Hubbard Model. I. Degeneracy in the Atomic Light*

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The atomic limit of the Hubbard Hamiltonian is extremely degenerate. The ground-state degeneracy, in particular, makes the zero-temperature Green's function for this limit ambiguous. The manifestations of the degeneracy in the one- and two-particle Green's functions are found. The degeneracy gives rise to nonlocal spatial correlation of physical significance which must be taken into account in narrow-band-regime perturbation schemes for the model.

I. INTRODUCTION

THE Hubbard model[1] is essentially a cell model describing electron motion in a crystal with the electronic Coulomb repulsion screened out except between electrons in the same cell. In its simplest form, only a single s band is considered; that is, there is only one spatial state per lattice site. The strength of the term in the Hamiltonian that contains hopping from cell to cell, or, equivalently, from lattice site to lattice site, is characterized by the parameter Δ. This parameter is closely related to the bandwidth. In Hubbard's notation, the Coulomb energy associated with two electrons of opposite spin on the same site is I. The narrow band limit $kT \ll \Delta \ll I$ of this model is very interesting and is related to the problems of itinerant magnetism and the electrical properties of many materials. In this paper,[2] we will clarify the mathematical and physical implications of the extreme degeneracy which becomes important for $kT=0$, $\Delta \ll I$.

Any attempt to solve the Hubbard model in this narrow-energy-band limit faces two serious (and not unrelated) obstacles. First, we are dealing with a large potential energy and, hence, may not use any of the ordinary perturbation expansions in powers of the potential. Second, any expansion in powers of the hopping parameter must be done with caution because of the degeneracy. For zero Δ, or no hopping, a complete set of energy eigenstates can be labeled simply by the up- and down-spin occupation numbers for all the sites. However, the eigenvalues of the Hamiltonian depend in this limit only on the total number of doubly occupied sites in the eigenstate. This means that there is degeneracy of very high multiplicity reflecting the number of ways that electrons can be arranged on a lattice under the constraint that the number of doubly occupied sites is fixed by the energy. Most important, the ground state is, in general, extremely degenerate. The multiplicity of the ground state can be so large that degenerate perturbation theory in its usual form may not be employed. However, it is essential that any approximation that takes advantage of the smallness of the kinetic energy incorporate the essence of degenerate perturbation theory. The point is that for finite hopping the degeneracy is broken and the ground state is unique. As the hopping vanishes, the ground state evolves into a particular one of its many degenerate ground states. Certain phase relations persist between electrons on *different* sites. One manifestation of these phase relations, which we will explicitly verify, is that the one-particle Green's function which describes single-particle propagation is nonlocal *even* for vanishing kinetic energy. Another manifestation we find is that the nonlocal spin-density correlation function which describes the coupling between both parallel and antiparallel spins on different sites is nonvanishing. Hence, there are zeroth-order nonlocal correlations even though the zero-order Hamiltonian is a sum of commuting parts, each of which refers only to a single site.

Harris and Lange[3] have enumerated other physical manifestations of these phase relations. They exactly solve the two-site problem and then, by applying some very general moment techniques to the N-site case, show that these phase relations are essential if one is to get the correct first-order terms in an expansion in the hopping parameters.

Many solutions to the Hubbard Hamiltonian have been proposed for the $\Delta \ll I$ regime. All of these solutions either explicitly or implicitly utilize the fact that Δ/I is small. Usual Green's functions or equations of motion decoupling neglect the zero-order manifestations of the ground-state degeneracy. Any procedure which intends to calculate Δ finite and use the $\Delta=0$ model as a jumping-off point must begin with the proper solutions which fully reflect the spatial coherence implied by the degeneracy.

After defining necessary quantities in Sec. II, we derive, in Sec. III, the full implications of the ground-state degeneracy as manifest in the Green's functions and correlation functions for $\Delta=0$.

II. FORMALISM AND DEFINITIONS

The Hubbard Hamiltonian is

$$\mathcal{H} = \sum_{ij\sigma} T_{ij} c_{i\sigma}{}^{\dagger} c_{j\sigma} + \tfrac{1}{2} I \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}. \tag{1}$$

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The operator $c_{i\sigma}^\dagger$ creates an electron with spin σ ($\sigma=\pm1$) in a Wannier state centered at the lattice site labeled by the position vector R_i. These operators are related to Bloch-state creation and annihilation operators by

$$c_{i\sigma}^\dagger=\frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i}c_{\mathbf{k},\sigma}^\dagger. \tag{2}$$

The operators $c_{i\sigma}^\dagger$ have the usual Fermion equal-time anticommutation relation

$$\{c_{i\sigma}^\dagger,c_{j\sigma'}\}=\delta_{R_iR_j}\delta_{\sigma,\sigma'}. \tag{3}$$

The coefficients in the first (or hopping term) are related to the Bloch energies by

$$T_{ij}=\frac{1}{N}\sum_{\mathbf{k}}\epsilon(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}. \tag{4}$$

Without loss of generality we will choose our zero of energy such that $T_{ii}=0$. Using Eqs. (1) and (4), we may rewrite the hopping term in (1) in the more familiar form

$$\mathcal{H}_0=\sum_{\mathbf{k},\sigma}\epsilon(\mathbf{k})c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}. \tag{5}$$

The interaction term in Eq. (1) represents the screened Coulomb potential. Note that essentially all it does is count the number of doubly occupied sites. Here, the operator $n_{i\sigma}$ is defined, as usual, as

$$n_{i\sigma}=c_{i\sigma}c_{i\sigma}^\dagger. \tag{6}$$

The parameter Δ, mentioned earlier, is defined by

$$\Delta=\left(\frac{1}{N}\sum_{ij}|T_{ij}|^2\right)^{1/2}. \tag{7}$$

The following Green's functions will be needed [in these definitions, $(\ )_+$ is the time-ordered product; the subscript in the operator $c_{1\sigma}^\dagger$ refers to site R_1 and time t_1]:

$$G_{11'\sigma}=-i\langle(c_{1\sigma}c_{1'\sigma}^\dagger)_+\rangle, \tag{8}$$

$$\Gamma_{11'\sigma}=-i\langle(n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^\dagger)_+\rangle, \tag{9}$$

$$W_{11'2'}{}^{\sigma}=-i\langle(c_{1\sigma}c_{1-\sigma}c_{2'-\sigma}^\dagger c_{1'\sigma}^\dagger)_+\rangle, \tag{10}$$

$$D_{12}{}^{\sigma\sigma'}=\langle(n_{1\sigma}n_{2\sigma'})_+\rangle-\langle n_{1\sigma}\rangle\langle n_{2\sigma'}\rangle, \tag{11}$$

$$S_{12,\sigma}=\langle(c_{1\sigma}c_{1-\sigma}^\dagger c_{2-\sigma}c_{2\sigma}^\dagger)_+\rangle. \tag{12}$$

The Fourier transforms are defined with a factor $e^{+i\omega t}$ for the unprimed time variables, and $e^{-i\omega t'}$ for the primed time variables. Much of the paper is devoted to finding these functions in the atomic limit.

If $G_{11'\sigma}$ and $\Gamma_{11'\sigma}$ are functions of $t_1-t_{1'}$ then $G_{R_1R_{1'}\sigma}(\omega_1\omega_{1'})$ and $\Gamma_{R_1R_{1'}\sigma}(\omega_1\omega_{1'})$ may be written as

$$G_{R_1R_{1'}\sigma}(\omega_1\omega_{1'})=2\pi\delta(\omega_1-\omega_{1'})G_{R_{1'}R_1\sigma}(\omega) \tag{13}$$

and

$$\Gamma_{R_1R_{1'}\sigma}(\omega_1\omega_{1'})=2\pi\delta(\omega_1-\omega_{1'})\Gamma_{R_1R_{1'}\sigma}(\omega_1). \tag{14}$$

We shall be interested in evaluating these functions in the limit of $\Delta\to0$. In that limit, the time dependence of the operators $c_{1\sigma}$ is given by

$$i(\partial/\partial t_1)c_{1\sigma}=[c_{1\sigma},\mathcal{H}_{\text{at}}], \tag{15}$$

where

$$\mathcal{H}_{\text{at}}=\tfrac{1}{2}I\sum_{i\sigma}n_{i\sigma}n_{i-\sigma}. \tag{16}$$

Since we are working at zero temperature, the expectation value is over the ground state of H_{at}. But now we encounter the difficulty. Because of the degeneracy, there are many ground states of H_{at}. Corresponding to this ambiguity in the ground state, there is an ambiguity in the Green's functions. The correct ground state is fixed by the condition that if we slowly turn on the hopping and then slowly turn it off, we return to the same state. The correct Green's functions correspond to those unique functions one obtains by evaluating the unambiguous Green's functions for finite hopping and then taking the zero hopping limit.

In this paper, we establish the nature of the ambiguity in the one-particle Green's function. We then express all ambiguity in higher-order functions in terms of that which appears in the one-particle function. This process clarifies the physical manifestations of the degeneracy.

III. ATOMIC-LIMIT GREEN'S FUNCTIONS

A. One-Particle Green's Function

In this section we find the most general form for the one-particle Green's function for the Hubbard Hamiltonian in the limit of zero hopping, that is, the atomic limit. This function then satisfies the equations

$$i(\partial/\partial t_1)G_{11'\sigma}=\delta_{11'}+I\Gamma_{11'\sigma}, \tag{17}$$

$$\omega G_{R_1R_{1'}\sigma}(\omega)=\delta_{R_1R_{1'}}+I\Gamma_{R_1R_{1'}\sigma}(\omega). \tag{18}$$

In Sec. III B we show that the correct expression for $\Gamma_{R_1R_{1'}\sigma}(\omega)$ including the boundary condition is

$$\Gamma_{R_1R_{1'}\sigma}(\omega)=[\langle n_{1-\sigma}\rangle/(\omega-I+i\epsilon)]\delta_{R_1R_{1'}}. \tag{19}$$

Also, we only consider spatially homogeneous systems so that $\langle n_{1\sigma}\rangle$ is independent of R_1. In the following, we will take $n_\sigma=\langle n_{1\sigma}\rangle$.

Consider $G_{R_1R_{1'}\sigma}(\omega)$ split into two parts:

$$G_{R_1R_{1'}\sigma}(\omega)=\tilde{G}_{R_{1'}R_1\sigma}(\omega)+2\pi i\delta(\omega)g_{R_1R_{1'}\sigma}, \tag{20}$$

where $\tilde{G}_{R_1R_{1'}\sigma}(\omega)$ is that part not proportional to a δ function in frequency. Equation (18) is actually only sufficient to determine $\tilde{G}_{R_1R_{1'}\sigma}(\omega)$ as follows:

$$\omega\tilde{G}_{R_1R_{1'}\sigma}(\omega)=\delta_{R_1R_{1'}}+I\Gamma_{R_1R_{1'}\sigma}(\omega),$$

$$\tilde{G}_{R_1R_{1'}\sigma}(\omega)=\frac{\delta_{R_1R_{1'}}}{\omega+i\epsilon}\left(1+\frac{n_{-\sigma}I}{\omega-I+i\epsilon}\right)$$

$$=\delta_{R_1R_{1'}}\left(\frac{1-n_{-\sigma}}{\omega+i\epsilon}+\frac{n_{-\sigma}}{\omega-I+i\epsilon}\right). \tag{21}$$

In Eq. (21) we have arbitrarily imposed a certain boundary condition on the portion contributing to a zero-frequency pole. The difference between $\tilde{G}_{R_1R_{1'}\sigma}(\omega)$ defined for this boundary condition and a similar function defined for the opposite boundary condition $[1/(\omega-i\epsilon)]$ is proportional to a δ function in frequency. This ambiguity may be absorbed into our definition of $g_{R_1R_{1'}\sigma}$. Using Eqs. (20) and (21), we have for the most general solution to Eq. (17) for less than one electron per site,

$$G_{R_1R_{1'}\sigma}(\omega)=\delta_{R_1R_{1'}}\left(\frac{1-n_{-\sigma}}{\omega+i\epsilon}+\frac{n_{-\sigma}}{\omega-I+i\epsilon}\right)+2\pi i\delta(\omega)g_{R_1R_{1'}\sigma}. \quad (22)$$

Note that the diagonal portion of $g_{R_1R_{1'}\sigma}$ is determined by the number condition

$$\langle n_{1\sigma}\rangle=-i\lim_{\alpha\to0^+}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{i\alpha\omega}G_{R_1R_1\sigma}(\omega)$$
$$=-i\lim_{\alpha\to0^+}\int_c\frac{d\omega}{2\pi}e^{i\alpha\omega}G_{R_1R_1\sigma}(\omega)$$
$$=\lim_{\alpha\to0^+}\int_c\frac{d\omega}{2\pi}e^{i\alpha\omega}2\pi\delta(\omega)g_{R_1R_1\sigma}=g_{R_1R_1\sigma}. \quad (23)$$

Here the contour C is closed in the upper half-plane. The off-diagonal portion $g_{R_1\neq R_{1'}\sigma}$ is unspecified, and, indeed, the arbitrariness in this function corresponds to the arbitrariness in our choice of a degenerate ground state. To choose this function prematurely would be to prejudice the possible manifestations of the degeneracy. Rather, we will leave this function unspecified. This function can only be determined in the $\Delta\to0$ limit.

From Eq. (17) we see that $G_{11'\sigma}$ for $R_1\neq R_{1'}$ is independent of t_1 abd $t_{1'}$. Hence, from Eq. (20),

$$G_{11'\sigma}|_{R_1\neq R_{1'}}=ig_{R_1\neq R_{1'}\sigma}. \quad (24)$$

In particular, for $t_{1'}=t_{1+}$, and for $R_1\neq R_{1'}$, we have

$$G_{11'\sigma}|_{t_{1'}=t_1^+}=i\langle c_{1'\sigma}^+c_{1\sigma}\rangle|_{t_{1'}=t_1}=ig_{R_1R_{1'}\sigma}. \quad (25)$$

From Eqs. (23) and (25), we have

$$g_{R_1R_{1'}\sigma}=\langle c_{1'\sigma}^+c_{1\sigma}\rangle|_{t_{1'}=t_1}. \quad (26)$$

B. Two-Particle Green's Function $\Gamma_{11'\sigma}$

Having obtained the most general form for the one-particle Green's function in the limit of zero hopping, we turn to the two-particle Green's function. The very interesting result is that for paramagnetic ground states, the ambiguity in this latter function may be expressed in terms of the function $g_{R_1R_{1'}\sigma}$. First, we obtain an expression for a particular two-particle Green's function ($\Gamma_{11'\sigma}$), and then we consider the general two-particle Green's function ($G_{121'2'}{}^{\sigma\sigma'}$).

The ground state of the Hubbard Hamiltonian as $\Delta\to0$ is a certain linear combination of the ground states of $H_{\rm at}$. Furthermore, for the number of electrons less than the number of sites, none of the ground states of $H_{\rm at}$ contain any doubly occupied sites. Hence the ground state of H for $\Delta\to0$ does not contain any doubly occupied sites. Denoting this ground state by $|0\rangle$, we then have, for all R_1, t_1,

$$n_{1\sigma}n_{1-\sigma}|0\rangle=0. \quad (27)$$

$\Gamma_{11'\sigma}$ can be written as

$$\Gamma_{11'\sigma}=-i\langle(c_{1\sigma}n_{1\sigma}n_{1-\sigma}c_{1'\sigma}{}^\dagger)_+\rangle. \quad (28)$$

Further, for $\Delta\to0$ the commutation relations of operators referring to different sites at different times are equal to their equal-time commutators. This may be seen from the following sets of equations, where we define $H_{\rm at}{}^i$ as $In_{i\downarrow}n_{i\uparrow}$ (in these equations, we restrict $R_1\neq R_2$, but keep t_1 and t_2 general):

$$\{c_{1\sigma},c_{2\sigma'}{}^\dagger\}=c_{1\sigma}c_{2\sigma'}{}^\dagger+c_{2\sigma'}{}^\dagger c_{1\sigma}, \quad (29)$$

but

$$c_{1\sigma}c_{2\sigma'}{}^\dagger=e^{iH_{\rm at}t_1}c_{R_1\sigma}e^{-iH_{\rm at}t_1}e^{iH_{\rm at}t_2}c_{R_2\sigma'}e^{-iH_{\rm at}t_2},$$
$$=e^{iH_{\rm at}{}^1t_1}c_{R_1\sigma}e^{-iH_{\rm at}{}^1t_1}e^{iH_{\rm at}{}^2t_2}c_{R_2\sigma'}{}^\dagger e^{-iH_{\rm at}{}^2t_2}$$
$$=e^{iH_{\rm at}{}^1t_1}c_{R_1\sigma}e^{iH_{\rm at}{}^2t_2}e^{-iH_{\rm at}{}^1t_1}c_{R_2\sigma'}{}^\dagger e^{-iH_{\rm at}{}^2t_2}$$
$$=e^{i(H_{\rm at}{}^1t_1+H_{\rm at}{}^2t_2)}c_{R_1\sigma}c_{R_2\sigma'}{}^\dagger e^{-i(H_{\rm at}{}^1+H_{\rm at}{}^2t_2)}. \quad (30)$$

These manipulations used the commutation relations

$$[H_{\rm at}{}^1,H_{\rm at}{}^2]=0,\quad [c_{R_1\sigma},H_{\rm at}{}^2]=0. \quad (31)$$

Hence,

$$\{c_{1\sigma},c_{2\sigma'}{}^\dagger\}|_{R_1\neq R_2}=e^{i(H_{\rm at}{}^1t_1+H_{\rm at}{}^2t_2)}\times\{c_{R_1\sigma}c_{R_2\sigma'}{}^\dagger\}|_{R_1\neq R_2}e^{-i(H_{\rm at}{}^1t_1+H_{\rm at}{}^2t_2)}=0. \quad (32)$$

In these last few equations, $c_{R_1\sigma}$ has been used to represent that operator referring to the site at R_1 at some reference time zero. It follows that

$$[n_{1\sigma}n_{1-\sigma},c_{1'\sigma}{}^\dagger]|_{R_1\neq R_{1'}}=0. \quad (33)$$

We see from Eq. (28) that for $\Delta\to0$,

$$\Gamma_{11'\sigma R_1\neq R_{1'}}=0. \quad (34)$$

This information may be used to solve the following equation of motion for $\Gamma_{11'\sigma}$:

$$i(\partial/\partial t_1)\Gamma_{11'\sigma}=\delta_{11'}\langle n_{1-\sigma}\rangle+I\Gamma_{11'\sigma}. \quad (35)$$

(Our ground state is assumed to be translationally invariant, so that $\langle n_{1-\sigma}\rangle$ is independent of R_1.)

Using Eq. (35), we obtain

$$(\omega_1-I)\Gamma_{R_1R_{1'}\sigma}(\omega_1\omega_{1'})=2\pi\delta(\omega_1-\omega_{1'})\delta_{R_1R_{1'}}n_{-\sigma}. \quad (36)$$

In order to solve Eq. (36) with the proper boundary condition, we will need to consider the spectral form for $\Gamma_{11'\sigma}$. One may obtain a spectral form for $\Gamma_{11'\sigma}$ in precisely the same way one obtains a spectral form for $G_{11'\sigma}$. $\Gamma_{R_1R_{1'}\sigma}(\omega)$ may be expressed

$$\Gamma_{R_1R_{1'}\sigma}(\omega)=\int\frac{d\bar\omega}{2\pi}\frac{A_{R_1R_{1'}\sigma}{}^\Gamma(\bar\omega)}{\omega-\bar\omega+i\epsilon\,\mathrm{sgn}(\bar\omega-\mu)}. \quad (37)$$

In opposition to $G_{11'\sigma}$, the function $\Gamma_{11'\sigma}$ has no ambiguity for $R_1 \neq R_{1'}$. From Eq. (34) we see the off-diagonal terms vanish. Hence, Eq. (37) may be rewritten as

$$\Gamma_{R_1R_{1'}\sigma}(\omega)=\delta_{R_1R_{1'}}\int\frac{d\bar{\omega}}{2\pi}\frac{A_{R_1R_{1'}}{}^{\Gamma}(\bar{\omega})}{\omega-\bar{\omega}+i\epsilon\,\mathrm{sgn}(\bar{\omega}-\mu)}. \quad (38)$$

Using Eqs. (36) and (14) we get

$$\begin{aligned}\Gamma_{R_1R_{1'}\sigma}(\omega)&=\delta_{R_1R_{1'}}\int\frac{d\bar{\omega}}{2\pi}\frac{2\pi n_{-\sigma}\delta(\bar{\omega}-I)}{\omega-\bar{\omega}+i\epsilon\,\mathrm{sgn}(\bar{\omega}-\mu)}\\ &=\delta_{R_1R_{1'}}\frac{n_{-\sigma}}{\omega-I+i\epsilon\,\mathrm{sgn}(I-\mu)}\\ &=\delta_{R_1R_{1'}}\frac{n_{-\sigma}}{\omega-I\times i\epsilon}, \quad (39)\end{aligned}$$

since for $n<N$, $\mu\to 0$ as $\Delta\to 0$.

As an aside, note that this restriction $n<N$ (number of electrons less than the number of sites) is not an essential one. For $n>N$, the ground state of H (as $\Delta\to 0$) does not contain any empty sites. We may use this information to make corresponding arguments for this case.

C. General Two-Particle Green's Function

We now seek an expression relating the general two-particle Green's function G_2 to the one-particle Green's function G_1.

For any Δ, and for $G^0{}_{12}{}^{-1}$ defined by

$$G^0{}_{12}{}^{-1}=\delta(t_1-t_2)\delta_{R_1R_2}i(\partial/\partial t_2)\,, \quad (40)$$

we have[4]

$$(G^0{}_{12}{}^{-1}+T_{12})G_{21'\sigma}=\delta_{11'}+I\Gamma_{11'\sigma}. \quad (41)$$

For finite Δ, there is no ambiguity in the one-particle Green's function, and the solution to Eq. (41) has a well-defined inverse which allows us to write

$$G^0{}_{12}{}^{-1}-T_{12}=(\delta_{13}+I\Gamma_{13\sigma})G^{-1}{}_{32\sigma}. \quad (42)$$

We will need the following specially defined higher-order Green's functions[5]:

$$\Gamma_{121'2'}{}^{\sigma\sigma'}=-\langle(n_{1-\sigma}c_{1\sigma}c_{2\sigma'}c_{2'\sigma'}{}^{\dagger}c_{1'\sigma}{}^{\dagger})_+\rangle\,, \quad (43)$$

$$\Gamma^*{}_{121'2'}{}^{\sigma\sigma'}=-\langle(n_{1-\sigma}c_{1\sigma}n_{2-\sigma'}c_{2\sigma'}c_{2'\sigma'}{}^{\dagger}c_{1'\sigma}{}^{\dagger})_+\rangle. \quad (44)$$

The equation of motion for $G_{121'2'}{}^{\sigma\sigma'}$ for any Δ is

$$\begin{aligned}&(G^0{}_{11'}{}^{-1}-T_{11'})G_{121'2'}{}^{\sigma\sigma'}\\ &\qquad=\delta_{11'}G_{22'\sigma'}-\delta_{12'}G_{21'\sigma}\delta_{\sigma\sigma'}+I\Gamma_{121'2'}. \quad (45)\end{aligned}$$

The left-hand side may be rewritten with Eq. (42) as

$$\begin{aligned}&(G^0{}_{11'}{}^{-1}-T_{11'})G_{121'2'}{}^{\sigma\sigma'}\\ &\qquad=(\delta_{13}+I\Gamma_{13\sigma})G_{31'}{}^{-1}G_{321'2'}{}^{\sigma\sigma'}. \quad (46)\end{aligned}$$

Now for any Δ, we have

$$\begin{aligned}(G^0{}_{2\bar{2}\sigma'}{}^{-1}-T_{2\bar{2}})\Gamma_{1\bar{2}1'2'}{}^{\sigma\sigma'}&=\delta_{22'}\Gamma_{11'\sigma}-\delta_{21'}\Gamma_{12'\sigma}\delta_{\sigma\sigma'}\\ &\quad+W_{11'2'}{}^{\sigma}\delta_{12}\delta_{\sigma',-\sigma}+I\Gamma^*{}_{121'2}{}^{\sigma\sigma'}. \quad (47)\end{aligned}$$

Hence,

$$\begin{aligned}&(G^0{}_{1\bar{1}\sigma}{}^{-1}-T_{1\bar{1}})(G^0{}_{2\bar{2}\sigma'}{}^{-1}-T_{2\bar{2}})G_{\bar{1}\bar{2}1'2'}{}^{\sigma\sigma'}\\ &\quad=\delta_{11'}\delta_{22'}+I\delta_{11'}\Gamma_{22'\sigma}-\delta_{12'}\delta_{21'}\delta_{\sigma\sigma'}-I\delta_{12'}\Gamma_{21'\sigma}\delta_{\sigma\sigma'}\\ &\qquad+I\delta_{22'}\Gamma_{11'\sigma}-I\delta_{21'}\Gamma_{12'\sigma}\delta_{\sigma\sigma'}+I\delta_{12}W_{11'2'}{}^{\sigma}\delta_{\sigma',-\sigma}\\ &\qquad+I^2\Gamma^*{}_{121'2'}{}^{\sigma\sigma'}. \quad (48)\end{aligned}$$

Using Eq. (42), inverting the corresponding G_1' terms, and using the symmetry $\sum_2 A_{12}B_{21'}=\sum_2 B_{12}A_{21'}$ for functions only of difference coordinates, we obtain

$$\begin{aligned}&(\delta_{1\bar{1}}+I\Gamma_{11'\sigma})(\delta_{2\bar{2}}+I\Gamma_{2\bar{2}\sigma'})G_{\bar{1}\bar{2}1'2'}{}^{\sigma\sigma'}\\ &\quad=G_{11'\sigma}G_{22'\sigma'}-G_{12'\sigma}G_{21'\sigma}\delta_{\sigma\sigma'}+IG_{11'\sigma}G_{2\bar{2}\sigma'}\Gamma_{\bar{2}2'\sigma}\\ &\qquad-IG_{12'\sigma}G_{2\bar{2}\sigma}\Gamma_{\bar{2}1'\sigma}\delta_{\sigma\sigma'}+IG_{22'\sigma'}G_{1\bar{1}\sigma}\Gamma_{\bar{1}1'\sigma}\\ &\qquad-IG_{21'\sigma}G_{1\bar{1}\sigma}\Gamma_{\bar{1}2'\sigma}\delta_{\sigma\sigma'}+IG_{1\bar{2}\sigma}G_{2\bar{2}-\sigma}W_{\bar{2}1'2'}{}^{\sigma}\delta_{-\sigma,\sigma'}\\ &\qquad+I^2G_{1\bar{1}\sigma}G_{2\bar{2}\sigma'}\Gamma^*{}_{121'2'}{}^{\sigma\sigma'}. \quad (49)\end{aligned}$$

Equation (49) may be rewritten as

$$\begin{aligned}&(\delta_{1\bar{1}}+I\Gamma_{1\bar{1}\sigma})(\delta_{2\bar{2}}+I\Gamma_{2\bar{2}\sigma})\\ &\qquad\times(G_{\bar{1}\bar{2}1'2}{}^{\sigma\sigma'}-G_{\bar{1}1'\sigma}G_{\bar{2}2'\sigma}+G_{\bar{1}2'\sigma}G_{\bar{2}1'\sigma}\delta_{\sigma\sigma'})\\ &\quad=IG_{1\bar{2}\sigma}G_{2\bar{2}-\sigma}W_{\bar{2}1'2'}{}^{\sigma}\delta_{\sigma',-\sigma}+I^2G_{1\bar{1}\sigma}G_{2\bar{2}\sigma'}\Gamma^*{}_{\bar{1}\bar{2}1'2'}{}^{\sigma\sigma'}\\ &\qquad-I^2\Gamma_{1\bar{1}\sigma}\Gamma_{2\bar{2}\sigma'}[G_{\bar{1}1'0}G_{\bar{2}2'\sigma'}-G_{\bar{1}2'\sigma}G_{\bar{1}2'\sigma}G_{\bar{2}1'\sigma}\delta_{\sigma\sigma'}]. \quad (50)\end{aligned}$$

This becomes

$$\begin{aligned}&G_{121'2'}{}^{\sigma\sigma'}-G_{11'\sigma}G_{22'\sigma'}+G_{12'\sigma}G_{21'\sigma}\delta_{\sigma\sigma'}\\ &\quad=(\delta_{1\bar{1}}+I\Gamma_{1\bar{1}\sigma})^{-1}(\delta_{2\bar{2}}+I\Gamma_{2\bar{2}\sigma'})^{-1}\\ &\qquad\times IG_{\bar{3}\sigma}G_{\bar{2}3-\sigma}W_{\bar{3}1'2'}{}^{\sigma}\delta_{\sigma',-\sigma}\\ &\qquad+I^2G_{13\sigma}G_{24\sigma'}(\delta_{3\bar{1}}+I\Gamma_{3\bar{1}\sigma})^{-1}\\ &\qquad\times(\delta_{4\bar{2}}+I\Gamma_{4\bar{2}\sigma'})^{-1}\Gamma^*{}_{\bar{1}\bar{2}1'2'}{}^{\sigma\sigma'}\\ &\qquad-I^2[(\delta_{1\bar{1}}+I\Gamma_{1\bar{1}\sigma})^{-1}\Gamma_{\bar{1}3\sigma}][(\delta_{2\bar{2}}+I\Gamma_{2\bar{2}\sigma'})^{-1}\\ &\qquad\times\Gamma_{\bar{2}4\sigma'}](G_{31'\sigma}G_{42'\sigma'}-G_{32'\sigma}G_{41'\sigma}\delta_{\sigma\sigma'}). \quad (51)\end{aligned}$$

This equation expresses the two-particle Green's function in terms of the one-particle function, the function Γ, which is unambiguous and known, and the functions W and Γ^*. The $\Delta\to 0$ limit for W and Γ^* must now be analyzed.

D. Analysis of Γ^*

For $\Delta\to 0$, we have

$$\begin{aligned}&[i(\partial/\partial t_1)-I]\Gamma^*{}_{121'2}{}^{\sigma\sigma}\\ &\qquad=\delta_{11'}(-i)\langle(n_{1-\sigma}n_{2-\sigma}c_{2\sigma}c_{2'\sigma}{}^{\dagger})_+\rangle\\ &\qquad\quad-\delta_{12'}(-i)\langle(n_{1-\sigma}n_{2-\sigma}c_{2\sigma}c_{1'\sigma}{}^{\dagger})_+\rangle, \quad (52)\end{aligned}$$

$$\begin{aligned}&[i(\partial/\partial t_1)-I][i(\partial/\partial t_2)-I]\Gamma^*{}_{121'2}{}^{\sigma\sigma}\\ &\qquad=(\delta_{11'}\delta_{22'}-\delta_{12'}\delta_{21})\langle n_{1-\sigma}n_{2-\sigma}\rangle, \quad (53)\end{aligned}$$

$$\begin{aligned}&[i(\partial/\partial t_1)-I]\Gamma^*{}_{121'2'}{}^{\sigma,-\sigma}\\ &\qquad=\delta_{11'}(-i)\langle(n_{1-\sigma}n_{2\sigma}c_{2-\sigma}c_{2'-\sigma}{}^{\dagger})_+\rangle\\ &\qquad\quad-\delta_{12'}(-i)\langle(c_{1\sigma}c_{1-\sigma}{}^{\dagger}n_{2\sigma}c_{2-\sigma}c_{1'\sigma}{}^{\dagger})_+\rangle, \quad (54)\end{aligned}$$

[4] We implicitly sum and/or integrate over repeated indices so that, for example, in Eq. (47) we sum over sites R_2 and integrate over time t_2.

[5] The Fourier transforms of these functions are defined in the same way as for the functions defined in Eqs. (8)–(12).

$$[i(\partial/\partial t_1)-I][i(\partial/\partial t_2)-I]\Gamma^*{}_{121'2'}{}^{\sigma,-\sigma}$$
$$=\delta_{11'}\delta_{22'}\langle n_{1-\sigma}n_{2-\sigma}\rangle$$
$$+i\delta_{12}(\delta_{11'}\Gamma_{12'-\sigma}+\delta_{12'}\Gamma_{21'\sigma})$$
$$-\delta_{12'}\delta_{21'}\langle(c_{1\sigma}c_{1-\sigma}{}^{\dagger}v_{2-\sigma}c_{2\sigma}{}^{\dagger})_+\rangle. \quad (55)$$

These equations allow us to relate the function Γ^* to the functions D and S defined in Eqs. (11) and (12).

E. Analysis of W

It was necessary to invoke the spectral form of $\Gamma_{11'\sigma}$ in order to obtain its correct boundary condition (see Sec. III B). Now $W_{11'2'}{}^{\sigma}$ has no simple spectral form, since it is a function of two time differences. However, it will be possible to use the previously determined boundary condition on $\Gamma_{11'\sigma}$ to fix the boundary condition for $W_{11'2'}{}^{\sigma}$.

Consider $W_{11'2}{}^{\sigma}$ for $\Delta\to 0$. Equation (10) may be rewritten as

$$W_{11'2'}{}^{\sigma}=-i\langle(c_{1\sigma}c_{1-\sigma}n_{1\sigma}n_{1-\sigma}c_{2'-\sigma}{}^{\dagger}c_{1'\sigma}{}^{\dagger})_+\rangle. \quad (56)$$

For $n<N$, the function $W_{11'2'}{}^{\sigma}$ vanishes unless $R_1=R_{1'}$ and/or $R_{2'}$. This information will be used to solve the following equation of motion for $\Delta\to 0$ in a fashion similar to that employed for $\Gamma_{11'\sigma}$:

$$[i(\partial/\partial t_1)-I]W_{11'2'}{}^{\sigma}=i\delta_{11'}G_{12-\sigma}+i\delta_{12'}G_{11'\sigma}, \quad (57)$$

and, therefore,

$$(\omega_1-I)W_{R_1R_{1'}R_{2'}}{}^{\sigma}(\omega_1\omega_{1'}\omega_{2'})$$
$$=i\delta_{R_1R_{1'}}G_{R_2R_{2'}-\sigma}(\omega_1-\omega_{1'},\,\omega_{2'})$$
$$+i\delta_{R_1R_{2'}}G_{R_1R_{1'}\sigma}(\omega_1-\omega_{2'},\,\omega_{1'}). \quad (58)$$

This gives

$$W_{R_1R_{1'}R_{2'}}{}^{\sigma}(\omega_1\omega_{1'}\omega_{2'})=\frac{2\pi i\delta(\omega_1-\omega_{1'}-\omega_{2'})}{\omega_{1'}+\omega_{2'}-I+i\epsilon x(\omega_{1'}\omega_{2'})}$$
$$\times[\delta_{R_1R_{1'}}G_{R_1R_{2'}-\sigma}(\omega_{2'})+\delta_{R_1R_{2'}}G_{R_1R_{1'}\sigma}(\omega_{1'})]. \quad (59)$$

Here x $(=\pm 1)$ can at *most* depend on the frequencies. This follows since $W_{11'2'}{}^{\sigma}$ vanishes unless $R_1=R_{1'}$ and/or $R_{2'}$. Hence, there is no spatial ambiguity left in Eq. (58) as opposed to the ambiguity in Eq. (18).

We define

$$x(\omega_{1'}\omega_{2'})\,|_{\,\omega_{1'}+\omega_{2'}=I}=y(\omega_{1'}) \quad (60)$$

and

$$W_{R_1R_{1'}R_{2'}}{}^{\sigma}(\omega_1\omega_{1'}\omega_{2'})$$
$$=2\pi\delta(\omega_1-\omega_{1'},\,\omega_{2'})\tilde{W}_{R_1R_{1'}R_{2'}}{}^{\sigma}(\omega_{1'}\omega_{2'}). \quad (61)$$

The boundary condition in Eq. (59) is only essential when $\omega_{1'}+\omega_{2'}=I$, hence x may be replaced by y. Having reduced the arbitrariness in the boundary condition to (at most) a dependence on $\omega_{1'}$, we may relate $W_{11'2'}{}^{\sigma}$ to $\Gamma_{11'\sigma}$ to fix this condition:

$$\Gamma_{11'\sigma}=-W_{11'2'}{}^{\sigma}\big|_{\substack{R_1=R_{2'}\\ t_{2'}=t_1{}^+}}=-\lim_{\alpha\to 0^+}\int\frac{d\omega_1}{2\pi}\int\frac{d\omega_{1'}}{2\pi}\int\frac{d\omega_{2'}}{2\pi}$$
$$\times e^{-i(\omega_1t_1-\omega_{1'}t_{1'}-\omega_{2'}t_{2'})}e^{i\omega_{2'}\alpha}W_{R_1R_2R_{2'}}{}^{\sigma}(\omega_1\omega_{1'}\omega_{2'})$$
$$=-\lim_{\alpha\to 0^+}\int\frac{d\omega_{1'}}{2\pi}\int\frac{d\omega_{2'}}{2\pi}e^{-i\omega_{1'}(t_1-t_{1'})}$$
$$\times e^{i\omega_{2'}\alpha}\tilde{W}_{R_1R_{1'}R_{2'}}{}^{\sigma}(\omega_{1'}\omega_{2'}). \quad (62)$$

Fourier transforming, we get

$$\frac{n_{-\sigma}\delta_{R_1R_{1'}}}{\omega_{1'}-I+i\epsilon}=-i\lim_{\alpha\to 0^+}\int\frac{d\omega_{2'}}{2\pi}\frac{e^{i\omega_{2'}\alpha}}{\omega_{1'}+\omega_{2'}-I+i\epsilon y(\omega_{1'})}$$
$$\times[\delta_{R_1R_{1'}}G_{R_1R_1-\sigma}(\omega_{2'})+G_{R_1R_{1'}\sigma}(\omega_{1'})]. \quad (63)$$

This is an identity for all $\omega_{1'}$.

Further, we recall that

$$n_{-\sigma}=-i\lim_{\alpha\to 0^+}\int\frac{d\omega_{2'}}{2\pi}e^{i\omega_{2'}\alpha}G_{R_1R_1-\sigma}(\omega_{2'}). \quad (64)$$

This then fixes $y(\omega_{1'})$ as independent of $\omega_{1'}$ and equal to $+1$.

All ambiguity in the pole positions is thus resolved and we have

$$W_{R_1R_{1'}R_{2'}}{}^{\sigma}(\omega_1\omega_{1'}\omega_{2'})=\frac{2\pi i\delta(\omega_1-\omega_{1'}-\omega_{2'})}{\omega_1-I+i\epsilon}$$
$$\times[\delta_{R_1R_{1'}}G_{R_1R_{2'}-\sigma}(\omega_{2'})+\delta_{R_1R_{2'}}G_{R_1R_{1'}\sigma}(\omega_{1'})]. \quad (65)$$

F. Compilation of G_2

Sections III A–III E must be compiled to give the general two-particle Green's functions. Using Eqs. (53) and (55) for the Γ^* functions, now expressed in terms of the functions D and S of Eqs. (11) and (12), and the fact that the Fourier transform of $(\delta_{11'}+I\Gamma_{11'\sigma})^{-1}$ is given by

$$\delta_{R_1R_{1'}}\times 2\pi\delta(\omega_1-\omega_{1'})\frac{\omega_1-I}{\omega_1-I(1-n_{-\sigma})}, \quad (66)$$

we get the following expression for the Fourier transform of the general G_2 in Eq. (51):

$$G_{R_1R_2R_{1'}R_{2'}}{}^{\sigma\sigma'}(\omega_1\omega_2\omega_{1'}\omega_{2'})-G_{R_1R_{1'}\sigma}(\omega_1\omega_{1'})G_{R_2R_{2'}\sigma}(\omega_2\omega_{2'})+G_{R_1R_{2'}\sigma}(\omega_1\omega_{2'})G_{R_2R_{1'}\sigma}(\omega_2\omega_{1'})\delta_{\sigma\sigma'}$$
$$=\frac{I(\omega_1-I)(\omega_2-I)}{[\omega-I(1-n_{-\sigma})][\omega_2-I(1-n_{-\sigma'})]}G_{R_1R_{\bar{2}}\sigma}(\omega_1)G_{R_2R_{\bar{2}}\sigma'}(\omega_2)W_{R_{\bar{2}}R_{1'}R_{2'}}{}^{\sigma}(\omega_1+\omega_2,\,\omega_{1'},\,\omega_{2'})\delta_{-\sigma,\sigma'}$$
$$+\frac{I^2G_{R_1R_{\bar{1}}\sigma}(\omega)G_{R_2R_{\bar{2}}\sigma'}(\omega_2)}{[\omega_1-I(1-n_{-\sigma})][\omega_2-I(1-n_{-\sigma'})]}\{D_{R_{\bar{1}}R_{\bar{2}}}{}^{-\sigma,-\sigma'}(\omega_1-\omega_{1'},\,\omega_2-\omega_{2'})\delta_{R_1R_{1'}}\delta_{R_{\bar{2}}R_{2'}}$$
$$-D_{R_{\bar{1}}R_{\bar{2}}}{}^{-\sigma,-\sigma'}(\omega_1-\omega_{2'},\,\omega_2-\omega_{1'})\delta_{R_{\bar{1}}R_{2'}}\delta_{R_{\bar{2}}R_{1'}}\delta_{\sigma,\sigma'}-S_{R_{\bar{1}}R_{\bar{2}}}(\omega_1-\omega_2,\,\omega_2-\omega_{1'})\delta_{R_{\bar{1}}R_{2'}}\delta_{R_{\bar{2}}R_{1'}}\delta_{\sigma,-\sigma'}$$
$$+2\pi i\delta(\omega_1+\omega_2-\omega_{1'}-\omega_{2'})\delta_{R_{\bar{1}}R_{\bar{2}}}[\delta_{R_{\bar{1}}R_{1'}}\Gamma_{R_{\bar{1}}R_{2'}-\sigma}(\omega_{2'})+\delta_{R_{\bar{1}}R_{2'}}\Gamma_{R_{\bar{2}}R_{1'}\sigma}(\omega_{1'})]\delta_{\sigma,-\sigma'}\}. \quad (67)$$

Equation (67) relates the two-particle Green's function to the one-particle Green's function. It is still an implicit relationship since on the right-hand side we have certain density and spin correlation functions which are unknown. However, this equation may be used to generate a series of coupled equations relating these spin correlation functions to themselves and to G_1, and this is done in Sec. III G. They are then solved giving explicit expressions for all two-particle functions in terms of G_1 alone. These expressions are then analyzed. Using these results one may obtain the general G_2 in terms of G_1.

Before proceeding with this program, it will be convenient to return once more to time coordinates. We define

$$F_{11'\sigma}=\int\frac{d\omega_1}{2\pi}e^{-i\omega_1(t_1-t_{1'})}\frac{G_{R_1R_{1'}\sigma}(\omega)}{\omega_1-I(1-n_{-\sigma})},\qquad(68)$$

$$\bar{F}_{11'\sigma}=\int\frac{d\omega_1}{2\pi}e^{-i\omega_1(t_1-t_{1'})}\frac{(\omega_1-I)G_{R_1R_{1'}\sigma}(\omega_1)}{\omega_1-I(1-n_{-\sigma})}.\qquad(69)$$

It follows from the form of G_1 that these integrals are well defined, regardless of how one goes around the point $\omega_1=I(1-n_{-\sigma})$ in the integration. In terms of F and $\bar{F}$, we have

$$\begin{aligned}G_{121'2}{}^{\sigma\sigma'}&-G_{11'\sigma}G_{22'\sigma}+G_{12'\sigma}G_{21'\sigma}\delta_{\sigma\sigma'}\\&=I\bar{F}_{1\bar{2}}\bar{F}_{2\bar{2}-\sigma}W_{\bar{2}1'2'}{}^{\sigma}\delta_{-\sigma,\sigma'}\\&\quad+I^2F_{11'\sigma}F_{22'\sigma}D_{1'2'}{}^{-\sigma,-\sigma'}\\&\quad-I^2F_{12'\sigma}F_{21'\sigma}D_{2'1'}{}^{-\sigma,-\sigma'}\delta_{\sigma'\sigma}\\&\quad-I^2F_{12'\sigma}F_{21'-\sigma}S_{2'1'\sigma}\delta_{-\sigma,\sigma'}\\&\quad+i\Gamma^2(F_{11'\sigma}F_{21'-\sigma}\Gamma_{1'2'-\sigma}\\&\qquad+F_{12'\sigma}F_{22'-\sigma}\Gamma_{2'1'\sigma})\delta_{-\sigma,\sigma'}.\end{aligned}\qquad(70)$$

G. Correlation Functions D and S

In Eq. (70), G_2 is expressed in terms of the functions D and S. These functions, however, are themselves particular projections of the general two-particle Green's function. In this section we find and solve the equations for D and S which are implicit in Eq. (70).

We define n_σ^+ and n_0^- by

$$n_\sigma^+=F_{11^+\sigma},\quad n_\sigma^-=F_{11^-\sigma}.\qquad(71)$$

Using Eq. (70) and the definition of D, we get

$$\begin{aligned}D_{12}{}^{\sigma\sigma}&=-G_{121^+2^+}{}^{\sigma\sigma}+G_{11'\sigma}G_{22^+\sigma}\\&=G_{12\sigma}G_{21\sigma}-I^2(n_\sigma^+)^2D_{12}{}^{-\sigma,-\sigma}\\&\qquad+I^2F_{12\sigma}F_{21\sigma}D_{21}{}^{-\sigma,-\sigma}.\end{aligned}\qquad(72)$$

We will only consider a nonmagnetic ground state and, in this special case,

$$D_{12}{}^{\sigma\sigma}=D_{12}{}^{-\sigma,-\sigma}=D_{21}{}^{\sigma\sigma}\qquad(73)$$

and

$$D_{12}{}^{\sigma\sigma}=\frac{G_{12\sigma}G_{21\sigma}}{1+(n_\sigma^+I)^2-I^2F_{12\sigma}F_{21\sigma}}.\qquad(74)$$

Again using Eq. (70), we get

$$\begin{aligned}D_{12}{}^{\sigma,-\sigma}&=-G_{121^+2^+}{}^{\sigma,-\sigma}+G_{11^+\sigma}G_{22^+-\sigma}\\&=-I\bar{F}_{1\bar{2}\sigma}F_{2\bar{2}-\sigma}W_{\bar{2}12}{}^{\sigma}\\&\quad-iI^2(n_\sigma^+F_{21-\sigma}\Gamma_{12-\sigma}-n_{-\sigma}^+F_{12\sigma}\Gamma_{21\sigma})\\&\qquad-I^2n_\sigma^+n_{-\sigma}^+D_{12}{}^{-\sigma,\sigma}+I^2F_{12\sigma}F_{21-\sigma}S_{21\sigma}\end{aligned}\qquad(75)$$

and

$$\begin{aligned}S_{12,\sigma}&=G_{122^-1}{}^{-\sigma,-\sigma}\\&=G_{12\sigma}G_{21-\sigma}+I\bar{F}_{1\bar{2}\sigma}\bar{F}_{2\bar{2}-\sigma}W_{\bar{2}21}{}^{\sigma}\\&\quad+iI^2(n_{-\sigma}^-F_{12\sigma}\Gamma_{21-\sigma}-n_\sigma^-F_{21-\sigma}\Gamma_{12\sigma})\\&\qquad+I^2F_{12\sigma}F_{21-\sigma}D_{21}{}^{-\sigma,\sigma}-I^2n_\sigma^-n_{-\sigma}^-S_{12\sigma}.\end{aligned}\qquad(76)$$

Further symmetry following from our restriction to the nonmagnetic case is contained in the equations

$$D_{12}{}^{\sigma,-\sigma}=D_{12}{}^{-\sigma,\sigma}=D_{21}{}^{\sigma,-\sigma}=D_{21}{}^{-\sigma,\sigma},\qquad(77)$$

$$S_{12\sigma}=S_{12-\sigma}=S_{21\sigma},\qquad(78)$$

and

$$W_{\bar{2}12}{}^{\sigma}=W_{\bar{2}21}{}^{\sigma}=W_{\bar{2}12}{}^{-\sigma}.\qquad(79)$$

From Eqs. (71), (68), and (69), we can calculate the following relationships:

$$\begin{aligned}n_\sigma^+=F_{11^+\sigma}&=\lim_{\alpha\to0^+}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{i\alpha\omega}}{\omega-I(1-n_{-\sigma})}\\&\quad\times\left(\frac{1-n_{-\sigma}}{\omega+i\epsilon}+\frac{n_{-\sigma}}{\omega-I+i\epsilon}+2\pi i\delta(\omega)g_{11\sigma}\right)\\&=\frac{ig_{11\sigma}}{-I(1-n_{-\sigma})}=\frac{-in_{-\sigma}}{I(1-n_{-\sigma})},\end{aligned}\qquad(80)$$

$$\begin{aligned}n_\sigma^-=F_{11-\sigma}&=\lim_{\alpha\to0^+}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\alpha\omega}}{\omega-I(1-n_{-\sigma})}\\&\quad\times\left(\frac{1-n_{-\sigma}}{\omega+i\epsilon}+\frac{n_{-\sigma}}{\omega-I+i\epsilon}+2\pi i\delta(\omega)g_{11\sigma}\right)\\&=-i\left(\frac{1-n_{-\sigma}}{-I(1-n_{-\sigma})}+\frac{n_{-\sigma}}{In_{-\sigma}}\right)\\&\qquad+\frac{ig_{11\sigma}}{-I(1-n_{-\sigma})}=n_\sigma^+.\end{aligned}\qquad(81)$$

Incorporation of the symmetries, and simplifications of Eqs. (77)–(81) into Eqs. (75) and (76), leads to

$$\begin{aligned}D_{12}{}^{\sigma,-\sigma}&=-I\bar{F}_{1\bar{2}}\bar{F}_{2\bar{2}-\sigma}W_{\bar{2}12}{}^{\sigma}\\&\quad-iI^2(n_\sigma^+F_{21-\sigma}\Gamma_{12-\sigma}+n_\sigma^+F_{12\sigma}\Gamma_{21\sigma})\\&\qquad-I^2n_\sigma^+n_{-\sigma}^+D_{12}{}^{\sigma,-\sigma}+I^2F_{12\sigma}F_{21-\sigma}S_{12\sigma}\end{aligned}\qquad(82)$$

and

$$\begin{aligned}S_{12,\sigma}&=G_{12\sigma}G_{21-\sigma}+I\bar{F}_{1\bar{2}\sigma}\bar{F}_{2\bar{2}-\sigma}W_{\bar{2}21}{}^{\sigma}\\&\quad+iI^2(n_{-\sigma}^+F_{12\sigma}\Gamma_{21-\sigma}+n_\sigma^+F_{21-\sigma}\Gamma_{12\sigma})\\&\qquad+I^2F_{12\sigma}F_{21-\sigma}D_{12}{}^{\sigma,-\sigma}-I^2n_\sigma^+n_{-\sigma}^+S_{12\sigma}.\end{aligned}\qquad(83)$$

These are simply algebraic equations and their solution gives (for the nonmagnetic case)

$$D_{12}{}^{\sigma,-\sigma}=\frac{G_{12\sigma}G_{21-\sigma}I^2F_{12\sigma}F_{21-\sigma}-X_{12\sigma}[1+(n_\sigma{}^+I)^2-I^2F_{12\sigma}F_{21-\sigma}]}{[1+(n_\sigma{}^+I)^2]^2-[I^2F_{12\sigma}F_{21-\sigma}]^2} \tag{84}$$

and

$$S_{12,\sigma}=\frac{G_{12\sigma}G_{21-\sigma}[1-(n_\sigma{}^+I)^2]+X_{12\sigma}[1-(n_\sigma{}^+I)^2+I^2F_{12\sigma}F_{21-\sigma}]}{[1+(n_\sigma{}^+I)^2]^2-[I^2F_{12\sigma}F_{21-\sigma}]^2}, \tag{85}$$

where

$$X_{12\sigma}=I\bar{F}_{12\sigma}\bar{F}_{2\bar{2}-\sigma}W_{\bar{2}12}{}^\sigma+iI^2(n_\sigma{}^+F_{21-\sigma}\Gamma_{12-\sigma}+n_{-\sigma}{}^+F_{12\sigma}\Gamma_{21-\sigma})\,. \tag{86}$$

IV. CONCLUSION

We should note carefully what has been achieved in deriving the above expressions. All quantities appearing in the Eqs. (84) and (85) are known once one knows the one-particle Green's function. To the same extent, all quantities appearing in Eqs. (70) or (67) for the general two-particle function are known. The path we have taken in evaluating G_2 and G_1 for the Hamiltonian H_{at} is complicated, but guarantees that the time-independent parts of these functions which manifest the ground-state degeneracy have not been lost or prejudiced. Seemingly simpler or more straightforward solutions of the hiearchy of Green's function equations obscure the important spatial dependence we have shown to exist. The ambiguity in G_1, expressed through the function $g_{11'\sigma}$, appears in the general two-particle Green's function and in the density and spin correlation functions in a complicated way and will play an essential role in determining properties of the model in the narrow-band, or $\Delta/I\ll 1$, regime.

An inspection of Eqs. (84) and (85) shows that, just as for $i\neq j$,

$$\lim_{\Delta\to 0}\langle c_{i\sigma}{}^\dagger c_{j\sigma}\rangle\neq 0\,, \tag{87}$$

because of the degeneracy

$$\lim_{\Delta\to 0}(\langle n_{i\sigma}n_{j\sigma}\rangle-\langle n_{i\sigma}\rangle\langle n_{j\sigma}\rangle)\neq 0 \tag{88}$$

and

$$\lim_{\Delta\to 0}\langle c_{i\sigma}{}^\dagger c_{i-\sigma}c_{j-\sigma}{}^\dagger c_{j\sigma}\rangle\neq 0\,. \tag{89}$$

Thus the degeneracy leads to nonlocal spatial coherence in the density and spin correlations in the zero-hopping limit.

The function embodying the ambiguity, $g_{ij\sigma}$, cannot be determined without going to the finite Δ problem. In fact, $g_{ij\sigma}$ depends on the details of the hopping that is turned off as $\Delta\to 0$.

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