8

Conserving Approximations vs. Two-Particle Self-Consistent Approach

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ABSTRACT The conserving approximation scheme to many-body problems was developed by Kadanoff and Baym using the functional-derivative approach. Another approach for the Hubbard model also satisfies conservation laws, but in addition it satisfies the Pauli principle and a number of sum rules. A concise formal derivation of that approach, using functional derivatives, is given in this conference paper to highlight formal analogies and differences with conserving approximations.

1 Introduction

Although quantum many-body theory is in principle exact, any practical application of the formalism necessarily leads to the violation of some exact results. For example, it was noticed long ago that whenever infinite subsets of diagrams are resummed, conservation laws will be violated if certain rules are not followed. As another example of a possible inconsistency, one can obtain a relation between number of particles, chemical potential, and temperature from either a Green function or from a derivative of the free energy. How can we make sure that the diagrammatic series for the Green function and that for the free energy give the same result? Both of these problems, namely, obtaining response functions that satisfy conservation laws and making sure that the free energy is "thermodynamically consistent" with the Green function, can be solved using an approach that was developed by Kadanoff and Baym [1, 2] many years ago. This approach, described in the paper by Bickers (Chapter 6) in these proceedings, allows one to obtain so-called "conserving approximations" [3] that have been extensively used in the last decade. However, as in any approximate calculations, some exact identities are not satisfied by conserving approximations [4,6]. For example, the Pauli principle is violated, integration over the coupling constant of the potential energy obtained from susceptibilities does not lead back to the starting free energy, and the irreducible verticies generated by a functional derivative of the self-energy are not the same

as the vertex corrections entering the self-energy itself.[1] In addition, since there is an infinite number of choice of diagrams for the Luttinger–Ward functional, there is also an infinite number of conserving approximations and it is difficult to decide on the validity of an approximation based on the criterion of conservation only. Further criticism has appeared in [4] and [5].

In this chapter, we wish to present a new derivation of a *nondiagrammatic* approach to the *repulsive* Hubbard model that was developed a few years ago [4]. An analogous derivation in the case of the *attractive* Hubbard model was presented at this workshop by Bumsoo Kyung and has already appeared [7, 8]. Here, we go back to our earlier results on the repulsive Hubbard model, but we use a formal approach that highlights analogies and differences with conserving approximations. This chapter will strive to be concise with the explicit purpose of being clear without getting lost in details. The published derivation for the attractive Hubbard model contains more of these details [7].

In Section 2 we first present a derivation of conserving approximations that can be extended, in Section 3, to the derivation of our nondiagrammatic approach. This derivation focuses first on response functions and on the self-consistent determination of irreducible spin and charge vertices. That determination is done in such a way that the Pauli principle in its simplest form is satisfied. In other words, crossing symmetry (Chapter 6) is satisfied only for field operators on a single site, all at the same time. This is the so-called two-particle self-consistent (TPSC) part of the approach . We then improve our approximation for the self-energy by using the TPSC results in the exact non Hartree–Fock part of the self-energy. Vertices and Green function entering the final expression are at the same level of approximation. No Migdal theorem is assumed. The effects of transverse and longitudinal fluctuations are considered in separate subsections before the final expression can be written down. The internal-accuracy check [4] is also presented and used in the derivation. We end up in Section 4 with a discussion of extensions of the approach that are now being developed. The appendix addresses a technical detail.

2 Functional Derivative Formalism and Conserving Approximations

In this section, we first discuss single-particle properties, then response functions and, finally, we present the Hartree–Fock approximation as an example of a conserving approximation. The latter will be helpful as a

[1] In FLEX for example, the structure of the self-energy is the same as if Migdal's theorem was applicable.

starting point for the derivation of the two-particle self-consistent (TPSC) approach in the next section.

2.1 Single-Particle Properties

Following functional methods of the Schwinger school [1, 2, 9], we begin with the generating function with source fields ϕ_σ and field destruction operators ψ in the grand canonical ensemble

$$\ln Z[\phi] = \ln \mathrm{Tr}\big[e^{-\beta(\widehat{H}-\mu\widehat{N})}\mathrm{T}_\tau\big(e^{-\psi^\dagger_{\overline{\sigma}}(\overline{1})\phi_{\overline{\sigma}}(\overline{1},\overline{2})\psi_{\overline{\sigma}}(\overline{2})}\big)\big]. \tag{2.1}$$

We adopt the convention that 1 stands for the position and imaginary time indices $(\mathbf{r}_1, \tau_1)$. The overbar means summation over every lattice site and integration over imaginary-time from 0 to β. T_τ is the time-ordering operator.

The propagator in the presence of the source field is obtained from functional differentiation

$$G_\sigma(1,2;\{\phi\}) = -\langle\psi_\sigma(1)\psi^\dagger_\sigma(2)\rangle_\phi = -\frac{\delta \ln Z[\phi]}{\delta\phi_\sigma(2,1)}. \tag{2.2}$$

From now on, *the time-ordering operator in averages,* $\langle\ \rangle$, *is implicit.* Physically relevant correlation functions are obtained for $\{\phi\} = 0$ but it is extremely convenient to keep finite $\{\phi\}$ in intermediate steps of the calculation.

Using the equation of motion for the field ψ and the definition of the self-energy, one obtains the Dyson equation in the presence of the source field [2, p. 43]

$$(G_0^{-1} - \phi)G = 1 + \Sigma G; \quad G^{-1} = G_0^{-1} - \phi - \Sigma \tag{2.3}$$

where, from the commutator of the interacting part of the Hubbard Hamiltonian H, one obtains

$$\Sigma_\sigma(1,\bar{1};\{\phi\})G_\sigma(\bar{1},2;\{\phi\}) = -U\langle\psi^\dagger_{-\sigma}(1^+)\psi_{-\sigma}(1)\psi_\sigma(1)\psi^\dagger_\sigma(2)\rangle_\phi. \tag{2.4}$$

The imaginary time in 1^+ is infinitesimally larger than in 1.

2.2 Response Functions

Response (four-point) functions for spin and charge excitations can be obtained from functional derivatives $(\delta G/\delta\phi)$ of the source-dependent propagator. Following the standard approach and using matrix notation to abbreviate the summations and integrations we have

$$\begin{gathered} GG^{-1} = 1 \\ \frac{\delta G}{\delta\phi}G^{-1} + G\frac{\delta G^{-1}}{\delta\phi} = 0. \end{gathered} \tag{2.5}$$

Using the Dyson equation (2.3) $G^{-1} = G_0^{-1} - \phi - \Sigma$,S we may rewrite this as

$$\frac{\delta G}{\delta \phi} = -G\frac{\delta G^{-1}}{\delta \phi}G = G \circ G + G\frac{\delta \Sigma}{\delta \phi}G, \tag{2.6}$$

where the symbol $\circ$ reminds us that the neighboring labels of the propagators have to be the same as those of the ϕ in the functional derivative. If perturbation theory converges, we may write the self-energy as a functional of the propagator. From the chain rule, one then obtains an integral equation for the response function in the particle-hole channel that is the analog of the Bethe–Salpeter equation in the particle-particle channel

$$\frac{\delta G}{\delta \phi} = G \circ G + G\left[\frac{\delta \Sigma}{\delta G}\frac{\delta G}{\delta \phi}\right]G. \tag{2.7}$$

The labels of the propagators in the last term are attached to the self-energy, as in (2.6).[2] Vertices appropriate for spin and charge responses are given, respectively, by

$$U_{\rm sp} = \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} - \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow}; \quad U_{\rm ch} = \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} + \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow}. \tag{2.8}$$

2.3 Hartree–Fock and RPA as an Example

As an example of calculation of response functions, consider the Hartree–Fock approximation which corresponds to factoring the four-point function in the definition of the self-energy (2.4) as if there were no correlations,

$$\Sigma^{\rm H}_\sigma(1,\bar{1};\{\phi\})G^{\rm H}_\sigma(\bar{1},2;\{\phi\}) = UG^{\rm H}_{-\sigma}(1,1^+;\{\phi\})G^{\rm H}_\sigma(1,2;\{\phi\}). \tag{2.9}$$

Multiplying the above equation by $(G^{\rm H}_\sigma)^{-1}$, we are left with

$$\begin{aligned} \Sigma^{\rm H}_\sigma(1,2;\{\phi\}) &= UG^{\rm H}_{-\sigma}(1,1^+;\{\phi\})\delta(1-2), \\ \left.\frac{\delta \Sigma^{\rm H}_\uparrow(1,2;\{\phi\})}{\delta G^{\rm H}_\downarrow(3,4;\{\phi\})}\right|_{\{\phi\}=0} &= U\delta(1-2)\delta(3-1)\delta(4-2), \end{aligned} \tag{2.10}$$

which, when substituted in the integral equation (2.7) for the response function, tells us that we have generated the random phase approximation (RPA) with, from (2.8), $U_{\rm sp} = U_{\rm ch} = U$.

3 Another Approach

The approach developed in [4], consists of two steps, corresponding to the following two subsections. First, one computes response functions from the

[2] To remind ourselves of this, we may also adopt an additional "vertical matrix notation" convention and write (2.6) as $\delta G/\delta\phi = G \circ G + G\big[\frac{\delta\Sigma/\delta G}{\delta G/\delta\phi}\big]G$.

TPSC approach, inspired by earlier work of Singwi [10]. Second, one generates an improved approximation for the self-energy starting from an exact expression for Σ that explicitly separates the infinite-frequency limit from the lower-frequency contribution. The method also contains an internal-accuracy check that is discussed in the last subsection.

3.1 First Step: Two-Particle Self-Consistency for $G^{(1)}$, $\Sigma^{(1)}$, $\Gamma^{(1)}_{\rm sp} = U_{\rm sp}$, and $\Gamma^{(1)}_{\rm ch} = U_{\rm ch}$

In conserving approximations, the self-energy is obtained from a functional derivative $\Sigma[G] = \delta\Phi[G]/\delta G$ of Φ the Luttinger–Ward functional, which is itself computed from a set of diagrams. To liberate ourselves from diagrams, we start instead from the exact expression for the self-energy (Eq. 2.4) and notice that when label 2 equals 1^+, the right-hand side of this equation is equal to double-occupancy $\langle n_\uparrow n_\downarrow\rangle$. Factoring as in Hartree–Fock amounts to assuming no correlations. Instead, we should insist that $\langle n_\uparrow n_\downarrow\rangle$ should be obtained self-consistently. After all, in the Hubbard model, there are only two local four point functions: $\langle n_\uparrow n_\downarrow\rangle$ and $\langle n^2_\uparrow\rangle = \langle n^2_\downarrow\rangle$. The latter is given exactly, through the Pauli principle, by $\langle n^2_\uparrow\rangle = \langle n^2_\downarrow\rangle = \langle n_\uparrow\rangle = \langle n_\downarrow\rangle = n/2$, when the filling n is known. In a way, $\langle n_\uparrow n_\downarrow\rangle$ in the self-energy equation (2.4), can be considered as an initial condition for the four point function when one of the points, 2, separates from all the others which are at 1. When that label 2 does not coincide with 1, it becomes more reasonable to factor *à la* Hartree–Fock. These physical ideas are implemented by postulating

$$\Sigma^{(1)}_\sigma(1,\bar{1};\{\phi\})G^{(1)}_\sigma(\bar{1},2;\{\phi\}) = A_{\{\phi\}}G^{(1)}_{-\sigma}(1,1^+;\{\phi\})G^{(1)}_\sigma(1,2;\{\phi\}), \quad (3.1)$$

where $A_{\{\phi\}}$ depends on external field and is chosen such that the exact result[3]

$$\Sigma_\sigma(1,\bar{1};\{\phi\})G_\sigma(\bar{1},1^+;\{\phi\}) = U\langle n_\uparrow(1)n_\downarrow(1)\rangle_\phi \quad (3.2)$$

is satisfied. It is easy to see that the solution is

$$A_{\{\phi\}} = U\frac{\langle n_\uparrow(1)n_\downarrow(1)\rangle_\phi}{\langle n_\uparrow(1)\rangle_\phi\langle n_\downarrow(1)\rangle_\phi}. \quad (3.3)$$

Substituting $A_{\{\phi\}}$ back into our *ansatz* (3.1) we obtain the self-energy by right-multiplying by $\left(G^{(1)}_\sigma\right)^{-1}$:

$$\Sigma^{(1)}_\sigma(1,2;\{\phi\}) = A_{\{\phi\}}G^{(1)}_{-\sigma}(1,1^+;\{\phi\})\delta(1-2). \quad (3.4)$$

[3]If we had chosen $2 \to 1^-$ instead of $2 \to 1^+$ we would have found $\langle n_\downarrow(1)(n_\uparrow(1)-1)\rangle$ on the right-hand side of (3.2), as discussed in the Appendix. Since we are interested in using the local limit of ΣG as an initial condition for spin and charge correlations, it is more natural to focus on $2 \to 1^+$ since in that case it is $\langle n_\downarrow(1)n_\uparrow(1)\rangle$ that appears on the right-hand side, a quantity that follows directly from the spin and charge correlations and where spin up and spin down are treated on equal footing. See also the appendix.

We are now ready to obtain irreducible vertices using the prescription of the previous section (Eq. 2.8), namely, through functional derivatives of Σ with respect to G. In the calculation of $U_{\rm sp}$, the functional derivative of $\langle n_\uparrow n_\downarrow\rangle/(\langle n_\uparrow\rangle\langle n_\downarrow\rangle)$ drops out, so we are left with[4]

$$U_{\rm sp} = \left.\frac{\delta\Sigma_\uparrow^{(1)}}{\delta G_\downarrow^{(1)}}\right|_{\{\phi\}=0} - \left.\frac{\delta\Sigma_\uparrow^{(1)}}{\delta G_\uparrow^{(1)}}\right|_{\{\phi\}=0} = A_{\{\phi\}=0} = U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}. \tag{3.5}$$

The renormalization of this irreducible vertex may be physically understood as coming from Kanamori–Brueckner screening [4]. To close the system of equations, we need to know double-occupancy. It may be found self-consistently using the fluctuation-dissipation theorem and the Pauli principle. First notice that the Pauli principle, $\langle n_\sigma^2\rangle = \langle n_\sigma\rangle$, implies that

$$\langle (n_\uparrow - n_\downarrow)^2\rangle = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle - 2\langle n_\uparrow n_\downarrow\rangle \tag{3.6}$$

while the fluctuation-dissipation theorem tells us that $\langle (n_\uparrow - n_\downarrow)^2\rangle$ is given by the equal-time equal-position imaginary-time susceptibility $\chi_{\rm sp}$. Since $\chi_{\rm sp}^{-1}(q) = \chi_0^{-1}(q) - \frac{1}{2}U_{\rm sp}$ with $q \equiv (\mathbf{q}, 2\pi nT)$, this is equivalent to the equation

$$\frac{T}{N}\sum_q \frac{\chi_0(q)}{1 - \frac{1}{2}U_{\rm sp}\chi_0(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle \tag{3.7}$$

that, with (3.5) for $U_{\rm sp}$, gives us double-occupancy.

The functional-derivative procedure generates an expression for the charge vertex $U_{\rm ch}$ which involves the functional derivative of $\langle n_\uparrow n_\downarrow\rangle/(\langle n_\uparrow\rangle\langle n_\downarrow\rangle)$ which contains six point functions that one does not really know how to evaluate. But, if we again assume that the vertex $U_{\rm ch}$ is a constant, it is simply determined by the requirement that charge fluctuations also satisfy the fluctuation-dissipation theorem and the Pauli principle,

$$\frac{T}{N}\sum_q \frac{\chi_0(q)}{1 + \frac{1}{2}U_{\rm ch}\chi_0(q)} = n + 2\langle n_\uparrow n_\downarrow\rangle - n^2. \tag{3.8}$$

Note that, in principle, $\Sigma^{(1)}$ also depends on double-occupancy, but since $\Sigma^{(1)}$ is a constant, it is absorbed in the definition of the chemical potential, and we do not need to worry about it in this case. That is why the noninteracting irreducible susceptibility $\chi_0(q)$ appears in the expressions for the susceptibility, even though it should be evaluated with $G^{(1)}$ that contains $\Sigma^{(1)}$. One can check that spin and charge conservation are satisfied by our susceptibilities.

Detailed comparisons with quantum Monte Carlo simulations (QMC) [4,5,11,12] have shown that (3.5), (3.7), and (3.8) give predictions that are

[4]For $n > 1$, all particle occupation numbers must be replaced by hole occupation numbers.

quantitative at the few percent level, in regions of parameter space where size effects are negligible. This remains true even at couplings of the order of the bandwidth and when second-neighbor hopping t' is present [13]. QMC size effects become important at half-filling below a crossover temperature T_X where the renormalized-classical regime appears. Even though (3.5) for $U_{\rm sp}$ fails at $n = 1$, $t' = 0$ in this regime, by assuming that $\langle n_\uparrow n_\downarrow \rangle$ is temperature independent below T_X one obtains a qualitatively correct description of the renormalized-classical regime. The universality class of our theory, however, is $O(N = \infty)$ instead of $O(N = 3)$ [14]. A rough estimate of the renormalized chemical potential (or equivalently of $\Sigma^{(1)}$), is given in the appendix.

3.2 Second Step: An Improved Self-Energy $\Sigma^{(2)}$

Collective modes are less influenced by details of the single-particle properties than the other way around. We thus wish now to obtain an improved approximation for the self-energy that takes advantage of the fact that we have found accurate approximations for the low-frequency spin and charge fluctuations. We begin from the general definition of the self-energy (Eq. 2.4) obtained from Dyson's equation. The right-hand side of that equation can be obtained either from a functional derivative with respect to an external field that is diagonal in spin, as in our generating function (Eq. 2.1), or by a functional derivative of $\langle \psi_{-\sigma}(1)\psi^\dagger_\sigma(2)\rangle_{\phi_t}$ with respect to a transverse external field ϕ_t. These two approaches will be considered in turn below. They give a self-energy formula that takes into account, respectively, longitudinal and transverse fluctuations. Crossing symmetry, rotational symmetry and sum rules will dictate the final formula for the improved self-energy $\Sigma^{(2)}$ that will be presented at the end of the subsection on the consistency check.

3.2.1 Longitudinal Channel

The right-hand side of the general definition of the self-energy (Eq. 2.4) may be written as

$$\Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},2) = -U\left[\left.\frac{\delta G_\sigma(1,2;\{\phi\})}{\delta\phi_{-\sigma}(1^+,1)}\right|_{\{\phi\}=0} - G_{-\sigma}(1,1^+)G_\sigma(1,2)\right]. \quad (3.9)$$

The last term is the Hartree–Fock contribution. It gives the exact result for the self-energy in the limit $\omega \to \infty$ [4]. The $\delta G_\sigma/\delta\phi_{-\sigma}$ term is thus a contribution to lower frequencies and it comes from the spin and charge fluctuations. Right-multiplying the last equation by G^{-1} and replacing the lower energy part $\delta G_\sigma/\delta\phi_{-\sigma}$ by its general expression in terms of irreducible

vertices (Eq. 2.7) we find

$$\Sigma_\sigma^{(2)}(1,2) = UG_{-\sigma}^{(1)}(1,1^+)\delta(1-2) - UG_\sigma^{(1)}(1,\bar{3})\left[\frac{\delta\Sigma_\sigma^{(1)}(\bar{3},2;\{\phi\})}{\delta G_{\bar{\sigma}}^{(1)}(\bar{4},\bar{5};\{\phi\})}\bigg|_{\{\phi\}=0}\frac{\delta G_{\bar{\sigma}}^{(1)}(\bar{4},\bar{5};\{\phi\})}{\delta\phi_{-\sigma}(1^+,1)}\bigg|_{\{\phi\}=0}\right]. \quad (3.10)$$

Every quantity appearing on the right-hand side of that equation has been taken from the TPSC results. This means in particular that the irreducible vertices $\delta\Sigma_\sigma^{(1)}/\delta G_{\sigma'}^{(1)}$ are at the same level of approximation as the Green functions $G_\sigma^{(1)}$ and self-energies $\Sigma_\sigma^{(1)}$. In approaches that assume that Migdal's theorem applies to spin and charge fluctuations, one often sees renormalized Green functions $G^{(2)}$ appearing on the right-hand side along with unrenormalized vertices, $\delta\Sigma_\sigma/\delta G_{\sigma'} \to U$.

In terms of $U_{\rm sp}$ and $U_{\rm ch}$ in Fourier space, the above formula [5] reads

$$\Sigma_\sigma^{(2)}(k)_{\rm long} = Un_{-\sigma} + \frac{U}{4}\frac{T}{N}\sum_q\left[U_{\rm sp}\chi_{\rm sp}^{(1)}(q) + U_{\rm ch}\chi_{\rm ch}^{(1)}(q)\right]G_\sigma^{(1)}(k+q). \quad (3.11)$$

3.2.2 Transverse Channel

In the transverse channel, the calculation basically has to be redone from scratch. It is closely analogous to the attractive Hubbard model case, for which detailed calculations have been published [7]. We will thus be concise. The generating function in a transverse field is

$$\ln Z[\phi_t] = \ln {\rm Tr}\left[e^{-\beta(\widehat{H}-\mu\widehat{N})}{\rm T}_\tau\left(e^{-\psi_\uparrow^\dagger(\bar{1})\phi_-(\bar{1},\bar{2})\psi_\downarrow(\bar{2})-\psi_\downarrow^\dagger(\bar{1})\phi_+(\bar{1},\bar{2})\psi_\uparrow(\bar{2})}\right)\right]. \quad (3.12)$$

The corresponding spin-space matrix Green function

$$\mathbf{G}(1,2;\{\phi_t\}) = -\begin{pmatrix}\langle\psi_\uparrow(1)\psi_\uparrow^\dagger(2)\rangle_{\phi_t} & \langle\psi_\uparrow(1)\psi_\downarrow^\dagger(2)\rangle_{\phi_t}\\ \langle\psi_\downarrow(1)\psi_\uparrow^\dagger(2)\rangle_{\phi_t} & \langle\psi_\downarrow(1)\psi_\downarrow^\dagger(2)\rangle_{\phi_t}\end{pmatrix} \quad (3.13)$$

obeys the matrix Dyson equation

$$\mathbf{G}^{-1}(1,2;\{\phi_t\}) = \mathbf{G}_0^{-1}(1-2) - \mathbf{\Sigma}(1,2;\{\phi_t\}) - \Phi_t \quad (3.14)$$

with

$$\Phi_t = \begin{pmatrix}0 & \phi_-\\ \phi_+ & 0\end{pmatrix} \quad (3.15)$$

and

$$\begin{aligned}&\mathbf{\Sigma}\,(1,\bar{1};\{\phi_t\})\,\mathbf{G}\,(\bar{1},2;\{\phi_t\})\\&\quad\equiv -U\begin{pmatrix}\langle\psi_\downarrow^\dagger(1^+)\psi_\downarrow(1)\psi_\uparrow(1)\psi_\uparrow^\dagger(2)\rangle_{\phi_t} & \langle\psi_\downarrow^\dagger(1^+)\psi_\downarrow(1)\psi_\uparrow(1)\psi_\downarrow^\dagger(2)\rangle_{\phi_t}\\ \langle\psi_\uparrow^\dagger(1^+)\psi_\uparrow(1)\psi_\downarrow(1)\psi_\uparrow^\dagger(2)\rangle_{\phi_t} & \langle\psi_\uparrow^\dagger(1^+)\psi_\uparrow(1)\psi_\downarrow(1)\psi_\downarrow^\dagger(2)\rangle_{\phi_t}\end{pmatrix}.\end{aligned}\tag{3.16}$$

We need to obtain, in turn, the renormalized vertex $U_{\rm sp}$ (Eq. 3.5), and finally find an improved formula for the self-energy $\Sigma^{(2)}$. Starting from the matrix equation $\mathbf{G}\mathbf{G}^{-1}=\mathbf{1}$ and following the procedure below (Eq. 2.5), one of the two response functions that do not vanish in zero external field obeys

$$\begin{aligned}\left.\frac{\delta G_{21}(1,2;\{\phi_t\})}{\delta\phi_+(3,4)}\right|_{\{\phi_t\}=0} &= G_{22}(1,3)G_{11}(4,2)\\&\quad+G_{22}(1,\bar{2})\left.\frac{\delta\Sigma_{21}(\bar{2},\bar{3};\{\phi_t\})}{\delta G_{21}(\bar{6},\bar{7};\{\phi_t\})}\right|_{\{\phi_t\}=0}\left.\frac{\delta G_{21}(\bar{6},\bar{7};\{\phi_t\})}{\delta\phi_+(3,4)}\right|_{\{\phi_t\}=0}G_{11}(\bar{3},2),\end{aligned}\tag{3.17}$$

where the subscripts denote matrix elements in spin-space. There is an analogous equation for $\delta G_{12}(1,2)/\delta\phi_-(3,4)$. Note that

$$\begin{aligned}\delta G_{21}(1,1)/\delta\phi_+(2,2) &= -\langle S_+(1)S_-(2)\rangle\\&= -\langle\psi_\uparrow^\dagger(1)\psi_\downarrow(1)\psi_\downarrow^\dagger(2)\psi_\uparrow(2)\rangle = -\chi_{+-}(1,2).\end{aligned}\tag{3.18}$$

The usual Hartree–Fock factorization for the self-energy would transform (3.17) into the RPA equation for transverse spin fluctuations $\langle S_+(1)S_-(2)\rangle$.

The value of $\Sigma^{(1)}$ and of the corresponding vertices at the TPSC level are obtained using steps analogous to those in the longitudinal channel. We factor the self-energy in the Hartree–Fock manner,

$$\begin{aligned}&\mathbf{\Sigma}^{(1)}(1,\bar{1};\{\phi_t\})\mathbf{G}^{(1)}(\bar{1},2;\{\phi_t\})\\&\qquad=-A_{\{\phi_t\}}\begin{pmatrix}G_{22}^{(1)}(1,1^+;\{\phi_t\}) & -G_{12}^{(1)}(1,1^+;\{\phi_t\})\\ -G_{21}^{(1)}(1,1^+;\{\phi_t\}) & G_{11}^{(1)}(1,1^+;\{\phi_t\})\end{pmatrix}\\&\qquad\qquad\begin{pmatrix}G_{11}^{(1)}(1,2;\{\phi_t\}) & G_{12}^{(1)}(1,2;\{\phi_t\})\\ G_{21}^{(1)}(1,2;\{\phi_t\}) & G_{22}^{(1)}(1,2;\{\phi_t\})\end{pmatrix}\end{aligned}\tag{3.19}$$

but we correct this factorization by the factor $A_{\{\phi_t\}}$ which is determined in such a way that when $2\to 1^+$ the exact result for the four point function on the right-hand side of (3.16) is recovered. Using

$$\langle\psi_\downarrow^\dagger(1^+)\psi_\downarrow(1)\psi_\uparrow(1)\psi_\downarrow^\dagger(1^+)\rangle_{\phi_t}=\langle\psi_\downarrow^\dagger(1^+)\psi_\downarrow^\dagger(1^+)\psi_\downarrow(1)\psi_\uparrow(1)\rangle_{\phi_t}=0$$

and the analogous result for the other off-diagonal element, we obtain the exact result for $2 \to 1^+$:

$$\mathbf{\Sigma}^{(1)}(1,\bar{1};\{\phi_t\})\mathbf{G}^{(1)}(\bar{1},1^+;\{\phi_t\}) = U \begin{pmatrix} \langle n_\downarrow(1) n_\uparrow(1)\rangle_{\phi_t} & 0 \\ 0 & \langle n_\uparrow(1) n_\downarrow(1)\rangle_{\phi_t} \end{pmatrix}. \quad (3.20)$$

Equating with the right-hand side of the approximate result (Eq. 3.19) when $2 \to 1^+$ determines the value of $A_{\{\phi_t\}}$ by a simple 2×2 matrix inversion. From this, one extracts the off-diagonal component of the self-energy and the corresponding irreducible vertex that is needed for response functions in (3.17):

$$\left.\frac{\delta\Sigma_{21}^{(1)}(1,2;\{\phi_t\})}{\delta G_{21}^{(1)}(3,4;\{\phi_t\})}\right|_{\{\phi_t\}=0} = -U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\delta(1-3)\delta(1-2)\delta(1-4). \quad (3.21)$$

Substituting in the equation for the response function (Eq. 3.17), one precisely recovers for the transverse spin fluctuations the same TPSC result as for the longitudinal fluctuations: $\chi_{\rm sp}^{-1}(q) = \chi_0^{-1}(q) - \frac{1}{2}U_{\rm sp}$ with $U_{\rm sp}$ given by (3.5). The determination of $U_{\rm sp}$ through the fluctuation-dissipation theorem leads again to (3.7). We thus recover the results expected from rotational invariance.

To move to the second level of approximation for the self-energy, we return to the exact definition for the self-energy (3.16) but this time in zero applied external field. The first diagonal component can be written as

$$\Sigma_{11}(1,2) = U\left.\frac{\delta G_{21}(1,\bar{2};\{\phi_t\})}{\delta\phi_+(1^+,1)}\right|_{\{\phi_t\}=0} G_{11}^{-1}(\bar{2},2). \quad (3.22)$$

If we use the exact result for the transverse response (Eq. 3.17), this takes the form

$$\Sigma_{11}(1,2) = UG_{22}(1,1^+)\delta(1-2) + UG_{22}(1,\bar{3})\left.\frac{\delta\Sigma_{21}(\bar{3},2;\{\phi_t\})}{\delta G_{21}(\bar{6},\bar{7};\{\phi_t\})}\right|_{\{\phi_t\}=0}\left.\frac{\delta G_{21}(\bar{6},\bar{7};\{\phi_t\})}{\delta\phi_+(1^+,1)}\right|_{\{\phi_t\}=0}, \quad (3.23)$$

where, as in the longitudinal case, the high-frequency Hartree–Fock result is now explicit. Substituting on the right-hand side the TPSC (i.e., level 1) results, we obtain an improved approximation for the self-energy due to transverse spin fluctuations. In momentum space, it reads

$$\Sigma_\sigma^{(2)}(k)_{\rm trans} = Un_{-\sigma} + \frac{U}{2}\frac{T}{N}\sum_q [U_{\rm sp}\chi_{\rm sp}^{(1)}(q)t]G_{-\sigma}^{(1)}(k+q). \quad (3.24)$$

3.3 Internal Accuracy Check

The equation (3.2) that relates $\mathrm{Tr}[\Sigma G]$ to double occupancy (potential energy) relates purely single-particle quantities, Σ and G, to a quantity that may be computed from two-particle quantities, namely, spin and charge correlation functions. In our approach, it can be checked [4] that $\frac{1}{2}\,\mathrm{Tr}[\Sigma^{(2)}G^{(1)}]$ is exactly equal to $U\langle n_\uparrow n_\downarrow\rangle$, with $\langle n_\uparrow n_\downarrow\rangle$ computed at the TPSC level. More specifically, we find,

$$\tfrac{1}{2}\,\mathrm{Tr}[\Sigma^{(2)}G^{(1)}] = \lim_{\tau\to 0^-}\frac{T}{N}\sum_k \Sigma^{(2)}_\sigma(k)G^{(1)}_\sigma(k)e^{-ik_n\tau} = U\langle n_\uparrow n_\downarrow\rangle. \qquad (3.25)$$

One can use the difference between $\frac{1}{2}\,\mathrm{Tr}[\Sigma^{(2)}G^{(1)}]$ and $\frac{1}{2}\,\mathrm{Tr}[\Sigma^{(2)}G^{(2)}]$ as an internal accuracy check of the theory. In the pseudogap regime at $n = 1$ for example, the breakdown of the theory is clearly indicated by the growing difference between the two quantities. Reference [8] gives a detailed table that illustrates these facts in the case of the attractive Hubbard model.

The $\mathrm{Tr}[\Sigma^{(2)}G^{(1)}]$ formula can also be used to help in the interpretation of the two different results obtained above for the self-energy (Eqs. 3.10 and 3.23). Without the approximation that the TPSC results should be used on the right-hand side, the results that follow from the corresponding exact expressions (Eqs. 3.10 and 3.23) would be identical. To resolve this problem, we follow [17]. Figure 1 of this paper shows the self-energy in terms of the fully reducible vertex $\Gamma(q, k-k', k+k'-q)$. In both formulas for the self-energy (Eqs. 3.11 and 3.24), the dependence of Γ on the particle-particle channel center of mass momentum $k+k'-q$ is neglected since this channel is not singular. The longitudinal version of the self-energy (Eq. 3.11) takes good care of the singularity of Γ when its first argument q is near (π,π). The transverse version does the same for the singular dependence near (π,π) of the second argument $k-k'$, which corresponds to the other particle-hole channel. One then expects that averaging the two possibilities gives a better approximation for Γ since it preserves crossing symmetry in the two particle-hole channels. Furthermore, one can verify that the longitudinal spin fluctuations in (3.11) contribute an amount $U\langle n_\uparrow n_\downarrow\rangle/2$ to the consistency condition $\frac{1}{2}\,\mathrm{Tr}(\Sigma^{(2)}_{\mathrm{long}}G^{(1)}) = U\langle n_\uparrow n_\downarrow\rangle$ and that each of the two transverse spin components also contribute $U\langle n_\uparrow n_\downarrow\rangle/2$ to $\frac{1}{2}\,\mathrm{Tr}(\Sigma^{(2)}_{\mathrm{trans}}G^{(1)}) = U\langle n_\uparrow n_\downarrow\rangle$. Hence, averaging (3.11) and the expression in the transverse channel (3.24) also preserves rotational invariance. In addition, one verifies numerically that the exact sum rule [4] $-\int d\omega'\ \mathrm{Im}[\Sigma_\sigma(\mathbf{k},\omega')]/\pi = U^2 n_{-\sigma}(1-n_{-\sigma})$ determining the high-frequency behavior is satisfied to a higher degree of accuracy. We thus obtain a self-energy formula that we

called [17] "symmetric":

$$\Sigma_\sigma^{(2)}(k)_{\rm sym} = Un_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_q [3U_{\rm sp}\chi_{\rm sp}^{(1)}(q) + U_{\rm ch}\chi_{\rm ch}^{(1)}(q)]G_\sigma^{(1)}(k+q). \quad (3.26)$$

$\Sigma_\sigma^{(2)}(k)_{\rm sym}$ is different from so-called Berk–Schrieffer type expressions [15] that do not satisfy [4] the consistency condition between one- and two-particle properties, $\frac{1}{2}\,{\rm Tr}(\Sigma G) = U\langle n_\uparrow n_\downarrow\rangle$.

4 Discussion and Extensions

The approach described above is valid in the weak to intermediate coupling regime. It involves two steps. First, a self-consistent determination of double-occupancy and renormalized vertices that enter the dynamical susceptibilities of the most important four-point correlation functions (density-density and spin-spin correlation functions). This is summarized by (3.5), (3.7), and (3.8). Conservation laws, such as charge and spin conservation, are satisfied. These results are then used to obtain an improved approximation for single-particle properties through the self-energy (Eq. 3.26). An internal accuracy check allows one to decide on the validity of the results in cases where QMC or other exact results are not available as references. The approach satisfies the Pauli principle, the Mermin–Wagner theorem, contains Kanamori–Brueckner screening, and does not assume a Migdal theorem in the calculation of the self-energy.

In addition to provide an accurate calculational tool for the Hubbard model, this methodology has allowed us to develop insight into the physics of this model. The physically most important result obtained to date is probably the detailed description of the physics of the pseudogap that appears *in two dimensions* in the renormalized-classical regime ($\hbar\omega \ll k_B T$) when the antiferromagnetic correlation length (superconducting correlation length in the case of the attractive model) becomes larger than the single particle thermal de Broglie wavelength [4, 5]. This physics explains a possible route to the destruction of the Fermi liquid in *two dimensions*. These results have been confirmed by extensive QMC calculations [12, 16, 17]. The pseudogap (depletion near $\omega = 0$) in ${\rm Im}\, G_\sigma^R(\mathbf{k}_F, \omega)$ appears along with precursors of the Bogoliubov quasiparticles (finite ω peaks) of the ordered state. To extrapolate more deeply in the pseudogap regime, where strictly speaking the above method fails, one assumes that double-occupancy becomes temperature independent below the crossover temperature T_X where one enters the renormalized-classical regime.

The above methodology has been applied successfully to the attractive Hubbard model [7, 8, 18]. It trivially applies to the Hubbard model with an

arbitrary hopping matrix. $\Sigma^{(2)}$ can also be used to obtain consistent thermodynamic predictions [19]. Extensions to multiband problems are nontrivial but are being developed [20]. Recently an extension of this approach has been used to obtain quantitative results for the spin and charge susceptibilities in the attractive Hubbard model [21]. Proceeding along the same lines for the repulsive Hubbard model, pairing correlations have been calculated [22]. They yield a dome shape dependence on doping of the d-wave superconductivity transition temperature T_c. The decrease of T_c near half-filling comes from the detrimental effect of opening a pseudogap. Phenomenological extensions to more complicated models with d-wave superconductivity and antiferromagnetism have also been proposed [23]. Future directions include generalizations to the pseudogap regime, to states with broken symmetry, [24] to longer-range interactions and to impurity models. It would also be extremely valuable to obtain the irreducible vertices $\delta\Sigma_\sigma^{(2)}/\delta G_{\sigma'}^{(2)}$ that are consistent with the best estimate of the self-energy.

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Appendix A An Approximate Formula for $\Sigma^{(1)}$

The equation (3.2) that was used to obtain finally

$$U_{\rm sp} = U\langle n_\uparrow n_\downarrow\rangle/(\langle n_\downarrow\rangle\langle n_\uparrow\rangle)$$

would be different if we had taken the limit $2 \to 1^-$ instead of $2 \to 1^+$ in the general expression for ΣG (Eq. 2.4). More specifically, at $\{\phi\} = 0$,

$$\begin{aligned}\Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},1^+) &= U\langle n_\downarrow(1)n_\uparrow(1)\rangle;\\ \Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},1^-) &= U\langle n_\downarrow(1)(n_\uparrow(1)-1)\rangle.\end{aligned} \tag{A.1}$$

Any approximation for the self-energy that has Hartree–Fock as its infinite-frequency limit will be such that the difference between the above two results, $\Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},1^+) - \Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},1^-) = U\langle n_\downarrow(1)\rangle$ is satisfied. The proof [7, (44)] is as follows:

$$\begin{aligned}\frac{T}{N}\sum_{\mathbf{k}}\sum_{ik_n}\left(\frac{\Sigma(\mathbf{k},ik_n)}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)-\Sigma(\mathbf{k},ik_n)}-\frac{U\langle n_\downarrow\rangle}{ik_n}\right)\left(e^{-ik_n0^-}-e^{-ik_n0^+}\right)\\ +\frac{T}{N}\sum_{\mathbf{k}}\sum_{ik_n}\left[\frac{U\langle n_\downarrow\rangle}{ik_n}\left(e^{-ik_n0^-}-e^{-ik_n0^+}\right)\right]=U\langle n_\downarrow\rangle.\end{aligned} \tag{A.2}$$

In this expression, the first sum vanishes because we have added and subtracted a term that makes it convergent at infinity without the need for convergence factors $e^{-ik_n0^\pm}$. Hence, only the last sum survives.

Since $\Sigma^{(1)}_\sigma(1,2)$ is a constant times $\delta(1-2)$, one can obtain two estimates of the constant depending on which of the two equations in (A.1) one starts from. By analogy with (A.2) one expects that the difference between these two estimates is related to the high-frequency behavior of the true result while the average of the two estimates is related to the low-frequency behavior. This average is

$$\frac{n}{2}\big(U+U_{\rm sp}(1-n)\big)\frac{1}{2-n}. \tag{A.3}$$

The exact result, $U/2$, is recovered at $n = 1$. For other fillings, the above formula gives a very rough estimate of the chemical potential shift induced by interactions. For example, for U up to $4t$ on 8×8 lattices and temperatures of order $t/4$ in energy units, one finds results that deviate by up to 20% from the QMC results. The corresponding procedure in the *attractive* Hubbard model case [7] seems to work better.