New self-consistent many-body perturbation theory: Application to the Hubbard model*

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A new many-body theory perturbationally consistent to all orders of the perturbation is presented and applied to the Hubbard problem as an example. Use is made of the recent Kim and Wilson commutator projection operator to derive the Dyson equation for the one-particle Green's function and an exact set of coupled differential equations for the damping or self-energy term which are solved self-consistently. The Hubbard I result follows in our first approximation and the Esterling-Lange (EL) -type result in the second. Since we keep the hopping finite throughout the calculation, no degeneracy problem is encountered as in EL.

I. INTRODUCTION

The purpose of this paper is to present a self-consistent many-body perturbation theory of the single-particle Green's function. The idea is to derive the Dyson equation in an easy and straightforward fashion by means of the Zwanzig-Mori[1] projection-operator method. This is accomplished through the useful commutation projection operator recently introduced by Kim and Wilson.[2] The present approach deviates from usual perturbation calculations by ensuring a self-consistent result in every order of perturbation. Basically this is achieved by developing, through the projection-operator approach, a chain of equations for the self-energy or damping term and its time derivatives in Zubarev fashion. The chain breaking in our approach lies in the neglect of commutators with appropriate parts of the Hamiltonian which are *internal* to the particular averages involved, but only *after* explicitly ensuring a perturbationally correct result. In order to demonstrate the usefulness and ease of such an approach we apply the method to the Hubbard model, which has recently received much attention in the solid-state community because of its great importance to many current phase-transition problems. The well-known Esterling–Lange-type result is reproduced, including terms of the two-site and three-site variety which they neglected. However, we might point out that the present method has not surmounted the well-known difficulties inherent to the Hubbard problem when treated in perturbation about the atomic limit.[3,4] For the exact nature of this limitation for the Hubbard problem and a more complete discussion of the types of system which are not bothered by such a restriction, the reader may directly consult the material following Eq. (3.39). A brief outline of the paper follows.

In Sec. II, after introduction of the Hubbard Hamiltonian, we use the Zwanzig-Mori projection-operator method in the format of Kim and Wilson to derive the Dyson equation for the Laplace-transformed single-particle Green's function. This is accomplished through the use of a linear combination of commutator projection operators of the Kim and Wilson variety. Section III contains basically three different exemplary orders of perturbation for the so-called damping term. The first of these is to use the unperturbed Liouville operator in the projection-operator-modified time propagator appearing in the damping term, keeping the full ensemble average for the remainder of the calculation. This leads trivially to the Hubbard first result. The next order of approximation is obtained by deriving an exact equation of motion for the damping term and again uses the unperturbed Liouville operator in the projection-operator-modified time propagator appearing in the inhomogeneous term of this equation. The third order of approximation consists of deriving an exact equation of motion for the mentioned inhomogeneous term. We obtain then a new inhomogeneous term which we treat perturbationally as before, and the continuance of this procedure directly generates any arbitrary order. Special mention is given to the inherent difficulties of our expansion in the hopping matrix elements t_{ij}. There exists two important neighborhoods in frequency space, $\overline{\omega}', \overline{\omega}' - I \sim O(t_{ij})$, where not all terms of order t_{ij} have been collected. Bari,[3] and later Esterling,[4] were the first to pinpoint this special difficulty with the Hubbard model. However, in problems where expansion about the Hartree-Fock result is valid, such difficulties do not arise.

II. BASIC THEORY

Consider the Hubbard Hamiltonian

$$H = H_I + H_u + H_t \quad , \tag{2.1}$$

where

$$H_I \equiv \frac{I}{2} \sum_{j,\sigma} n_{j-\sigma} n_{j\sigma} \quad , \tag{2.2}$$

$$H_\mu \equiv -\mu \sum_{j,\sigma} n_{j\sigma} \quad , \tag{2.3}$$

and

$$H_t \equiv \sum_{i,j,\sigma} t_{ij} C^\dagger_{i\sigma} C_{j\sigma}; \quad t_{jj} \equiv 0 \quad . \tag{2.4}$$

Here $C^\dagger_{j\sigma}$ ($C_{j\sigma}$) is the Fermion creation (destruction) operator for the Wannier state at lattice site $\vec{R}_j$; $n_{j\sigma} \equiv C^\dagger_{j\sigma} C_{j\sigma}$; I is the intra-atomic Coulomb repulsion, μ the chemical potential, and t_{ij} the hopping matrix element from site i to site j. It is also convenient to define the Liouville operators L_ρ in the following manner:

$$L_\rho \chi \equiv [H_\rho , \chi]_- \quad , \tag{2.5}$$

for $\rho = I$, μ, or t and χ any arbitrary operator. Here $[\ ,\ ]_-$ is the ordinary commutator, and we further define

$$L \equiv L_I + L_\mu + L_t \quad . \tag{2.6}$$

We shall now derive by the Zwanzig-Mori projection-operator method an exact equation of motion for the single-particle Green's function G defined by

$$G_{ij\sigma}(t) \equiv i \langle [C_{i\sigma} , C^\dagger_{j\sigma}(t)]_+ \rangle \quad , \tag{2.7}$$

with $C^\dagger_{j\sigma}(t)$ the usual Heisenberg operator

$$C^\dagger_{j\sigma}(t) \equiv e^{iHt} C^\dagger_{j\sigma} e^{-iHt} = e^{iLt} C^\dagger_{j\sigma}; \quad C^\dagger_{j\sigma}(t=0) \equiv C^\dagger_{j\sigma} . \tag{2.8}$$

Here $[\ ,\ ]_+$ is the anticommutator and the bracket $\langle \ldots \rangle$ signifies the grand canonical average is to be taken over the full H of Eq. (2.1). Use of Eq. (2.8) in Eq. (2.7) gives for our equation of motion

$$\frac{\partial}{\partial t} G_{ij\sigma}(t) = -\langle [C_{i\sigma} , L C^\dagger_{j\sigma}(t)]_+ \rangle \quad . \tag{2.9}$$

The essence of the projection-operator formalism of Zwanzig and Mori is to break up $C^\dagger_{j\sigma}(t)$ in the following way:

$$C^\dagger_{j\sigma}(t) = P C^\dagger_{j\sigma}(t) + (1-P) C^\dagger_{j\sigma}(t) \quad , \tag{2.10}$$

with P an appropriate projection operator. The time derivative of Eq. (2.9) is thus broken into two parts:

$$\frac{\partial}{\partial t} G_{ij\sigma}(t) = -\langle [C_{i\sigma} , L P C^\dagger_{j\sigma}(t)]_+ \rangle - \langle [C_{i\sigma} , L(1-P) C^\dagger_{j\sigma}(t)]_+ \rangle \quad . \tag{2.11}$$

We now choose a projection operator which projects out of the complete motion of $C^\dagger_{j\sigma}(t)$ the needed Green's function G and then relates in an exact fashion the complementary part $(1-P) C^\dagger_{j\sigma}(t)$ to G at another time τ. One gets in this simple manner, with a judiciously chosen P, the Dyson equation, as shown originally by Kim and Wilson.[2] To see how this is accomplished, let us define the anticommutator projection operator similar to that used by Kim and Wilson

$$P_{j\sigma} \chi = C^\dagger_{j\sigma} \langle [C_{j\sigma} , \chi]_+ \rangle \tag{2.12}$$

for arbitrary χ. We see immediately that we have a set of orthogonal projection operators, i.e., $P^2_{i\sigma} = P_{i\sigma}$, and

$$P_{i\sigma} P_{j\sigma} \chi = \delta_{ij} P_{j\sigma} \chi \quad . \tag{2.13}$$

We now choose P of Eq. (2.10) to be

$$P \equiv \sum_j P_{j\sigma} \quad , \tag{2.14}$$

which obviously satisfies the basic projection operator condition $P^2 = P$. From Eq. (2.8) we have

$$\frac{\partial}{\partial t} C^\dagger_{j\sigma}(t) = i L C^\dagger_{j\sigma}(t) \quad , \tag{2.15}$$

and therefore we can write

$$\begin{aligned} \frac{\partial}{\partial t}\left[\left(1 - \sum_l P_{l\sigma}\right) C^\dagger_{j\sigma}(t)\right] &= \left(1 - \sum_l P_{l\sigma}\right) \frac{\partial}{\partial t} C^\dagger_{j\sigma}(t) \\ &= i\left(1 - \sum_l P_{l\sigma}\right) L C^\dagger_{j\sigma}(t) \\ &= i\left(1 - \sum_l P_{l\sigma}\right) L \left(\sum_{l'} P_{l\sigma'}\right) C^\dagger_{j\sigma}(t) \\ &\quad + i\left(1 - \sum_l P_{l\sigma}\right) L \left(1 - \sum_{l'} P_{l'\sigma}\right) C^\dagger_{j\sigma}(t) \quad . \end{aligned} \tag{2.16}$$

Note that we have used the easily verified fact that the $P_{l\sigma}$ commute with the time differential operator, $\partial/\partial t$. The formal solution of Eq. (2.16) can be seen to be

$$\begin{aligned} \left(1 - \sum_l P_{l\sigma}\right) C^\dagger_{j\sigma}(t) &= e^{it(1-\Sigma_l P_{l\sigma})L} \left(1 - \sum_l P_{l\sigma}\right) C^\dagger_{j\sigma}(0) \\ &\quad + i \int_0^t d\tau\, e^{i\tau} \left(1 - \sum P_{l\sigma}\right) L \\ &\quad \times \left(1 - \sum_{l'} P_{l'\sigma}\right) L \left(\sum_l P_{l\sigma}\right) C^\dagger_{j\sigma}(t-\tau) \quad . \end{aligned} \tag{2.17}$$

Advantageously, with our particular choice of $P_{l\sigma}$ [see Eq. (2.12)] the initial term on the right-hand side of Eq. (2.17) is identically zero. Use of Eqs. (2.14) and (2.17) in Eq. (2.9) gives

$$\frac{\partial}{\partial t} G_{ij\sigma}(t) = i \sum_l \Omega_{il\sigma} G_{lj\sigma}(t) - \sum_l \int_0^t d\tau\, \gamma_{il\sigma}(\tau) G_{lj\sigma}(t-\tau) \ , \tag{2.18}$$

where the so-called frequency Ω and damping γ terms are given by

$$\Omega_{ij\sigma} \equiv \langle [C_{i\sigma}, LC^\dagger_{j\sigma}]_+\rangle \quad , \tag{2.19}$$

and

$$\gamma_{ij\sigma}(t) \equiv \left\langle \left[C_{i\sigma}, Le^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right) LC^\dagger_{j\sigma}\right]_+ \right\rangle. \tag{2.20}$$

Thus we have a formally closed equation for the single-particle Green's function $G_{ij\sigma}(t)$. This equation is easily solved by introducing the Laplace transform,

$$M_{il\sigma}(\bar{\omega}) \equiv \int_0^\infty dt\, e^{-i\bar{\omega}t} M_{il\sigma}(t) \quad , \tag{2.21}$$

where $\bar{\omega} \equiv \omega - i\epsilon$, $\epsilon = 0^+$, and M represents either G or γ. We see from standard arguments that $M_{il\sigma}(\bar{\omega})$ can be analytically continued into the lower half of the complex ω plane, as is done for the "advanced" Zubarev-type Green's functions. The inverse of Eq. (2.21) is

$$M_{il\sigma}(t) = \frac{1}{2\pi}\int_{c-i\infty}^{c+i\infty} d\omega\, e^{i\bar{\omega}t} M_{il\sigma}(\bar{\omega}) \quad . \tag{2.22}$$

We now take the Laplace transform of Eq. (2.18) to find

$$G_{ij\sigma}(\bar{\omega}) = \delta_{ij} + \sum_l \Omega_{il\sigma} G_{lj\sigma}(\bar{\omega}) + i\sum_l \gamma_{il\sigma}(\bar{\omega}) G_{lj\sigma}(\bar{\omega}) \quad , \tag{2.23}$$

noting from Eq. (2.7) that $G_{ij\sigma}(0) \equiv i\delta_{ij}$.

Now we can directly Fourier transform this result into momentum space $\vec{k}$ as follows. Define

$$M_{\vec{k}\sigma}(\bar{\omega}) = \sum_{(i-j)} e^{-i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} M_{ij\sigma}(\bar{\omega}) \quad , \tag{2.24a}$$

so that

$$M_{ij\sigma}(\bar{\omega}) = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} M_{\vec{k}\sigma}(\bar{\omega}) \quad , \tag{2.24b}$$

with N the number of lattice sites and $M = G$, γ, or Ω. Use of Eqs. (2.24) with Eq. (2.23) gives the Dyson equation,

$$G^{-1}_{\vec{k}\sigma}(\bar{\omega}) = \bar{\omega} - \Omega_{\vec{k}\sigma} - i\gamma_{\vec{k}\sigma}(\bar{\omega}) \quad , \tag{2.25}$$

which represents the starting point of the present work.

III. PERTURBATION CALCULATION

In this section we present our self-consistent perturbation scheme. For the purpose of this calculation we shall put the damping term $\gamma_{ij\sigma}(t)$ of Eq. (2.20) in a more useful form. We first move the initial L operator in the numerator of Eq. (2.20) to the left of $C_{i\sigma}$, thereby changing the sign so that

$$\gamma_{ij\sigma}(t) = -\left\langle \left[LC_{i\sigma}, \; e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right) LC^\dagger_{j\sigma}\right]_+ \right\rangle, \tag{3.1}$$

since, for any X and Y,

$$\langle [X, LY]_+\rangle = -\langle [LX, Y]_+\rangle \quad . \tag{3.2}$$

This arises basically from the cyclic invariance of the trace implied in the ensemble averaging. We shall also show that the first L on the right-hand side of Eq. (3.1) may be exactly replaced by L_I. For this purpose we need the easily verified identities

$$L_I\, C^\dagger_{j\sigma} = +In_{j-\sigma} C^\dagger_{j\sigma} \quad , \tag{3.3}$$

$$L_t\, C^\dagger_{j\sigma} = +\sum_k t_{kj}\, C^\dagger_{k\sigma} \quad , \tag{3.4}$$

$$L_\mu\, C^\dagger_{j\sigma} = -\mu C^\dagger_{j\sigma} \quad . \tag{3.5}$$

The only difference for these identities when $C_{j\sigma}$ replaces $C^\dagger_{j\sigma}$ is that the sign changes on the right-hand side of these expressions.

From the basic definition of our projection operator and using Eqs. (3.3)–(3.5), we can write

$$\begin{aligned}\left(1-\sum_l P_{l\sigma}\right) LC^\dagger_{j\sigma} &= In_{j-\sigma} C^\dagger_{j\sigma} + \sum_k t_{kj}\, C^\dagger_{k\sigma} - \mu C^\dagger_{j\sigma} \\ &\quad - \sum_l C^\dagger_{l\sigma}\left\langle\left[C_{l\sigma}, \left(In_{j-\sigma} C^\dagger_{j\sigma} + \sum_k t_{kj}\, C^\dagger_{k\sigma} - \mu C^\dagger_{j\sigma}\right)\right]\right\rangle \\ &= I(n_{j-\sigma} - \langle n_{j-\sigma}\rangle)\, C^\dagger_{j\sigma} \\ &= \left(1-\sum_l P_{l\sigma}\right) L_I\, C^\dagger_{j\sigma} \; . \end{aligned} \tag{3.6}$$

Equation (3.1) can be further simplified from the observation that the term $L_t + L_\mu$ operating on $C_{i\sigma}$ leads to a linear combination of terms $C_{k\sigma}$, with constant coefficients. Such a term, as we now demonstrate, does not make any contribution to $\gamma_{ij\sigma}(t)$. This follows immediately from the easily verified simple identities

$$\frac{\partial}{\partial t}\left\langle\left[C_{k\sigma}, \; e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right) L_I\, C^\dagger_{j\sigma}\right]_+\right\rangle = 0 \; , \tag{3.7a}$$

and

$$\left\langle\left[C_{k\sigma}, \left(1-\sum_l P_{l\sigma}\right) L_I\, C^\dagger_{j\sigma}\right]_+\right\rangle = 0 \quad . \tag{3.7b}$$

Thus we are able to write down immediately our exact starting formula for the damping function γ,

$$\gamma_{ij\sigma}(t) = -\left\langle\left[L_I\, C_{i\sigma}, \; e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right) L_I C^\dagger_{j\sigma}\right]_+\right\rangle. \tag{3.8}$$

As mentioned in the introduction, our first approximation is to approximate the full L in the exponential in γ by L_I+L_μ. Let us briefly sketch this procedure in order to demonstrate that this approximation is indeed the Hubbard first result. Starting with

$$\gamma_{ij\sigma}(t)\cong-\left\langle\left[L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})(L_I+L_\mu)}\times\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle, \quad (3.9)$$

we expand the exponential, since its effect can be calculated exactly. We recall from Eq. (3.6) that

$$\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger=I(n_{j-\sigma}-\langle n_{j-\sigma}\rangle)C_{j\sigma}^\dagger \ . \quad (3.10)$$

In the same way we can arrive at the nth-order term

$$\left[\left(1-\sum_l P_{l\sigma}\right)(L_I+L_\mu)\right]^n\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger = [I(1-\langle n_{j-\sigma}\rangle)-\mu]^n\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger \ . \quad (3.11)$$

Using this result we are able to write γ in the simple form

$$\gamma_{ij\sigma}(t)\cong\delta_{ij}I^2\langle n_{j-\sigma}\rangle(1-\langle n_{j-\sigma}\rangle)e^{it[I(1-\langle n_{j-\sigma}\rangle)-\mu]} \ . \quad (3.12)$$

Of course it is the Laplace transform of γ which we need, that being

$$\gamma_{ij\sigma}(\bar\omega)\cong\frac{-i\delta_{ij}I^2(1-\langle n_{j-\sigma}\rangle)\langle n_{j-\sigma}\rangle}{\bar\omega-[I(1-\langle n_{j-\sigma}\rangle)-\mu]} \ . \quad (3.13)$$

The "frequency" term $\Omega_{ij\sigma}$ is trivial to evaluate exactly. We find from Eqs. (3.3)–(3.5)

$$\begin{aligned}\Omega_{ij\sigma}&\equiv\langle[C_{i\sigma},\ LC_{j\sigma}^\dagger]_+\rangle\\&=\left\langle\left[C_{i\sigma},\ \left(In_{j-\sigma}C_{j\sigma}^\dagger+\sum_k t_{kj}C_{k\sigma}^\dagger-\mu C_{j\sigma}^\dagger\right)\right]_+\right\rangle\\&=\delta_{ij}I\langle n_{j-\sigma}\rangle+t_{ij}-\mu\delta_{ij} \ .\end{aligned} \quad (3.14)$$

Since in the end we need the Fourier transform of Eq. (3.14), we work that out here:

$$\begin{aligned}\Omega_{\vec k\sigma}&\equiv\sum_{(i-j)}e^{-i\vec k\cdot(\vec R_i-\vec R_j)}\Omega_{ij\sigma}\\&=\sum_{(i-j)}e^{-i\vec k\cdot(\vec R_i-\vec R_j)}(\delta_{ij}I\langle n_{j-\sigma}\rangle+t_{ij}-\mu\delta_{ij})\\&=I\langle n_{j-\sigma}\rangle+\epsilon_k-\mu \ ,\end{aligned} \quad (3.15)$$

where ϵ_k is the Fourier transform of t_{ij}. This is just the Hartree-Fock result.

Now, taking the Fourier transform of γ in Eq. (3.13), using $\Omega_{\vec k\sigma}$ of (3.15), we get as our first approximation to $G_{\vec k\sigma}^{-1}(\bar\omega)$ [Eq. (2.25)] the Hubbard first result, i.e.,

$$G_{\vec k\sigma}^{-1}(\bar\omega)=\bar\omega'-\epsilon_k-I\langle n_{j-\sigma}\rangle\bar\omega'/[\bar\omega'-I(1-\langle n_{j-\sigma}\rangle)] \ , \quad (3.16)$$

where $\bar\omega'\equiv\bar\omega+\mu$.

In order to develop the second approximation, we need an exact equation of motion for $\gamma_{ij\sigma}(t)$. From the definition for γ in Eq. (3.8) we can immediately write down its time derivative:

$$\begin{aligned}\frac{\partial}{\partial t}\gamma_{ij\sigma}(t)&=-i\left\langle\left[L_I C_{i\sigma},\ \left(1-\sum_l P_{l\sigma}\right)Le^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle\\&=-i\left\langle\left[L_I C_{i\sigma},\ Le^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle\\&\quad+i\sum_l\langle[L_I C_{i\sigma},\ C_{l\sigma}^\dagger]_+\rangle\left\langle\left[C_{l\sigma},\ Le^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle\\&=+i\left\langle\left[LL_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle\\&\quad-i\sum_l\langle[L_I C_{i\sigma},\ C_{l\sigma}^\dagger]_+\rangle\left\langle\left[LC_{l\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle \ ,\end{aligned} \quad (3.17)$$

where we have used Eqs. (3.2) and (2.12). We note that from Eqs. (3.3)–(3.5), Eq. (3.7), and Eq. (3.8) the last factor in the second term of Eq. (3.17) is essentially $\gamma_{lj\sigma}(t)$, since

$$\begin{aligned}&\left\langle\left[LC_{l\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle\\&=\left\langle\left[L_I C_{l\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle\\&\equiv-\gamma_{lj\sigma}(t) \ .\end{aligned} \quad (3.18)$$

For completion, we need the commutation average

$$\langle[L_I C_{i\sigma},\ C_{l\sigma}^\dagger]_+\rangle=-\delta_{il}I\langle n_{l-\sigma}\rangle \ , \quad (3.19)$$

and the identity

$$\begin{aligned}LL_I C_{i\sigma}&=(L_I+L_\mu)L_I C_{i\sigma}+L_t L_I C_{i\sigma}\\&=-(I-\mu)L_I C_{i\sigma}+L_t L_I C_{i\sigma} \ ,\end{aligned} \quad (3.20)$$

which again comes from using Eqs. (3.3) and (3.5). These identities allow us to write Eq. (3.17) in the interesting and useful form

$$\left(\frac{\partial}{\partial t} - i[I(1-\langle n_{j-\sigma}\rangle) - \mu]\right)\gamma_{ij\sigma}(t) = iA_{ij\sigma}(t) , \quad (3.21)$$

where

$$A_{ij\sigma}(t) \equiv \left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle . \quad (3.22)$$

The first approximation, Eq. (3.12), is now clear: $A_{ij\sigma}(t)$, which is explicitly $O(t_{ij})$, was set equal to zero in Eq. (3.21). Again in the spirit of the *first* approximation we now replace, in the exponential operator of $A_{ij\sigma}(t)$, $L_I + L_\mu$ for the full L to get the *second* approximation. Here we need the identity

$$e^{it(1-\Sigma_l P_{l\sigma})(L_I+L_\mu)}\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger$$
$$= Ie^{it[I(1-\langle n_{j-\sigma}\rangle)-\mu]}(n_{j-\sigma} - \langle n_{j-\sigma}\rangle) C_{j\sigma}^\dagger , \quad (3.23)$$

which follows directly from our previously derived identity, Eq. (3.11). We can now write for $A_{ij\sigma}(t)$

$$A_{ij\sigma}(t) \cong -e^{it[I(1-\langle n_{j-\sigma}\rangle)-\mu]} I^2 B_{ij\sigma} , \quad (3.24)$$

where

$$B_{ij\sigma} \equiv -\frac{1}{I^2}\left\langle\left[L_t L_I C_{i\sigma},\ \left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle . \quad (3.25)$$

By a bit of lengthy but straightforward algebra of the variety amply demonstrated heretofore, we can write the Fourier transform of $B_{ij\sigma}$ in a more recognizable form:

$$B_{\vec{k}\sigma} \equiv \sum_j t_{ij}\langle C_{i\sigma}^\dagger C_{j\sigma}\rangle$$
$$- \sum_{(i-j)} e^{-i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} t_{ij}(\langle\Delta n_{i-\sigma}\Delta n_{j-\sigma}\rangle + \langle C_{j\sigma}^\dagger C_{j-\sigma} C_{i-\sigma}^\dagger C_{i\sigma}\rangle)$$
$$+ \sum_{(i-j)} e^{-i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} t_{ij}\langle C_{j\sigma}^\dagger C_{j-\sigma}^\dagger C_{i-\sigma} C_{i\sigma}\rangle$$
$$-\sum t_{ij}\langle(C_{i-\sigma}^\dagger C_{j-\sigma} + C_{j-\sigma}^\dagger C_{i-\sigma})n_{j\sigma}\rangle , \quad (3.26)$$

where

$$B_{ij\sigma} \equiv \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} B_{\vec{k}\sigma} , \quad (3.27)$$

and

$$\Delta n_{j-\sigma} \equiv n_{j-\sigma} - \langle n_{j-\sigma}\rangle . \quad (3.28)$$

The second approximation arises from the substitution of Eq. (3.24) into Eq. (3.21) to obtain

$$\left(\frac{\partial}{\partial t} - i[I(1-\langle n_{j-\sigma}\rangle) - \mu]\right)\gamma_{ij\sigma}(t)$$
$$\cong -ie^{it[I(1-\langle n_{j-\sigma}\rangle)-\mu]} I^2 B_{ij\sigma} . \quad (3.29)$$

Taking the Laplace and Fourier transforms of Eq. (3.29), we get

$$\gamma_{\vec{k}\sigma}(\overline{\omega}) \cong \frac{-i\gamma_{\vec{k}\sigma}(t=0)}{\overline{\omega} - [I(1-\langle n_{j-\sigma}\rangle) - \mu]} + \frac{iI^2 B_{\vec{k}\sigma}}{\{\overline{\omega} - [I(1-\langle n_{j-\sigma}\rangle) - \mu]\}^2} . \quad (3.30)$$

With this result we can immediately write the inverse Green's function

$$G_{\vec{k}\sigma}^{-1}(\overline{\omega}) = \overline{\omega}' - \epsilon_k - \frac{I\langle n_{j-\sigma}\rangle\overline{\omega}'}{\omega' - I(1-\langle n_{j-\sigma}\rangle)} + \frac{I^2 B_{\vec{k}\sigma}}{[\omega' - I(1-\langle n_{j-\sigma}\rangle)]^2} . \quad (3.31)$$

It is worthy of mention that this form represents the Esterling–Lange-type[5] result in its more complete form.

To develop our third approximation we need the exact equation of motion for our A term. We find from Eq. (3.22)

$$\frac{\partial}{\partial t}A_{ij\sigma}(t) = i\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\right.\right.$$
$$\left.\left.\times\left(1-\sum_l P_{l\sigma}\right)L\left(1-\sum_l P_{l\sigma}\right)L_I C_{i\sigma}^\dagger\right]_+\right\rangle$$
$$= i\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\right.\right.$$
$$\left.\left.\times\left(1-\sum_l P_{l\sigma}\right)(L_I + L_\mu)\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle$$
$$+ i\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\right.\right.$$
$$\left.\left.\times\left(1-\sum_l P_{l\sigma}\right)L_t\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger\right]_+\right\rangle . \quad (3.32)$$

But, from Eq. (3.11) for the case $n=1$, we can write

$$\left(1-\sum_l P_{l\sigma}\right)(L_I + L_\mu)\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger$$
$$= [I(1-\langle n_{j-\sigma}\rangle) - \mu]\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger . \quad (3.33)$$

Again from Eqs. (3.3) and (3.5) we see that

$$\left(1-\sum_l P_{l\sigma}\right)L_t\left(1-\sum_l P_{l\sigma}\right)L_I C_{j\sigma}^\dagger$$
$$= \left(1-\sum_l P_{l\sigma}\right)L_t L_I C_{j\sigma}^\dagger . \quad (3.34)$$

Use of Eqs. (3.33) and (3.34) in Eq. (3.32) yields

$$\left(\frac{\partial}{\partial t} - i[I(1-\langle n_{j-\sigma}\rangle) - \mu]\right)A_{ij\sigma}(t)$$
$$= i\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})L}\left(1-\sum_l P_{l\sigma}\right)L_t L_I C_{j\sigma}^\dagger\right]_+\right\rangle$$
$$\equiv iI^2 D_{ij\sigma}(t) . \quad (3.35)$$

We now clearly see the nature of the second approximation: $D_{ij\sigma}(t)$ of Eq. (3.35) is taken as zero. Although this appears as correct perturbation procedure since D is explicitly proportional to the hopping $(t_{ij})^2$, a bit of caution is in order. In fact such a procedure is not correct for the Hubbard model in the atomic limit. We shall demonstrate that the frequency dependence of D, or it's Laplace transform, possesses "dangerous poles" in the vicinity of $\overline{\omega}'$ and $\overline{\omega}'-I$ in this limit. We might note at this point that D has a structure similar to γ of Eq. (3.8), except that $L_t L_I$ has replaced L_I in the numerator of the expression. Keeping the full $D_{ij\sigma}(t)$ for the moment we find for the Laplace-Fourier transform of A in Eq. (3.35) the result

$$A_{\vec{k}\sigma}(\overline{\omega}) = iI^2\left[B_{\vec{k}\sigma} - iD_{\vec{k}\sigma}(\omega)\right] / \{\overline{\omega} - [I(1-\langle n_{j-\sigma}\rangle) - \mu]\} . \tag{3.36}$$

Also if we do likewise to γ in Eq. (3.21) we find

$$\gamma_{\vec{k}\sigma}(\overline{\omega}) = -i[\gamma_{\vec{k}\sigma}(t=0) + iA_{\vec{k}\sigma}(\omega)] / \{\overline{\omega} - [I(1-\langle n_{j-\sigma}\rangle) - \mu]\} . \tag{3.37}$$

Finally substitution of Eqs. (3.36) and (3.37) into Eq. (2.25) yields the exact result,

$$G_{\vec{k}\sigma}^{-1}(\omega) = \overline{\omega}' - \epsilon_k - \frac{I\langle n_{j-\sigma}\rangle\overline{\omega}'}{[\overline{\omega}' - I(1-\langle n_{j-\sigma}\rangle)]} + \frac{I^2[B_{\vec{k}\sigma} - iD_{\vec{k}\sigma}(\overline{\omega})]}{[\overline{\omega}' - I(1-\langle n_{j-\sigma}\rangle)]^2} . \tag{3.38}$$

The third approximation result follows directly in the footsteps of the others, i.e., replacement of $L_I + L_u$ for L in the exponential operator in D,

$$D_{ij\sigma}(t) \simeq \frac{1}{I^2}\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\sum_l P_{l\sigma})(L_I+L_u)} \times \left(1-\sum_l P_{l\sigma}\right) L_t L_I C_{j\sigma}^\dagger\right]_+\right\rangle . \tag{3.39}$$

This calculation of Eq. (3.39) is no longer simple because of the $\sum_l P_{l\sigma}$ in the exponential operator. However, it follows a path so similar to that of earlier approximations that we relegate the explicit calculation to the Appendix. The result has the troublesome form

$$D_{\vec{k}\sigma}(\overline{\omega}) \approx A_{\vec{k}\sigma}^{(1)}/\overline{\omega}' + A_{\vec{k}\sigma}^{(2)}/(\overline{\omega}' - I) , \tag{3.40}$$

where the $A_{\vec{k}\sigma}^{(i)}$'s are static averages explicitly proportional to $(t_{ij})^2$. The unwanted feature here is that we are looking for the zeros of $G_{\vec{k}\sigma}^{-1}(\overline{\omega})$ [see Eq. (3.38)], and these occur in the neighborhood $\overline{\omega}'$, $\overline{\omega}' - I \approx O(t_{ij})$ for small t_{ij}; so $D_{\vec{k}\sigma}(\overline{\omega})$ of Eq. (3.40) is of the same order as $B_{\vec{k}\sigma}$, and thus our procedure has not collected all the terms in $G_{\vec{k}\sigma}^{-1}(\overline{\omega})$ which are first order in t_{ij}. This is a manifestation of the inherent difficulty of expanding about the atomic limit pointed out by Bari and later by Esterling.

That this troublesome feature is indeed peculiar to the Hubbard-like atomic-limit Hamiltonian is best illustrated by expanding instead about the kinetic-energy (hopping) term. Here in Eq. (3.39) L would be replaced by $L_t + L_u$, and we find that in this approximation something like

$$D_{\vec{k}\sigma}(\overline{\omega}) \approx \sum_{\vec{k}} \frac{X_{\vec{k}\sigma}}{\overline{\omega}' - \epsilon_{\vec{k}}} , \tag{3.41}$$

with again $X_{\vec{k}\sigma}$ a static average proportional to $(t_{ij})^2$. We see here that $D_{\vec{k}\sigma}(\overline{\omega})$ involves a sum (or integral) over $\vec{k}$, yielding a term which has no dangerous poles in the neighborhood of $G_{\vec{k}\sigma}^{-1}(\overline{\omega}) \approx 0$, and can be replaced in normal "damping-like" fashion by a frequency-*independent* complex number of order $(t_{ij})^2$. Recapitulating, we see that if an expansion is done about the unperturbed system containing a "band" of energies we will not have difficulty. On the other hand, an expansion about an unperturbed system with a finite number of levels yield the trouble depicted in Eq. (3.40).

Returning to the complete definition of $D_{ij\sigma}(t)$ in Eq. (3.35) we find that we can no longer find a single and useful equation of motion satisfied by D. Thus our self-consistent perturbation taken involves an iteration of the operator $e^{it(1-\sum_l P_{l\sigma})L}$ in D. We note the operator identity

$$\begin{aligned} e^{it(A+B)} &= e^{itA} + i\int_0^t e^{i\tau A} B e^{i(t-\tau)(A+B)} d\tau \\ &= e^{itA} + i\int_0^t e^{i\tau A} B e^{i(t-\tau)A} d\tau + \cdots \end{aligned} \tag{3.42}$$

for any A and B. Our essential approximation involves breaking up $(1-\sum_l P_{l\sigma})L$ into two parts and using Eq. (3.42). Such a breakup in perturbation fashion would be to choose $A = (1-\sum_l P_{l\sigma})L_0$ and $B = (1-\sum_l P_{l\sigma})L_v$, where L_0 means take the commutator with respect to the unperturbed part H_0 and L_v means take the commutator with respect to potential part V of the Hamiltonian H. Note that such an approximation to the exponential operator is internal to the outer averaging process and in this sense is like chain breaking, and that it is of course self consistent at every stage of the perturbation, withstanding atomic-limit- (finite level) type expansions. Also the equivalent of infinite-order perturbation theory (i.e., diagrammatic-like expansions) can be done trivially by this method and will be reported elsewhere. Finally, we wish to point out for large I the projection operator, Eq. (7.12), which projects out the kinetic-energy (hopping) term is really not appropriate here. One would really like to project out the intra-atomic Coulomb repulsion term. This can easily be done by modifying the definition of the projection operator. Such a procedure leads to a "D" term which is proportional to $(t_{ij})^2$ alone and not $I^2(t_{ij})^2$ and is more convenient to handle for large I. This calculation will also be reported in a later paper.

It is apparent that the above approach is particularly suited to a whole range of solid state problems where there exists the possibility of a phase transition. Recent treatments of some problems in superconductivity have convinced us that the method may serve as a powerful approach to strong-coupling problems such as vibrational relaxation in molecular solids and liquids. We ought to mention that the main ideas of this article have been stated in an earlier note.[6]

APPENDIX: EVALUATION OF $D_{ij\sigma}(t)$

In this section we present the details of the calculation leading to (3.40).

$$D_{ij\sigma}(t) \cong \frac{1}{I^2}\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(1-\Sigma_l P_{l\sigma})(L_I+L_\mu)} \times\left(1-\sum_l P_{l\sigma}\right)L_t L_I C_{j\sigma}^\dagger\right]_+\right\rangle \equiv \overline{D}_{ij\sigma}(t) \ . \quad \text{(A1)}$$

We again write, as in Eq. (3.42),

$$e^{it(A+B)} = e^{itA} + i\int_0^t d\tau\, e^{i(t-\tau)A}\, B e^{i\tau(A+B)} \quad \text{(A2)}$$

for any operators A and B. Here we set $A = L_I + L_\mu$ and $B = -\sum_l P_{l\sigma}(L_I+L_\mu)$ and use (A2) in (A1) to find

$$\overline{D}_{ij\sigma}(t) = d_{ij\sigma}(t) - i\sum_l \int_0^t d\tau\, a_{il\sigma}(t-\tau) M_{lj\sigma}(\tau) \ , \quad \text{(A3)}$$

where

$$d_{ij\sigma}(t) = \frac{1}{I^2}\left\langle\left[L_t L_I C_{i\sigma},\ e^{it(L_I+L_\mu)} \times\left(1-\sum_l P_{l\sigma}\right)L_t L_I C_{j\sigma}^\dagger\right]_+\right\rangle , \quad \text{(A4)}$$

where

$$a_{il\sigma}(t) = (1/I)\langle[L_t L_I C_{i\sigma},\ e^{it(L_I+L_\mu)} C_{l\sigma}^\dagger]_+\rangle \ , \quad \text{(A5)}$$

and where

$$M_{lj\sigma}(t) \equiv \frac{1}{I}\left\langle\left[C_{l\sigma},\ (L_I+L_\mu) e^{it(1-\Sigma_l P_{l\sigma})(L_I+L_\mu)} \times\left(1-\sum_l P_{l\sigma}\right)L_t L_I C_{j\sigma}^\dagger\right]_+\right\rangle . \quad \text{(A6)}$$

We again apply (A2) to (A6) to find

$$M_{lj\sigma}(t) = m_{lj\sigma}(t) - i\sum_{l_1}\int_0^t d\tau\, r_{ll_1}(t-\tau) M_{l_1 j\sigma}(\tau) \ , \quad \text{(A7)}$$

where

$$m_{lj\sigma}(t) \equiv \frac{1}{I}\left\langle\left[C_{l\sigma},\ (L_I+L_\mu) e^{it(L_I+L_\mu)} \times\left(1-\sum_l P_{l\sigma}\right)L_t L_I C_{j\sigma}^\dagger\right]_+\right\rangle , \quad \text{(A8)}$$

and

$$\begin{aligned} r_{ll_1}(t) &\equiv \langle[C_{l\sigma},\ (L_I+L_\mu) e^{it(L_I+L_\mu)} C_{l_1\sigma}^\dagger]_+\rangle \\ &= \delta_{ll_1}[e^{it(I-\mu)}(I-\mu)\langle n_{l-\sigma}\rangle - e^{-it\mu}\,\mu(1-\langle n_{l-\sigma}\rangle)] \\ &\equiv \delta_{ll_1} r(t) \ . \end{aligned} \quad \text{(A9)}$$

Use of (A9) in (A7) and taking the Laplace transform gives

$$M_{lj\sigma}(\overline{\omega}) = m_{lj\sigma}(\overline{\omega})/[1+ir(\overline{\omega})] \ . \quad \text{(A10)}$$

We now take the Laplace transform of (A3) inserting (A10) for $M_{lj\sigma}(\overline{\omega})$, to obtain

$$\overline{D}_{ij\sigma}(\overline{\omega}) = d_{ij\sigma}(\overline{\omega}) - i\sum_l \frac{a_{il\sigma}(\overline{\omega})\, m_{lj\sigma}(\overline{\omega})}{1+ir(\overline{\omega})} \ . \quad \text{(A11)}$$

Now d and m can be decomposed further. From (A4) and (A5) we find

$$d_{ij\sigma}(t) = f_{ij\sigma}(t) - \sum_l a_{il\sigma}(t)\, b_{lj\sigma} \ , \quad \text{(A12)}$$

where

$$f_{ij\sigma}(t) \equiv (1/I^2)\langle[L_t L_I C_{i\sigma},\ e^{it(L_I+L_\mu)} L_t L_I C_{j\sigma}^\dagger]_+\rangle \ , \quad \text{(A13)}$$

and

$$b_{lj\sigma} \equiv (1/I)\langle[C_{l\sigma},\ L_t L_I C_{j\sigma}^\dagger]_+\rangle \ . \quad \text{(A14)}$$

The $f_{ij\sigma}(t)$ explicitly involves *three-site* correlations. From (A8), (A9), and (A14)

$$m_{lj\sigma}(t) = h_{lj\sigma}(t) - \sum_{l_1} r_{ll_1}(t)\, b_{l_1 j\sigma} \ , \quad \text{(A15)}$$

where

$$h_{lj\sigma}(t) \equiv (1/I)\langle[C_{l\sigma},\ (L_I+L_\mu) e^{it(L_I+L_\mu)} L_t L_I C_{j\sigma}^\dagger]_+\rangle \quad \text{(A16)}$$

and involves *two-site* correlations. Consider the Fourier transforms of (A11), (A12), and (A15). We obtain

$$D_{k\sigma}(\overline{\omega}) = d_{k\sigma}(\overline{\omega}) - i\frac{a_{k\sigma}(\overline{\omega})\, m_{k\sigma}(\overline{\omega})}{1+ir(\overline{\omega})} \ . \quad \text{(A17a)}$$

$$d_{k\sigma}(\overline{\omega}) = f_{k\sigma}(\overline{\omega}) - a_{k\sigma}(\overline{\omega})\, b_{k\sigma} \ , \quad \text{(A17b)}$$

$$m_{k\sigma}(\overline{\omega}) = h_{k\sigma}(\overline{\omega}) - r(\overline{\omega})\, b_{k\sigma} \ . \quad \text{(A17c)}$$

Use of (A17b) and (A17c) in (A17a) yields for $\overline{D}_{k\sigma}(\overline{\omega})$

$$\overline{D}_{\vec{k}\sigma}(\overline{\omega}) = f_{\vec{k}\sigma}(\overline{\omega}) - a_{\vec{k}\sigma}(\overline{\omega})\frac{b_{\vec{k}\sigma} + ih_{\vec{k}\sigma}(\overline{\omega})}{1+ir(\overline{\omega})} \ . \quad \text{(A18)}$$

What we have accomplished here is to remove the projection operator from the exponential, and we are left with all the time dependence in the form $e^{it(L_I+L_\mu)}$, which is easily calculable. That the form, Eq. (3.40), arises is now simply verified.

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