)}[p]$ is obtained similarly.

The same calculation may be applied to the second, third and fourth terms in the self-energy correction Σ_{σ} obtained in Eq. (4.14). The second term may be written in the form of the first term in Eq. (5.14) of I and, since its functional structure is essentially the same as $\overline{\xi}_0$ given by Eq. (5.1), the effect of $\delta \langle N \rangle / \delta \epsilon$, etc., can be calculated exactly the same manner as before modifying the Fourier transform of the second term as follows:

$$\sum_{R''} \frac{n_{\overline{\sigma}}(1-n_{\overline{\sigma}})I^2 \epsilon_{R''R'}}{[\omega - (1-n_{\overline{\sigma}})I]^2 - n_{\overline{\sigma}}(1-n_{\overline{\sigma}})I^2}$$

$$\times \left(\delta_{RR''} - \frac{\varphi_{RR''\sigma}^{(D'')}(R''R';\omega)}{D_{R''R'\sigma}^{''} + \varphi_{RR\sigma}^{(D'')}(R''R';\omega)} \right), \tag{5.21}$$

where $\varphi^{(D'')}$ is the same as φ defined by Eq. (5.14) except that $D_{R_1R_2\sigma}$ involved in *b* given by Eq. (5.6) is replaced by

$$D_R'' = \{ w - [1 - \langle N_{R\overline{\sigma}}(t) \rangle] I \}^2 - n_{\overline{\sigma}}(1 - n_{\overline{\sigma}}) I^2.$$
 (5.22)

The third, fourth terms in Σ_{σ} can be expanded in powers of ξ' and η' defined by Eq. (4.12) and the same calculation may be applied to ξ' and η' individually. The results are to modify the Fourier transforms of x', y', z', and v' given by Eq. (4.13) into the following form:

$$x_{RR''}'' \pm y_{RR''}'' = \sum_{R_1} \left(\frac{P_{R_1} + \phi_{R_1}^{(p)}(R_1R'';\omega)}{D'_{R_1R''} \pm (1-f)\lambda(\frac{1}{2} - n_{\sigma})} \right) \left(\delta_{RR_1} - \frac{\varphi_{RR_1\sigma}^{(D'\pm)}(R_1R'';\omega)}{D'_{R_1R''} \pm (1-f)\lambda(\frac{1}{2} - n_{\sigma}) + \varphi_{RR_1\sigma}^{(D'\pm)}(R_1R'';\omega)} \right),$$

$$z_{RR''}'' \pm v_{RR''}'' = \sum_{R_1} \left(\frac{Q_{R_1R''} + \phi_{R_1R''}^{(Q)}(R_1R'';\omega)}{D'_{R_1R''} \mp (1-f)\lambda(\frac{1}{2} - n_{\sigma})} \right) \left(\delta_{RR_1} - \frac{\varphi_{RR_1\sigma}^{(D'\pm)}(R_1R'';\omega)}{D'_{R_1R''} \mp (1-f)\lambda(\frac{1}{2} - n_{\sigma}) + \varphi_{RR_1\sigma}^{(D'\pm)}(R_1R'';\omega)} \right),$$

$$(5.23)$$

where $\phi^{(P)}$, $\phi^{(Q)}$, and $\varphi^{(D'\pm)}$ are parallel to ϕ and φ defined by Eqs. (5.14)-(5.16) except for an appropriate replacement of D involved in $b^{(\pm)}[D]$ by P, Q, or (D'^{\pm}) , where

$$P_{R} = \lambda_{\overline{\sigma}}(Rt)^{3} f_{\overline{\sigma}}(Rt) I^{-1} \{ [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle] \mp [\frac{1}{2} - \langle N_{R\overline{\sigma}}(t) \rangle] \},$$

$$Q_{RR''} = \lambda_{\overline{\sigma}}(Rt)^{3} f_{\overline{\sigma}}(Rt) I^{-1} \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle,$$

$$(D'^{\pm})_{RR''} = [1 - f_{\overline{\sigma}}(Rt) \mu_{\overline{\sigma}}(Rt)] [1 - \mu_{\overline{\sigma}}(Rt)] - f_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(Rt)^{2} [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle]$$

$$+ f_{\overline{\sigma}}(Rt) \lambda_{\overline{\sigma}}(Rt)^{2} \langle C_{R''\sigma}^{\dagger}(t) C_{R\sigma}(t) \rangle \langle C_{R\sigma}^{\dagger}(t) C_{R''\sigma}(t) \rangle \pm [1 - f_{\overline{\sigma}}(Rt)] \lambda_{\overline{\sigma}}(Rt) [\frac{1}{2} - \langle N_{R\sigma}(t) \rangle].$$

$$(5.24)$$

In summary, the self-energy correction $\boldsymbol{\Sigma}_{\sigma}$ is written

$$\Sigma_{RR'\sigma}(\omega) = \sum_{R''} \left(\frac{(1-2n_{\sigma})\epsilon_{R'R''} \langle C_{R'\sigma}^{\dagger} C_{R''\sigma}^{\dagger} \rangle + \phi_{RR'\sigma}^{(p)} (R'R'';\omega)}{(\frac{1}{2} - n_{\sigma}^{-})^2 - (\frac{1}{2} - n_{\sigma})^2 + \langle C_{R'\sigma}^{\dagger} C_{R''\sigma}^{-} C_{R''\sigma}^{-} \rangle \langle C_{R''\sigma}^{\dagger} C_{R'\sigma}^{-} \rangle} \right)$$

$$\times \left(\delta_{RR'} - \frac{\varphi_{RR'\sigma}(R'R'';\omega)}{(\frac{1}{2} - n_{\sigma})^{2} - (\frac{1}{2} - n_{\sigma})^{2} + \langle C_{R'\sigma}^{+} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{+} C_{R'\sigma} \rangle + \varphi_{RR\sigma}(R'R'';\omega)} \right)$$

$$+ \sum_{R''} \left(\frac{2\epsilon_{R'R''} \langle C_{R''\sigma}^{+} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{+} C_{R'\sigma} \rangle + \phi_{RR''\sigma}^{(q)}(R''R';\omega)}{(\frac{1}{2} - n_{\sigma})^{2} - (\frac{1}{2} - n_{\sigma})^{2} + \langle C_{R'\sigma}^{+} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{+} C_{R'\sigma} \rangle} \right)$$

$$\times \left(\delta_{RR''} - \frac{\varphi_{RR''\sigma}(R''R';\omega)}{(\frac{1}{2} - n_{\sigma})^{2} - (\frac{1}{2} - n_{\sigma})^{2} + \langle C_{R'\sigma}^{+} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{+} \rangle \langle C_{R''\sigma}^{+} C_{R'\sigma} \rangle + \varphi_{RR\sigma}(R''R';\omega)} \right)$$

$$+ \sum_{R''} \left[\left(\left[n_{\sigma}(1 - n_{\sigma})I^{2} + K_{R''}\right] \epsilon_{R''R'} + f \sum_{R'''} L_{R''R''}' \epsilon_{R'''R'} \right) \right/ \left\{ \left[\omega - (1 - n_{\sigma})I^{2} - n_{\sigma}(1 - n_{\sigma})I^{2} - K_{R''}' \right\} \right]$$

$$\times \left(\delta_{RR''} - \frac{\varphi_{RR''\sigma}(R''R';\omega)}{D_{R''R'\sigma}'} + \varphi_{RR\sigma}'(R''R';\omega)} \right),$$

$$(5.25)$$

where

$$K'_{R} = (I^{2}/\lambda^{2}f) \sum_{R''} 2x''_{RR''} \epsilon_{RR''} \langle C^{\dagger}_{R\overline{o}} C_{R''\overline{o}} \rangle, \quad L'_{RR''} = (I^{2}/\lambda^{2}f) 2v''_{RR''} \epsilon_{RR''} \langle C^{\dagger}_{R\overline{o}} C_{R''\overline{o}} \rangle, \quad (5.26)$$

and $x''_{RR''}$ and $v''_{RR''}$ are given by Eq. (5.23).

If K', L', and the ϕ 's are all zero, the above result is exactly equal to the result in Paper I given by Eq. (5.14) of I. If all ϕ 's are zero, K' and L' given by Eqs. (5.23) and (5.26) become equal to K and L given by Eq. (4.16) and hence the above result is exactly the same as the complete solution of the restricted equation given by Eq. (4.15), illustrating the way the self-energy correction Σ_{σ} has been improved.

The first term in Eq. (4.15), which has been the source of the difficulty involved in the complete solution of the restricted equation, is now modified as shown in the first two terms in Eq. (5.25). Note, in particular, that the newly obtained terms may be rewritten

$$\sum_{R''} \frac{(1-2n_{\sigma}) \epsilon_{RR''} \langle C_{R\sigma}^{\dagger} C_{R'\sigma} \rangle + \phi_{RR\sigma}^{(p)}(RR'';\omega)}{(\frac{1}{2}-n_{\sigma})^{2}-(\frac{1}{2}-n_{\sigma})^{2}+\langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle + \varphi_{RR\sigma}(RR'';\omega)} + \frac{2\epsilon_{RR'} \langle C_{R\sigma}^{\dagger} C_{R'\sigma} \rangle \langle C_{R'\sigma}^{\dagger} C_{R\sigma} \rangle + \phi_{RR\sigma}^{(q)}(RR';\omega)}{(\frac{1}{2}-n_{\sigma})^{2}-(\frac{1}{2}-n_{\sigma})^{2}+\langle C_{R\sigma}^{\dagger} C_{R'\sigma} \rangle \langle C_{R'\sigma}^{\dagger} C_{R\sigma} \rangle + \varphi_{RR\sigma}(RR';\omega)} + \cdots,$$
(5.27)

where the dots represent terms involving $\varphi_{RR'\sigma}$ with $R \neq R'$. Here the terms involving $\varphi_{RR'\sigma}$ are higher-order corrections not included in the result in Eq. (4.15). In the nonmagnetic solution where $n_{\overline{\sigma}} = n_{\sigma}$, the denominators in the above expression, $\langle C_{R\sigma}^{\dagger} C_{R''\sigma} C_{R\sigma} \rangle + \varphi_{RR\sigma} (RR''; \omega)$, may become abnormally small in the absence of ϕ and ϕ , since $\langle C_{R\sigma}^{\dagger} C_{R'\sigma} \rangle = (1/N) \sum_{k} n_{k\sigma} e^{ik(R-R')}$ vanishes when the lower band is nearly empty or nearly filled. However, the correction term $\varphi_{RR\sigma} (RR'')$ is of the same order as the leading term $\langle C_{R\sigma}^{\dagger} C_{R''\sigma} C_{R\sigma} \rangle$ in the denominators, making the values of the first two terms in Eq. (5.27) completely different. The order of magnitude of ϕ and ϕ may be estimated as follows. Use of the expansion for $\delta \langle N_{R\overline{\alpha}} \rangle / \delta \in (\overline{\sigma})$, etc., given by Eq. (B4) of I in Eq. (5.6) yields

$$\zeta_{RR\sigma}^{(\pm)}(RR';tt',t') = -\lambda i G_{RR\sigma}(tt') \sum_{R_3} (1-2n_{\sigma}) \{ \epsilon_{RR_3} [i G_{RR\overline{\sigma}}(t't) G_{R_3R\overline{\sigma}}(tt')] \pm \epsilon_{R_3R} [i G_{RR_3\overline{\sigma}}(t't) G_{RR\overline{\sigma}}(tt')] \} + \cdots,$$
(5.28)

where the Fourier transform of $iG_{RR\sigma}(tt')iG_{RR\overline{\sigma}}(tt')G_{R_{3}R\overline{\sigma}}(tt')$ may be calculated as follows:

$$\Gamma(z_{\nu}) = \int_{t'}^{t'-i\beta} dt \, iG_{RR\overline{\sigma}}(tt') \, iG_{RR\overline{\sigma}}(tt') \, G_{R_{3}R\overline{\sigma}}(tt') \, e^{iz_{\nu}(t-t')} = - \int \int \int \left(\frac{d\omega}{2\pi}\right)^{3} \frac{1 + e^{\beta(\mu - \omega_{1} + \omega_{2} - \omega_{3})}}{(1 + e^{-\beta(\omega_{1} - \mu)}) \left(e^{\beta(\omega_{2} - \mu)} + 1\right) \left(1 + e^{-\beta(\omega_{3} - \mu)}\right)} \frac{A_{RR\sigma}(\omega_{1}) A_{RR\overline{\sigma}}(\omega_{2}) A_{R_{3}R\overline{\sigma}}(\omega_{3})}{z_{\nu} - \omega_{1} + \omega_{2} - \omega_{3}} , \quad (5.29)$$

where $z_v = (\pi v/-i\beta) + \mu$. The above integral is nonvanishing if ω_1 and ω_3 are above and ω_2 below the Fermi level or ω_1 and ω_3 below and ω_2 above the Fermi level, and, if the spectrum is continu-

ous, the value of $\Gamma(\omega)$ will be small as long as ω is not in the bottom or the top of the spectrum. In the strong-coupling limit, however, the band is split into two and the width of each split band, Δ ,

$$\Gamma(z_{\nu}) \sim (1 - n_{\sigma}) n_{\overline{\sigma}} \langle C_{R_{\overline{\sigma}}}^{\dagger} C_{R_{\sigma}}^{\dagger} \rangle / \Delta .$$
(5.30)

By inserting this and the Fourier transform of

$$iG_{RR\sigma}(tt')iG_{RR_{3}\overline{\sigma}}(t't)G_{RR\overline{\sigma}}(tt')$$

into ϕ given by Eqs. (5.10) and (5.15), we finally find that

$$\phi_{RR\sigma}(RR'';\omega) \sim (1-2n_{\sigma}) \epsilon_{RR''} / \Delta \sim 1-2n_{\sigma} , \quad (5.31)$$

because $\epsilon_{RR''} \sim \Delta$. When the lower band is nearly filled, $(1-2n_{o})$ and $\langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle$ are of the same order and vanish. Hence $\phi_{RR\sigma}(RR'';\omega)$ will be greater than the leading term in the denominators, $\langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle \langle C_{R''\sigma}^{\dagger} C_{R\sigma} \rangle$, and also the numerators, $(1-2n_{\sigma}) \epsilon_{RR''} \langle C_{R\sigma}^{\dagger} C_{R''\sigma} \rangle$ and $2\epsilon_{RR'} \langle C_{R\sigma}^{\dagger} C_{R'\sigma} \rangle \times \langle C_{R'\sigma}^{\dagger} C_{R\sigma} \rangle$, in Eq. (5.27). This suggests that the obvious defect found in the solution in Sec. IV is removed by including the effect of $\delta \langle N \rangle / \delta \epsilon(\overline{\sigma})$, etc. In other circumstances, when the filling differs significantly from $\frac{1}{2}$ or away from the narrow band limit, the solution of Sec. IV might not be deficient.

VI. DISCUSSION

The solution obtained in Sec. IV is the complete self-consistent solution of the basic Eq. (2.1) under the restrictions that $\pi [\Delta]$ is neglected and that functional derivatives $\delta \epsilon$ involved are replaced by the $\delta_0 \epsilon$'s which operate only on $\epsilon(\sigma)$ or $\epsilon(\overline{\sigma})$ as they occur explicitly, and not on $\langle N \rangle$ and $\langle C^{\dagger}C \rangle$ in which they occur implicitly, i.e., $\delta \langle N \rangle / \delta_0 \epsilon = 0$

Dept. of Physics, University of Chicago, Chicago, Ill. ¹T. Arai, M. H. Cohen, and M. P. Tosi, preceding paper, and $\delta \langle C^{\dagger}C \rangle / \delta_0 \epsilon = 0$. In principle, this result may be obtained by the iterative perturbation method developed in Paper I. However, such an approach is not only very complicated to carry out, but it is also difficult to ascertain if all possible terms are really included in the final result. In the present approach, the self-energy correction Σ_σ is expanded in powers of $\epsilon(\sigma)$ and $\epsilon(\overline{\sigma})$ as is shown in Eq. (3.5) and the parameters x, y, z, and v defined by Eqs. (3.19), (4.1), and (4.12) are determined by solving Eqs. (3.11), (3.14), and (3.17)exactly. Since, by inspection, Eq. (3.5) is the most general form for the self-energy correction under the proposed restrictions, it is easily recognized that the result obtained in Eqs. (4.14) or (4.15) is the complete solution. In the course of the calculation, we have also confirmed that the result in Paper I is exact through terms linear in ε.

The complete solution of the restricted equation given by Eq. (4.15) still exhibits the difficulty noted in Paper I that the second term in Eq. (5.14) of I becomes abnormally large for a half-filled case in the split band limit. As we have discussed in the end of Sec. V, this difficulty is removed by including the effect of $\delta \langle N \rangle / \delta \epsilon$. The calculation shows that care must be taken in expanding the solution formally in powers of ϵ . Note that the calculation developed in Sec. V is not exact because of the approximation described in Eq. (5.17).

We shall discuss the physics involved in the results obtained so far in a third paper at a formal and qualitative level and give numerical results in a subsequent publication.

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Phys. Rev. B <u>15</u>, 1817 (1977). This paper will be referred to as Paper I.

²T. Arai and M. Tosi, Solid State Commun. <u>14</u>, 947

^{(1974);} T. Arai, Phys. Rev. Lett. 33, 486 (1974).

³The idea is based on J. Schwinger, Proc. Natl. Acad. Sci. (U.S.) <u>37</u>, 452 (1951); see also, L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).

⁴J. Hubbard, Proc. R. Soc. A <u>276</u>, 238 (1963). This paper will be referred to as Hubbard I.