Nearest-Neighbor Repulsion and Competing Charge and Spin Order in the Extended Hubbard Model.

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We generalize the two-particle self-consistent approach (TPSC) to study the extended Hubbard model, where nearest-neighbor interaction is present in addition to the usual local screened interaction. Similarities and differences between the TPSC approach and the Singwi Tosi Land Sj\’olander (STLS) approximation for the electron gas are discussed. The accuracy of our extension of TPSC is assessed by comparisons with Quantum Monte Carlo calculations of Y. Zhang and J. Callaway, Phys. Rev. B 39, 9397 (1989). We observe that a positive off-site interaction enhances staggered charge fluctuations and reduces staggered magnetic order.

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I. INTRODUCTION

The electron gas with long-range Coulomb repulsion and the Hubbard model with screened on-site repulsion are two widely studied models that each describe large classes of materials. Both models are generally studied with quite different theoretical methods. However, by gradually increasing the range of the interaction in the Hubbard model and by reducing the density to average out lattice effects, one should be able to go continuously from the Hubbard to the Coulomb gas model. Is there one unified theoretical framework that allows us to treat both limiting cases?

To begin to answer this question, we generalize the Two-Particle Self-Consistent approach (TPSC)\textsuperscript{1,2} to study the extended Hubbard model, that includes nearest-neighbor repulsion in addition to the usual on-site repulsion. This model is interesting in its own right, independently of the above-mentioned theoretical question. Indeed, the extended Hubbard model allows one to study materials where competition between charge and spin order manifest themselves. In high-temperature superconductors, where screening is not perfect, understanding the extended Hubbard model is also of paramount importance.

Let us first motivate further our focus on the TPSC approach and then come back to the interesting physical phenomena that manifest themselves in the extended Hubbard model. Judging from comparisons with benchmark Quantum Monte Carlo calculations\textsuperscript{1,2,3,4,5,6} (in the absence of exact solutions), the TPSC approach provides us with the most accurate approximate solution to the Hubbard model at weak to intermediate coupling. A detailed critical comparison with other methods such as the Random Phase Approximation (RPA), the self-consistent renormalized theory and the fluctuation-exchange approximation is given in Ref.\textsuperscript{2}. In particular, TPSC satisfies the Pauli principle, the Mermin-Wagner theorem in two-dimensions includes Kanamori-Br"uckner screening and is non-perturbative although limited to interaction strengths less than the bandwidth. The TPSC approach is a close relative to the Singwi, Tosi, Land, Sj\’olander (STLS) method\textsuperscript{8} used in the electron gas problem. The STLS approximation has been first introduced to describe the structure functions of an electron liquid where it provided much better results compared to the RPA. This approximation has been applied to a variety of systems that contain Fermions, Bosons or classical particles in all physical dimensions and different geometries. Starting with the equation of motion for one-body density operator, the authors were faced with the well-known problem that the two-body density operator appeared in their equation. They solved the problem approximately by replacing the two-body density operator by a product of two one-body density operators and then correcting the result with the pair correlation function. The result of this factorization appears as a correction in the response functions of the system, the so-called local field factor. This factor is then determined by using a sum-rule derived from the fluctuation-dissipation theorem. The present paper will give a new point of view on the STLS method by comparing it to the TPSC approach. As we will show in more details, the main difference between the latter method and the STLS one, is the way we factorize the two-body density operator. It seems that for local vs non-local potentials, it is more accurate to use, respectively, local or non-local factorization and, as we will show in detail, a local factorization leads to better results for the extended Hubbard model. That is not all. It will become clear in the formalism used to derive TPSC that the STLS method also neglects some higher-order correlation functions. The same type of approximation will be necessary to be able to generalize TPSC to treat the extended Hubbard model. Otherwise, as in STLS, there is a shortage of sum-rules or conditions to find all unknowns that appear in the method.

We believe that accuracy of the approximation is crucial for a real understanding of physical properties and for meaningful comparisons to experiments. Bad approximations that agree with experiment only lead us astray. That is why we will benchmark our extension of
the TPSC approach against the highly accurate results that can obtained by Quantum Monte Carlo (QMC) simulations. We will carefully analyze the approximations involved in the method and discuss other possibilities for improvement.

Back to the extended Hubbard model. This model has a long history, so we can only discuss a small sample of the relevant literature. At half-filling, when the on-site interaction strength \( U \) tends to infinity so that super-exchange \( 4t^2/U \) vanishes, the effect of the nearest-neighbor repulsion \( V \) is to lead to an effective ferromagnetic interaction between localized spins. This is the physics of the so-called direct-exchange mechanism. The physics is quite different when \( U \) and \( 4V \) are of the same order and both in the weak to intermediate-coupling regime, namely less than or of the order of the bandwidth \( (W = 8t \text{ in } d = 2) \). In that case, there is a competition between staggered charge and spin orders. That charge ordering phenomenon is particularly relevant for manganites, vanadates and various organic conductors, as discussed in a recent theoretical paper that uses a new correlator-projection method. The relevant theoretical literature for these compounds focuses on the square lattice and on ladders for the quarter-filled case. The competition between charge and spin orders has also been studied in one-\(11,12,13\), two-\(14,15\), three-\(16,17,18\), two\(19,20,21\), three\(22\) and higher dimensions\(23\) at various fillings. The combined effect of charge fluctuations in addition to the usual spin fluctuation in favouring one type or another of unconventional superconductivity has also been studied using this model\(24,25,26\).

In the present paper, we are interested in the possibility that a generalization of TPSC to the extended Hubbard model can lead us to accurate estimations of the charge and spin structure factors and susceptibilities at finite temperature. We will use the QMC calculations of Ref. (30) as a benchmark. We note that methods that have been quite successful in one- or infinite dimension are generally not applicable in the two-dimensional case that we will consider. In \( d = 2 \), continuous symmetries can be broken only at zero temperature and, in addition, wave-vector dependencies that are neglected in high-dimension are generally not negligible.

In the following, we first present the theory and give the details of the calculation based on the functional derivative of the Dyson equation which gives us the response functions of the system. We also provide the equation of motion for the Wigner distribution function to show that the two different methods basically lead to the same set of equations. This also allows us to discuss the different types of factorizations. In Sec. II we present the results of our numerical calculations and compare them with QMC results to find the region where the method works properly or is precise enough. Finally, we discuss the influence of nearest-neighbor interaction \( V \) on spin and charge fluctuations.

**II. THEORY**

We first introduce the extended Hubbard Hamiltonian,

\[
H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle \sigma \sigma'} n_{i\sigma} n_{j\sigma'} - \mu \sum_{i} n_{i}
\]  

where \( c_{i\sigma} \) (\( c_{i\sigma}^\dagger \)) are annihilation (creation) operator for electrons of spin \( \sigma \) at site \( i \), \( n_{i\sigma} \) is the density operator, and \( t \) is the hopping matrix element. The quantities \( U \) and \( V \) are the on-site and nearest-neighbor interactions respectively and \( \mu \) is the chemical potential. Although we restrict ourselves to nearest-neighbor hopping, the generalization to an arbitrary hopping matrix \( t_{i,j} \) will be obvious to the reader. It only modifies the non-interacting dispersion relation. One can generalize the formalism to a system with longer interaction terms and also to a system with many bands. In the following, we first derive the TPSC approach using functional derivatives and then return to the approach that is more usual with the STLS approximation, namely the equation of motion for the one-body Wigner distribution function. These two derivations allow a deeper insight into the nature of the approximations. The reader may also choose the approach he is more familiar with.

**A. Functional derivative approach**

Following functional methods of the Schwinger school, we begin with the generating function \( Z[\phi_\sigma] \) with source fields \( \phi_\sigma \) in the grand canonical ensemble

\[
Z[\phi_\sigma] = -\text{Tr} [e^{-\beta H T \tau} S(\beta)]
\]  

where \( \beta = 1/T \), \( T \) is the temperature while \( S \) is defined as follows

\[
\ln S(\beta) = -\sum_{i,j,\sigma} \int_{0}^{\beta} d\tau d\tau' c_{i\sigma}^\dagger(\tau) c_{j\sigma}(\tau') \phi_{\sigma}(i,j,\tau,\tau')
\]  

where the brackets \( \langle \rangle \) represents a thermal average in the canonical ensemble, \( T \) is the time-ordering operator, and \( \tau \) is the imaginary time. The Green function can be calculated from the first functional derivative of the
where we have introduced the short-hand 1 to stand for both the site position and the corresponding imaginary time, as in the equation

\[
G_\sigma(1, 2) = - \left\langle T_\tau c_\sigma(\tau_1) c_\sigma^\dagger(\tau_2) \right\rangle = - \left\langle T_\tau c_\sigma(1) c_\sigma^\dagger(2) \right\rangle. 
\]

The equation of motion for the Green function has the following form \cite{31,33},

\[
G_\sigma(1, 2) = G_0^{-1}(1, 2) - \phi_\sigma(1, 2) - \Sigma_\sigma(1, 2),
\]

with the self-energy

\[
\Sigma_\sigma(1, 2) = - U \left\langle T_\tau c_\sigma^\dagger(1) c_\sigma(1) c_\sigma^\dagger(3) \right\rangle G_\sigma^{-1}(3, 2) = U \sum_{\sigma', a} \left\langle T_\tau c_{\sigma'}^\dagger(1 + a + 1) c_{\sigma'}(1 + a + 1) c_{\sigma'}(1) c_{\sigma'}^\dagger(3) \right\rangle G_\sigma^{-1}(3, 2).
\]

where \(\Sigma_\sigma(1, 2)\) is the equal-time pair correlation function which is related to the probability of finding one electron with spin \(\sigma'\) on site \(j\) when another electron with spin \(\sigma\) is held on site \(i\). More specifically,

\[
g_{\sigma\sigma'}(1, 2) \equiv \frac{\left\langle T_\tau c_\sigma^\dagger(1) c_\sigma(1) c_\sigma^\dagger(2) c_{\sigma'}(2) \right\rangle}{\left\langle T_\tau c_\sigma^\dagger(1) c_\sigma(1) \right\rangle} = \frac{\langle n_{\sigma'}(1) n_{\sigma'}(2) \rangle - \langle n_{\sigma'}(1) \rangle \langle n_{\sigma'}(2) \rangle}{\langle n_{\sigma'}(1) \rangle}.
\]

which is used in the STLS approximation. Further factorizations and additional details will be discussed in the following sections.

We want to calculate the spin and charge response functions. These can be obtained from the first functional derivative of the Green function with respect to the external source field. Taking the functional derivative on both sides of the identity \(G_\sigma(1, 3) G_\sigma^{-1}(3, 2) = \delta_{\sigma\sigma'} \delta(1, 2)\) and using the Dyson equation Eq. (7), we obtain the exact result

\[
\Pi_{\sigma\sigma'}(1, 2; 3, 3) \equiv - \frac{\delta G_\sigma(1, 2)}{\delta \phi_{\sigma'}(3, 3)} = G_\sigma(1, 4) \frac{\delta G_\sigma^{-1}(4, 5)}{\delta \phi_{\sigma'}(3, 3)} G_\sigma(5, 2)
\]

\[
= - \delta_{\sigma\sigma'} G_\sigma(1, 3) G_\sigma(3, 2) - \sum_{\sigma''} G_\sigma(1, 4) \frac{\delta \Sigma_{\sigma''}(4, 5)}{\delta G_{\sigma''}(6, 7)} \frac{\delta G_{\sigma''}(6, 7)}{\delta \phi_{\sigma''}(3, 3)} G_\sigma(5, 2).
\]
In turn, the first functional derivative of the self-energy with respect to the Green function can be evaluated from our approximate expression for the self-energy Eq. (9)

\[
\frac{\delta \Sigma_\sigma(4,5)}{\delta G_{\sigma'}(6,7)} = U \delta_{\sigma\sigma'} \delta(4,5) \delta(4,6) \delta(5,7) g_{\sigma\sigma}(4,4) + V \sum_a \delta(4,5) \delta(4 + a, 6) \delta(5 + a, 7) g_{\sigma\sigma}(4,4 + a) \\
+ U \delta(4,5) g_\sigma(4,4^+) \frac{\delta g_{\sigma\sigma}(4,4)}{\delta G_{\sigma'}(6,7)} + V \delta(4,5) \sum_{\sigma'', a} G_{\sigma''}(4,4^+) \frac{\delta g_{\sigma\sigma''}(4,4 + a)}{\delta G_{\sigma'}(6,7)}.
\]

The functional derivative of the pair correlation function with respect to the Green function is a three-body (six-point) correlation function that is not known. For the standard Hubbard model, it was shown that the unknown functional derivative (third term in the above equation) appears only in the charge response function. The authors in Ref. \[13\] approximated this functional by a constant whose value was obtained by enforcing the Pauli principle expressed as a sum-rule on spin and charge correlation functions. In our case, two other unknown functions that come from the last term in the above equation, appear in both the charge and spin response functions. We assume, and confirm with the numerical results of the following section, that these two unknown functionals do not give important contributions as long as \(4V\) is small compared to the bandwidth. Their contribution becomes more significant as \(V\) increases. By approximating the two unknown functions by two different constants, it should be possible to obtain them by using two extra sum-rules, such as the compressibility and spin susceptibility sum-rules. We leave this for future work and, at this point, we simply drop the \(\delta g_{\sigma\sigma''}(4,4 + a)/\delta G_{\sigma'}(6,7)\) term in the last line.

The spin and charge part of \(\Pi\) can now be obtained by combining Eqs. (11) and (12) in the form

\[
\Pi_{cc, ss}(1, 2; 3, 3) \equiv \sum_{\sigma\sigma'} (\sigma\sigma') \Pi_{\sigma\sigma'}(1, 2; 3, 3) = 2 [\Pi_{\sigma\sigma}(1, 2; 3, 3) \pm \Pi_{\sigma\bar{\sigma}}(1, 2; 3, 3)] \\
= -2G_\sigma(1, 3)G_\sigma(3, 2) - 2UG_\sigma(1, \bar{4})G_\sigma(\bar{4}, 2) g_{\sigma\bar{\sigma}}(\bar{4}, \bar{3}) \left[ \frac{\delta g_{\sigma}(\bar{4}, \bar{3})}{\delta \phi_{\bar{\sigma}}(3, 3)} \pm \frac{\delta G_\sigma(\bar{4}, \bar{3})}{\delta \phi_{\bar{\sigma}}(3, 3)} \right] \\
-2VG_\sigma(1, \bar{4})G_\sigma(\bar{4}, 2) \sum_{\sigma', a} g_{\sigma\sigma'}(\bar{4}, \bar{3} + a) \left[ \frac{\delta G_\sigma(\bar{4} + a, \bar{3} + a^+)}{\delta \phi_{\bar{\sigma}}(3, 3)} \pm \frac{\delta g_{\sigma\sigma'}(\bar{4}, \bar{3} + a)}{\delta \phi_{\bar{\sigma}}(3, 3)} \right].
\]

where \(\sigma = \pm\) (the third identity in the above equation is valid for a spin-unpolarized system).

To obtain the response functions of the system, we set the external potential to zero. When the minus sign (corresponding to the spin response function) is chosen in the last term, it drops out by rotational invariance in zero source fields. For the plus sign (corresponding to the charge response function), we assume that the functional derivative of the pair correlation respect to the density is a constant (after using an extra chain rule in the above equation). The final form of the charge and spin response functions, or equivalently susceptibilities, in Fourier space then have the following forms

\[
\chi_{cc}(q, \omega_n) = \frac{\chi^0(q, \omega_n)}{1 + \frac{\chi^0(q, \omega_n)}{2} U_{cc}(q)}
\]

where

\[
U_{ss}(q) = U g_{\sigma\bar{\sigma}}(0) - 4V g_{ss}(a) \sum_\alpha \cos(q_\alpha a),
\]

\[
U_{cc}(q) = U \left( g_{\sigma\bar{\sigma}}(0) + n g_{s\sigma}(0) \right) + 4V g_{cc}(a) \sum_\alpha \cos(q_\alpha a)
\]

and \(\omega_n = 2\pi n T\) is the Matsubara frequency. One can easily see the similarity of the above equations with what we had in Refs. \[12\] and also find out how easily these equations can be extended to a system with longer range of interaction and also to a system with many bands.
Finally the index \( \alpha \) takes the values \( \alpha = 1..D \), \( D \) being the dimension of the system, while the equal-time charge and spin pair correlation functions are defined by \( g_{cc,ss} = \sum_{\sigma \sigma'} \rho_{\sigma \sigma'} n_{\sigma n_{\sigma'}} / \rho \) (or simply \( g_{cc,ss}(r) = (g_{\sigma \sigma}(r) \pm g_{\sigma' \sigma'}(r))/2 \) for a spin-unpolarized system) with \( |r| = 0 \) or \( \alpha \) and \( \chi^0(q, \omega_n) \) is the response function for non-interacting electrons given by

\[
\chi^0(q, \omega_n) = \int \frac{dp}{BZ} f_0^0(p + q/2) - f_0^0(p - q/2),
\]

(18)

In the above formula \( \nu \) is the volume of the Brillouin zone (BZ), \( f_0^0(p) = 1/[1 + \exp[(\epsilon_q - \mu)/T]] \) is the Fermi-Dirac distribution function, and \( \epsilon_q = -2t \sum_{\alpha} \cos(q_{q},a) \) is the non-interacting particle dispersion relation. The pair correlation functions are related to the static structure functions by

\[
g_{cc}(r) = 1 + \frac{1}{n} \int_{BZ} \frac{d\mathbf{q}}{\nu} [S_{cc}(\mathbf{q}) - 1] \exp(i\mathbf{q} \cdot \mathbf{r})
\]

(19)

\[
g_{ss}(r) = \frac{1}{n} \int_{BZ} \frac{d\mathbf{q}}{\nu} [S_{ss}(\mathbf{q}) - 1] \exp(i\mathbf{q} \cdot \mathbf{r})
\]

(20)

where \( S_{cc,ss} = \sum_{\sigma \sigma'} \rho_{\sigma \sigma'}(\mathbf{q}) / \rho \) (or simply \( S_{ss,cc}(r) = S_{\sigma \sigma'}(r) \) for a spin-unpolarized system) are respectively the spin and charge static structure factors, with the spin-resolved static structure factor defined by \( S_{\sigma \sigma'}(r) \equiv [(\phi_{\sigma}(0) n_{\sigma}(r)) / \sqrt{n_{\sigma} n_{\sigma'}}] - \sqrt{n_{\sigma} n_{\sigma'}} \) and the Fourier transforms by,

\[
\sum_1 e^{i p r_1} \equiv \nu \delta(p), \quad \int \frac{dp}{\nu} e^{i p r_1} \equiv \delta_{r_1,0}.
\]

(21)

Finally the static structure factors are connected to the response functions by the fluctuation-dissipation theorem

\[
S_{\sigma \sigma'}(\mathbf{q}) = \frac{T}{\sqrt{n_{\sigma} n_{\sigma'}}} \sum_{\omega_n} \chi_{\sigma \sigma'}(\mathbf{q}, \omega_n).
\]

(22)

One should notice that the operators in the above equations act on some lattice sites which do not exist in the real system. Knowing that the Winger distribution functions (WDFs) are not a real physical functions we define them in this manner for the sake of simplicity in the notation. One can also define the WDFs in term of the operators which just act on the real lattice sites, but that makes the formalism a bit more tedious.

The density of particles of spin \( \sigma \) at position \( i \) is related to the OBWDF by

\[
n_{i \sigma}(\tau) = \int_{BZ} \frac{dp}{\nu} f_{i \sigma}(\mathbf{p}, \tau)
\]

(25)

with the same definitions of Fourier transforms as above, Eq. (21).

We first need to write the equation of motion for the operator \( c^\dagger \chi_{\sigma \sigma} \) to obtain the equation of motion for the OBWDF later on. This equation, after a bit of algebra,
can be written as,

\[-\frac{\partial c_{i,\sigma}}{\partial \tau} = [H, c_{i,\sigma}] = -\delta_{i}^{2}(c_{i,\sigma}) + Uc_{i,\sigma}c_{i,\sigma} + V_{i,\sigma}^{ext}c_{i,\sigma}\]

where \(\delta_{i}^{2}c_{i,\sigma}\) and \((j)_{i}\) means that the sum runs over all nearest-neighbors of site \(i\). Using the above equation, one can write the equation of motion for the OBWDF,

\[-\frac{\partial f_{i,\sigma}(p, \tau)}{\partial \tau} = -2it\sum_{\alpha} \sin(q_{\alpha})(\delta_{i}^{\alpha}f_{i,\sigma}(p, \tau)) - \sum_{l} \int_{BZ} \frac{dp_{l}}{\nu} c_{i,\sigma}(p-p_{l})r_{l}(V_{i+1/2,\sigma}^{ext} - V_{i-1/2,\sigma}^{ext})f_{i,\sigma}(p_{l}, \tau) - U\sum_{l} \int_{BZ} \frac{dp_{l}}{\nu} \int_{BZ} \frac{dp_{2}}{\nu} c_{i,\sigma}(p-p_{l}-p_{2})\delta_{i-1/2,\tau}(\delta_{i-1/2,\tau})f_{i,\sigma}(p_{l}, p_{2}, \tau).\]  

(27)

To derive the first term on the right-hand side of the above equation, we used the following identity, that we prove in the previous section, we factor the TBWDF as follows,

\[\delta_{i}^{2}(c_{i+1/2,\sigma})c_{i-1/2,\sigma} - c_{i+1/2,\sigma}\delta_{i}^{2}(c_{i-1/2,\sigma}) = c_{i+1/2,\sigma}c_{i-1/2,\sigma} - c_{i-1/2,\sigma}c_{i+1/2,\sigma} + c_{i+1/2,\sigma}c_{i-1/2,\sigma} - c_{i+1/2,\sigma}c_{i-1/2,\sigma} = \delta_{i}(c_{i+1/2,\sigma}c_{i-1/2,\sigma} - c_{i-1/2,\sigma}c_{i+1/2,\sigma}) = \delta_{i}\delta_{2i}(c_{i+1/2,\sigma}c_{i-1/2,\sigma}),\]

(28)

where \(\delta_{i}h_{i,\sigma} = h_{i+1/2,\sigma} - h_{i-1/2,\sigma}\) and \(\delta_{i}h_{i,\sigma} = h_{i+1,\sigma} - h_{i-1,\sigma}\) where \(h_{i}\) is a general function of the operators \(c_{i}\) and \(c_{i}^{\dagger}\), such as \(h_{i} = c_{i+1}c_{i+k}\) in which \(j \) and \(k\) are arbitrary numbers.

The TBWDF appears in the equation of motion for the OBWDF Eq. (27), which means that we have to make an approximation in order to obtain a closed set of equations. Proceeding by analogy with the previous section, we factor the TBWDF as follows,

\[f_{i,\sigma}(p, \tau) \approx f_{i,\sigma}(p, \tau) + \tilde{f}_{i,\sigma}(p, \tau)\]

(29)

where we define \(f_{i,\sigma}(p, \tau) \equiv f_{i,\sigma}(p, \tau) + \tilde{f}_{i,\sigma}(p, \tau)\) with \(f_{i,\sigma}(p, \tau)\) the deviation of the OBWDF from its average value due to presence of the external potential. In addition we assume that the external potential is weak enough that we can keep only the first term in the functional Taylor expansion of \(g_{\sigma\sigma}(\tau, i, i', \tau)\), which means that \(\tilde{f}_{i,\sigma}(p, \tau)\) and \(\tilde{n}_{\sigma}(\tau)\) are small. The first and third terms of the above equation do not contribute to the final form of the equation of motion for the OBWDF, Eq. (27). The functional dependence of \(g_{\sigma\sigma}(i, i', \tau)\) on \(n_{\sigma}(\tau)\) again appears in the above equation. We use the well-known local approximation \(\partial g_{\sigma\sigma}(i, i')/\partial n_{\sigma}(\tau) = \delta_{i,j}\partial g_{\sigma\sigma}(0)/\partial n_{\sigma}(\tau)\) where \(n_{\sigma}\) is the average number of particles per site with spin \(\sigma\). The final non-zero contribution from the above approximation for the TBWDF to the equation of the motion finally takes the following form,

\[K_{i,\sigma}(p, p', \tau) = f_{\sigma}(p, \tau)\tilde{f}_{i,\sigma}(p', \omega)g_{\sigma\sigma}(0) + f_{\sigma}(p, \tau)f_{\sigma}(p')\sum_{\omega} \frac{\partial g_{\sigma\sigma}(\omega)}{\partial n_{\sigma}}\tilde{n}_{\sigma}(\tau).\]

(31)
function \( f^0_\sigma(p) \). The final equation for \( \tilde{f}_\sigma(p, \tau) \) in Fourier space can finally be written as

\[
[\omega_n - 4t \sum_\alpha \sin(\frac{q_\alpha}{2} \sin(\rho_\alpha))] \tilde{f}_\sigma(q, p, \omega_n) = [f^0_\sigma(p + \frac{q}{2}) - f^0_\sigma(p - \frac{q}{2})]V^{\text{ext}}(q, \omega_n)
\]

\[
+ U \sum_1 \int_{BZ} \frac{dp_1}{\nu} \int_{BZ} \frac{dp_2}{\nu} e^{i(p-p_1) \cdot r_1} e^{-i(p-p_2) \cdot r_1} K_{\tau \sigma}(q, p, p', \omega_n).
\]

(32)

Now we can perform an integral over \( p \) to obtain an equation for the density \( \bar{n}_\sigma(q, \omega_n) \). The final form of this equation is

\[
\bar{n}_\sigma(q, \omega_n) = \chi^0_\sigma(q, \omega_n)V^{\text{ext}}(q, \omega_n) + U \chi^0_\sigma(q, \omega_n)[\bar{n}_\sigma(q, \omega_n)\tilde{g}_{\sigma \sigma}(0)] + \eta \sum_{\sigma'} \frac{\partial g_{\sigma \sigma}(0)}{\partial n_{\sigma'}} \bar{n}_{\sigma'}(q, \omega_n)
\]

(33)

where \( \chi^0_\sigma(q, \omega_n) \) is given by,

\[
\chi^0_\sigma(q, \omega_n) = \frac{\chi^0_\sigma(q, \omega_n)}{1 + \frac{\omega_n}{2} \chi^0_\sigma(q, \omega_n)}
\]

(34)

One can invert the equation for the change in density Eq. (33) in order to obtain the density in terms of the external potential to extract the susceptibility,

\[
\bar{n}_\sigma(q, \omega_n) = \chi_{cc}(q, \omega_n)V^{\text{ext}}(q, \omega_n) + \chi_{ss}(q, \omega_n)V^{\text{ext}}(q, \omega_n)
\]

where \( V^{\text{ext}}(q, \omega_n) = |V^{\text{ext}}(q, \omega_n) \pm V^{\text{ext}}(q, \omega_n)|/2 \), and the coefficients of the external potential are the response functions, which are given by following formulae,

\[
\chi_{cc,ss}(q, \omega_n) = \frac{\chi^0_\sigma(q, \omega_n)}{1 + \frac{\omega_n}{2} \chi^0_\sigma(q, \omega_n)}
\]

(35)

where \( \chi^0_\sigma(q, \omega_n) = \frac{1}{2} (\chi^0_\sigma(q, \omega_n) + \chi^0_\sigma(q, \omega_n)) \), \( U_{ss} = U \tilde{g}_{\sigma \sigma}(0) \) and \( U_{cc} = U [\tilde{g}_{\sigma \sigma}(0) + n \partial \tilde{g}_{\sigma \sigma}(0)/\partial n] \).

Eqs. (33) are the same as Eqs. (15) and Eq. (14) when we set \( V = 0 \). The extension of the above equations to the case \( V \neq 0 \) is straightforward and leads to exactly the same result as in the previous section. In the present case, the derivative of the pair correlation function with respect to the density can be evaluated if one wishes, but its contribution is not big enough to reproduce the QMC results as we will show in the next section. This problem is known in the context of the electron liquid.36

The authors add a extra unknown multiplier constant and fix it by the compressibility sum-rule. If they had used instead Pauli principle they would have recovered the TPSC equations.

C. Comments on the STLS approximation

We are now in a position to contrast the results of the above section with the STLS approximation. For the sake of simplicity, it is preferable to limit ourselves to the case \( V = 0 \). The factorization of the TBWDF that leads to the STLS approximation is given by

\[
f_{\tilde{W}_{\sigma \sigma}}(p, p', \tau) \approx f_{\tilde{W}_{\sigma \sigma}}(p, \tau)f_{\tilde{W}_{\sigma \sigma}}(p', \tau)g_{\sigma \sigma}(1, 1', \tau).
\]

(36)

This should be contrasted with the TPSC factorization appearing in Eq. (29) where the pair correlation function is taken “on-site”. At first glance the STLS factorization looks more reasonable because, as far as the TBWDF is concerned, the integral of the last formula with respect to \( p \) and \( p' \) leads to the exact result

\[
\langle \tilde{n}_{\sigma}(\tau)\tilde{n}_{\sigma'}(\tau) \rangle = \langle \tilde{n}_{\sigma}(\tau) \rangle \langle \tilde{n}_{\sigma'}(\tau) \rangle g_{\sigma \sigma}(i, 1', \tau).
\]

(37)

However, one must recall that in the equations of motion, the TBWDF appears weighted by the range-dependent potential appearing in the Hamiltonian. In particular, the form \( f_{\tilde{W}_{\sigma \sigma}}(p, p', \tau) \) is valid only for interactions with a finite range. With a local interaction, three of the creation-annihilation operators are at the same point, as is concerned, the integral of the last formula with respect to the density to recover the simplest result. The final forms of the response functions are given by

\[
\chi_{cc,ss}(q, \omega_n) = \frac{\chi^0_\sigma(q, \omega_n)}{1 + \frac{\omega_n}{2} \chi^0_\sigma(q, \omega_n)}
\]

(38)

where \( G_{\sigma \sigma}(q, \omega_n) \) is the local field factor for the qSTLS approximation. It can be written as

\[
G_{\sigma \sigma}(q, \omega_n) = -\frac{2}{n} \int_{BZ} \frac{dk}{\nu} S_{\sigma \sigma}(k - q) \chi^0_\sigma(q, k, \omega_n) \chi^0_\sigma(q, k, \omega_n)
\]

(39)

where \( \chi^0_\sigma(q, k, \omega_n) \) is the inhomogeneous free response function

\[
\chi^0_\sigma(q, k, \omega_n) = \int_{BZ} \frac{dp}{\nu} f^0_\sigma(p + \frac{k}{2}) - f^0_\sigma(p - \frac{k}{2}).
\]

(40)

The local field factor in the STLS approximation can be obtained by taking the following limit.
\[ G_{\sigma \bar{\sigma}}^{STLS}(q) = \lim_{\omega_n \to \infty} G_{\sigma \bar{\sigma}}(q, \omega_n) = -\frac{2}{n} \int_{BZ} \frac{d\nu}{\nu} S_{\sigma \bar{\sigma}}(\nu) \sum_{\alpha} \sin \left( \frac{q \alpha}{2} \right) \sin \left( \frac{k \alpha}{2} \right) \sum_{\alpha} \sin^2 \left( \frac{q \alpha}{2} \right). \]  

This integral can be simplified using \( k \to k + q \) so that the final result appears as \( q \) independent,

\[ G_{\sigma \bar{\sigma}}^{STLS} = -\frac{2}{nD} \int_{BZ} \frac{d\nu}{\nu} S_{\sigma \bar{\sigma}}(\nu) \sum_{\alpha} \cos \left( \frac{k \alpha}{2} \right). \]  

III. NUMERICAL RESULTS

We now present our numerical results obtained from Eqs. (15)-(22). Unless mentioned otherwise, we use \( U = 4 \) and \( n = 1 \) in all the figures, in units where \( \hbar = k_B = t = 1 \). We first present \( V = 0 \) results to contrast TPSC with other approaches and understand the source of the differences, then we move to the more general case.

A. TPSC, STLS and other approaches for \( V = 0 \).

In Fig. 1 we compare the static structure factors for different methods at \( U = 8, n = 1 \) and \( T = 1 \) as a function of momentum. The upper and lower curves are related to spin and charge components respectively.

![FIG. 1: The static structure factors for different methods at \( U = 8, n = 1 \) and \( T = 1 \) as a function of momentum. The upper and lower curves are related to spin and charge components respectively.](image)

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![FIG. 2: The inverse of the spin part of the static response function at specific momenta and \( V = 0, U = 4, n = 1 \) as a function of temperature. Symbols are QMC results extracted from [30].](image)

The inverse of the spin part of the static response function at specific momenta and \( V = 0, U = 4, n = 1 \) as a function of temperature. Symbols are QMC results extracted from [30].
can compare two more methods with STLS and TPSC. The local approximation (LA), represented by dots, consists in using for the effective interaction in the charge channel Eq. \( U_{\sigma\sigma} = U|g_{\sigma\sigma}(0) + n\partial g_{\sigma\sigma}(0)/\partial n| \). We call LA0, represented by dot-dashed line in Fig. 1, the approximation that neglects completely \( n\partial g_{\sigma\sigma}(0)/\partial n \). The difference between STLS and LA0 is very small. However, the difference between TPSC, LA, STLS (or LA0) is relatively large, demonstrating the importance of the functional derivative in this range of physical parameters. In the language of authors involved with the local approximation, since LA does not provide a satisfactory result, the multiplier factor in front of the derivative of the pair correlation function respect to the density is necessary. When this unknown multiplier is obtained from the Pauli sum-rule \( g_{\sigma\sigma}(0) = 0 \) instead of from the compressibility sum-rule, one recovers TPSC.

In TPSC, it suffices to know \( g_{\sigma\sigma}(0) \) to obtain the static spin structure factor. Could this quantity be determined from the compressibility sum-rule instead of from the sum-rule relating \( g_{\sigma\sigma}(0) \) to the integral of the structure factor? To answer this question, we show in Fig. 2 the TPSC results for the inverse of the static (\( \omega = 0 \)) spin response function (susceptibility) as a function of temperature, again for the \( V = 0 \) case, compared with QMC results of Ref. (30). Both short and long wave-length limits show a linear behavior in the intermediate and high temperature regimes, exhibiting a Curie law. The deviations from the Curie law appear at low temperature in both QMC and in TPSC. The agreement between TPSC and QMC is much better near wave vector \((\pi, \pi)\), even though the deviations are not large even around \((0, 0)\).

Hence, the spin susceptibility sum-rule is also very nearly satisfied with this method, meaning that the momentum independent correction factor, which is given by \( g_{\sigma\sigma}(0) \) in the effective interaction, corrects the result properly over the entire Brillouin zone\(^{38}\). However, to use the spin susceptibility sum-rule to fix the constant correction factor, one needs an independent way to find the spin-susceptibility.

Normally, the long wave-length behavior of the spin (charge) response function is related to the second derivative of the free energy with respect to magnetization \( m = n_\uparrow - n_\downarrow \) (density \( n \)) which can then be computed from the free-energy. In TPSC however, the free-energy requires further study\(^{38}\). In addition, given the less accurate results exhibited in Fig. 2 near \((0, 0)\), we consider it far more preferable to use the original TPSC method where \( g_{\sigma\sigma}(0) \) is determined by an integral over all wave vectors (Eqs. (20) and (22)) so as to satisfy the Pauli principle \( g_{\sigma\sigma}(0) = 0 \), which also involves a sum over all wave vectors.

### B. QMC vs generalization of TPSC for \( V \neq 0 \)

To judge the accuracy of TPSC, we plot in Fig. 3 the staggered static structure factors as a function of temperature, using QMC results of Ref. (31) as reference. The results for the charge structure factor are all smaller than the corresponding results for the spin structure factor. Our generalization for TPSC is plotted for \( V = 0, 0.5 \) and 1 while the QMC results, represented by symbols, are for \( V = 0.5 \) and 1. The figure clearly shows good agreement between our results and QMC in the high
temperature region or when \( V = 0.5 \). The deviation becomes significant when \( V = 1 \) and the temperature is low. This suggests that the effect of the functional derivative that we ignored in writing down Eqs. \( 15 \) and \( 14 \) becomes important when \( 4V^2 \) is of the order of the bandwidth (which is \( 8t \) here). Indeed the factor of four is necessary to account for the number of neighbors. The QMC data shows (not on the figure) that the tendency to staggered spin order disappears around \( V \approx 1.25 \) while in our case it persists to a higher value \( V \approx 2 \). This means that even though \( g_{\sigma\tilde{\sigma}}(a) \) decreases with increasing \( V \), the combination \( V g_{\sigma\tilde{\sigma}}(a) \) does not increase fast enough. The functional derivative must become important to take this effect into account. Note that in RPA, the spin structure factor is independent of \( V \).

Finally, Fig. 4 shows the staggered static charge and spin susceptibilities as a function of the temperature for the same parameters as the previous figure. All features are similar to what was mentioned in Fig. 3, except this fact that the correction factors do not correct the structure functions and response functions in the same manner. This is due to this assumption that these functions are local in time and space which certainly fails in certain region of the parameters even in the case \( V = 0 \).

### C. The effect of \( V \)

We finally turn to our main point, a more general overview of the effect of the nearest-neighbor interaction \( V \) over a wide range of parameters. In Fig. 5 we show the variation of \( g_{\sigma\tilde{\sigma}}(0) \) and \( g_{cc,ss}(a) \) as a function of temperature for \( V = 0, 0.5 \) and 1. We first notice that at \( V = 0 \), both \( g_{\sigma\tilde{\sigma}}(0) \) and \( g_{ss}(a) \) have a sharp decrease around \( T \approx 0.3 \). For \( g_{\sigma\tilde{\sigma}}(0) \) this means a decrease in the probability for finding two particles at the same place. In other words, there is an increase in the size of the local moment. The fact that \( g_{ss}(a) = (g_{\sigma\sigma}(a) - g_{\sigma\tilde{\sigma}}(a))/2 \) is negative means that the probability of finding two electrons at a distance \( a \) with opposite spins is larger than finding them there with the same spin. The decrease of \( g_{\sigma\tilde{\sigma}}(a) \) with temperature indicates a reinforcement of this tendency. These results reflect the tendency toward antiferromagnetic order (staggered spin order). Long-range spin-density wave order occurs only at zero temperature, as required by the Mermin-Wagner theorem in a two dimensional system, but the decrease in \( g_{\sigma\tilde{\sigma}}(0) \) and \( g_{ss}(a) \) reflects the beginning of the renormalized classical regime where the characteristic spin fluctuation frequency becomes smaller than temperature and where the antiferromagnetic correlation length begins to increase exponentially. By contrast, in the charge channel \( g_{cc}(a) \) does not show any strong change in the low temperature limit so there is no tendency to charge density wave order at these values of \( V \) within our present approximation even at very low temperature. We observe that as we increase the \( V \), the staggered spin fluctuations are depressed since \( g_{\sigma\tilde{\sigma}}(0) \) and \( g_{cc,ss}(a) \) do not decrease sharply.

How spin and charge fluctuations are influenced by \( V \) is best illustrated in Fig. 6 where we show the structure factors at \( T = 1 \), \( n = 1 \), \( U = 4 \), \( V = -0.5, 0 \) and 0.5. The upper and lower curves correspond respectively to the spin and charge components.
At this temperature, the antiferromagnetic correlation length begins to increase exponentially. We define it as the temperature where the ratio \( \chi_{ss}(q_x, q_y, 0)/\chi^0(q_x, q_y, 0) \) at its peak reaches the value 100. The rounding (foot) of the curves as the crossover temperature vanishes comes from this choice of ratio, which corresponds to fixing the correlation length at which we consider that we have entered the exponential regime related to the existence of long-range order at zero temperature. When the ratio is taken as larger, the rounding occurs over a narrower range of densities. In general there are quantum critical points at zero temperature where the exponential regime ends. In Fig. 7, the crossover temperature and the range of fillings where antiferromagnetic fluctuations are large both increase or decrease together. It is clear from this figure that positive \( V \) tends to suppress the staggered spin fluctuations while negative \( V \) leads to the opposite trend. As mentioned above, each site has four nearest-neighbor sites, and our method is quite accurate as long at \(|4V| < W\).

The apparent breaks in slope on the curves of the last figure correspond to a change from commensurate to incommensurate fluctuations. We have been using the terms antiferromagnetic and staggered rather loosely. Fig. 8 corrects this by presenting the peak position at the crossover temperature of the spin response function (or spin structure factor) as a function of filling factor for the same parameters as Fig. 7. The maximum in the spin fluctuations changes with temperature but, at the crossover temperature, it is at a wave vector that is commensurate near half-filling and then becomes incommensurate as we decrease \( n \). This comes mainly from the change in the peak position of the non-interacting susceptibility, but when \( V \) is finite there is an also effect that comes from the presence of the cosine functions in the effective interaction appearing in the denominator of Eq. (14). The range of fillings where commensurate fluctuations appear is increased when \( V < 0 \) and decreased when \( V > 0 \), concomitant with the tendency to increase or decrease the antiferromagnetic crossover temperature at half-filling.

![Image of Fig. 7: The crossover temperature as a function of filling factor for \( U = 4 \), and \( V = -0.4, -0.2, 0, 0.2, 0.4 \). Positive \( V \) reduces the strength of antiferromagnetic fluctuations while negative \( V \) has the opposite trend.](image)

![Image of Fig. 8: The wave-vector where the maximum of the spin response function appears at the crossover temperature, as a function of filling factor for \( U = 4 \), and \( V = -0.4, -0.2, 0, 0.2, 0.4 \). suppressed with increasing \( V \) while the charge fluctuations are enhanced. A negative value of \( V \) reverses the trend. For negative \( V \), pairing fluctuations should also become important but they are not considered here. In Fig. 7 we show the crossover temperature as a function of filling factor for \( V = -0.4, -0.2, 0, 0.2 \) and 0.4.

**IV. CONCLUSION AND SUMMARY**

We generalized the TPSC approach to the extended Hubbard model that contains nearest-neighbor repulsion \( V \) in addition to the usual on-site \( U \) term. That non-perturbative approach, which is a close relative of the STLS approach used for the electron gas, is valid in the weak to intermediate-coupling limit. The TPSC approach is usually studied in the functional derivative formalism and the STLS approach in the Wigner distribution function formalism, so we presented derivations in both languages to better illustrate the similarities and differences between the two approaches.

To derive either TPSC or STLS, two main approxima-
tions are necessary: First we must factor a four-point correlation function (two-body density matrix) and correct the factorization with the pair correlation function; second, we must treat the functional derivative of the pair correlation function with respect to a fictitious external potential. The STLS factorization of the pair correlation function does not take into account the range of the interaction whereas TPSC does. In particular, at $V = 0$, the STLS approximation involves the pair correlation function for all distances and does not enforce the Pauli principle. On the other hand, TPSC involves the calculation of $g_{\sigma\sigma}(0)$ only and, in addition, it enforces the Pauli principle $g_{\sigma\sigma}(0) = 0$. The Pauli principle gives an additional equation that allows an approximate evaluation of the functional derivative entering the charge channel when one neglects the momentum and frequency dependence of that functional derivative. The local approximation (where the functional derivative is replaced by a derivative with respect to density) is another approach, but it is less accurate than TPSC, as judged from comparisons with QMC. Analogous comparisons with the spin and charge structure factors obtained from QMC also show that TPSC is more accurate than STLS.

When $V \neq 0$, one uses the same type of factorization, but extra functional derivatives appear in TPSC. These extra derivatives cannot be determined from the same kind of simple sum-rules used for the $V = 0$ Hubbard model. Comparisons of numerical results with QMC show that for $4V < W$, one can neglect the extra functional derivatives. In principle, one could obtain these derivatives within the local approximation or, given an independent way to obtain the free energy, by enforcing the compressibility and spin susceptibility sum-rules. This is left for future work.

At $V = 0$, near half filling, there is a crossover temperature to the renormalized-classical regime where spin fluctuations near $(\pi, \pi)$ grow exponentially, diverging only at zero temperature in agreement with the Mermin-Wagner theorem in two dimensions. The effect of $V > 0$ is to decrease both the crossover temperature and the range of dopings over which this crossover occurs. The crossover to increasing commensurate $(\pi, \pi)$ fluctuations occurs over a narrower range near $n = 1$ when $V > 0$ than when $V = 0$. The opposite conclusions hold true for $V < 0$. All these effects are non-perturbative. They are beyond the reach of RPA where $V$ does not influence the spin fluctuations. Staggered charge fluctuations are enhanced by $V > 0$ and decreased by $V < 0$.

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APPENDIX A: OTHER POSSIBILITY FOR FACTORIZATION

Here we would like to return to Eq. (A2) in order to mention the Fock-type factorization of the $V$ term, which can be introduced as follows

\[
\Sigma'_\sigma(1, 2) = -V \sum_a G_\sigma(1, 1 + a) \delta(1 + a, 2) g_{xx}(1, 1 + a) \tag{A1}
\]

where $\Sigma'_\sigma(1, 2)$ is the extra contribution to the self-energy in Eq. (9) and $g_{xx}(a)$ is a new pair correlation function defined as

\[
g_{xx}(a) = \frac{\langle T_x c_{\downarrow}^{\dagger}(1 + a) c_{\sigma}(1) c_{\downarrow}(1) \rangle}{G_{\sigma}(1, 1 + a^+) G_{\sigma}(1 + a, 1^+)}. \tag{A2}
\]

This pair correlation function is related to the one for parallel spins by

\[
g_{xx}(a) = \frac{g_{\sigma\sigma}(a)n^2_\sigma}{G_{\sigma}(1, 1 + a^+) G_{\sigma}(1 + a, 1^+)}. \tag{A3}
\]

The Green function that appears in the definition of the pair correlation function Eq. (A2) can be written as

\[
G_{\sigma}(1 + a, 1^+) = \int \frac{dq}{\nu} \exp{i q \cdot a} n_{\sigma}(q) = \int \frac{dq}{\nu} [\cos(q \cdot a) + i \sin(q \cdot a)] n_{\sigma}(q) = n_{c}(a) + i n_{s}(a). \tag{A4}
\]

where $n_{\sigma}(q)$ is the momentum distribution $\langle c_{s}^{\dagger} c_{s} \rangle$. The extra contribution to the approximate self-energy is obtained by substituting Eq. (A3) and Eq. (A1) in Eq. (A1). The final form in Fourier space is

\[
\Sigma'_\sigma(q) = -2V n^2_{s} g_{\sigma\sigma}(a) \frac{n_{c}(a) \cos(q_{x}a) + \cos(q_{y}a)] + n_{s}(a) [\sin(q_{x}a) + \sin(q_{y}a)]}{n_{c}(a)^2 + n_{s}(a)^2}. \tag{A5}
\]

We stress that the $n_{s}(a)$ term is zero if we assume that the momentum distribution function (or the dispersion relation) is a symmetric function. In this case, the fi-
nal contribution of the above equation renormalizes the hopping term as follows
\[ t' = t + \frac{2Vn^2 \sigma \sigma}{n_e(a)}. \] (A6)

The effect of this renormalization for positive \( V \) is merely a depression in the structure functions. The effect is opposite for negative \( V \) and it can even lead to an instability when \( t' \approx 0 \). One also should notice that inclusion of \( n_s(a) \) in the self-energy leads to an asymmetric dispersion relation (or an asymmetric momentum distribution function) which in return gives a non-zero value for this quantity. The presence of a self-consistent asymmetry in the momentum distribution function is known as a Pomeranchuk instability, which can be related to presence of stripes in the system.\textsuperscript{28,29}

The extra term in the self-energy Eq. (A1) also leads to an extra contribution in the response functions. To evaluate this extra correction we need
\[
\frac{\delta \Sigma^I_{\sigma}(4,5)}{\delta G_{\sigma'}(6,7)} = -V \delta_{\sigma\sigma'} \sum_a \delta(4 + a, 5) \delta(4 + a, 7) g_{xx}(4, 4 + a) \delta G_{\sigma'}(6,7) \]
\[ -V \sum_a G_{\sigma}(4, 4 + a) \delta(4 + a, 5) \frac{\delta g_{xx}(4, 4 + a)}{\delta G_{\sigma'}(6,7)}. \] (A7)

By inserting the above equation in Eq. (11), after ignoring the second term which involves the functional derivative, one gets the following extra correction to the equation for the response functions
\[
\chi'_{\sigma\sigma}(1, 2) = V G_{\sigma}(1, 3) G_{\sigma '(3 + a, 1)} \frac{\delta G_{\sigma}(3, 3 + a)}{\delta \phi_{\sigma}(2,2)} g_{xx}(3, 3 + a). \] (A8)

One notices that the three point response function appears in the above correction for the two body response function. It is hard to determine this type of function in practice, but its contribution to the equation for the two-body response function can be estimated. Eq. (11) for parallel spins is our basic equation for this task. We replace 1 → 3, 2 → 3 + a and 3 → 1, then multiply both sides of the equation by \( V g_{xx}(1, 3) G_{\sigma}(3 + a, 1) g_{xx}(3, 3 + a) \) and finally performing a sum over the internal index 3. The final result is given by the following equation
\[
\chi'_{\sigma\sigma}(1, 2) = \chi^{1V}_{\sigma\sigma}(1, 2) + U g_{\sigma\sigma}(0) \chi^{1V}_{\sigma\sigma}(1, \bar{3}) \chi_{\sigma\sigma}(\bar{4}, 2) \\
+ V \sum_{a,\sigma'} g_{\sigma\sigma'}(a) \chi^{1V}_{\sigma\sigma}(1, \bar{4}) \chi_{\sigma\sigma'}(\bar{4} + a, 2) \\
+ U n_{\sigma} \sum_{a'} \frac{\delta g_{\sigma\sigma}(0)}{\delta n_{\sigma'}} \chi^{1V}_{\sigma\sigma}(1, \bar{4}) \chi_{\sigma\sigma'}(\bar{4}, 2) \] (A9)

where \( \chi^{1V}_{\sigma\sigma}(1, 2) \) is
\[
\chi^{1V}_{\sigma\sigma}(q, \omega_n) = V g_{xx}(a) G_{\sigma}(1, 3) G_{\sigma}(\bar{3}, 2) G_{\sigma}(1, \bar{3} + a) G_{\sigma}(\bar{3} + a, 2) \] (A10)

while 1V stands for the first order in \( V \) and (2) is a label for its equivalent diagram. One can replace \( \chi_{\sigma\sigma'}(1, 2) \) in Eq. (A9) which already contains \( \chi'_{\sigma\sigma}(1, 2) \). Eq. (A9) and Eq. (13) after equating labels 1 and 2 [in Eq. (13)] form a
set of coupled equations which in principle can be solved. Here we are not going to provide the final form of the equations and instead simply explain that the correction term is small compared to its counterparts. This can be easily understood from Eq. (A11) because $\chi^{1V(2)}(\nu, \omega_n)$ appears as a multiplicative factor and also as a separate factor in all terms, so having an estimate from this term tells us a lot about the importance of the correction term. This term can be easily evaluated and it has the following form in Fourier space

$$\chi^{1V(2)}(q, \omega_n) = g_{xx}(a) \int \frac{d\nu}{\nu} \int \frac{d\nu'}{\nu'} \frac{f_\sigma(k + \frac{q}{2}) - f_\sigma(k - \frac{q}{2})}{i\omega_n - (\epsilon_{k+\frac{q}{2}} - \epsilon_{k-\frac{q}{2}})} \delta V(|k - k'|),$$

(A11)

where $V(q) = V[\cos(q_x a) + \cos(q_y a)]$. The above function is proportional to one of the first order diagrams that appear in the perturbation expansion of the response functions. We evaluated the above equation numerically and compared the result with the other first order diagram, which is given by

$$\chi^{1V(1)}(q, \omega_n) = g_{\sigma'\sigma}(a)V(q)\chi^{0}_{\sigma\sigma}(q, \omega_n)^2.$$  

(A12)

We checked that Eq. (A11) is zero at half-filling within our numerical precision and its contribution away from half-filling is negligible compared to Eq. (A12).

**APPENDIX B: IMPROVED SELF-ENERGY (SECOND STEP OF THE TPSC APPROXIMATION)**

We can improve our approximation for the self-energy to include single-particle scattering off low-energy spin and charge fluctuations. These processes give momentum and frequency dependence to the self-energy. This improved self-energy leads to one-particle spectral functions that compare extremely well with QMC in the case of the usual Hubbard model. In the extended Hubbard model, the improved self-energy that includes the effects of longitudinal fluctuations can be obtained as follows. We first write the exact result

$$\Sigma(1, 2)G_\sigma(2, 3) = - U \langle T_\sigma c_\sigma^\dagger(1)c_\sigma(1)c_\sigma^\dagger(3) \rangle$$

$$- V \sum_{\sigma', a} \langle T_{\sigma' c_\sigma^\dagger(1 + a) c_\sigma(1 + a)c_\sigma^\dagger(3) \rangle$$

$$= - U \left[ \frac{\delta G_\sigma(1, 3)}{\delta \phi^{1++, 1+}_\sigma} - G_\sigma(1, 1^+)G_\sigma(1, 3) \right]$$

$$- V \sum_{\sigma', a} \left[ \frac{\delta G_\sigma(1, 3)}{\delta \phi^{1++, 1+}_\sigma} - G_\sigma(1 + a, 1 + a^+)G_\sigma(1, 3) \right].$$

(B1)

After replacing $3 \to 1^+$ and using rotational symmetry, we have

$$\Sigma(1, 2)G_\sigma(2, 1^+) = Un_\sigma n_\sigma g_{\sigma\sigma}(0) + 2Vn^2g_{cc}(a)$$

$$= U[\chi_{\sigma\sigma}(1, 1) + n_\sigma n_\sigma] + 2V[\chi_{cc}(1 + a) + n^2]$$

(B3)

which can be interpreted as a sum-rule relating one particle quantities to the left and two-particle quantities to the right. Note that the equalities

$$g_{\sigma\sigma}(0) = \frac{\chi_{\sigma\sigma}(1, 1)}{n_\sigma n_\sigma} + 1,$$

$$g_{cc}(a) = \frac{\chi_{cc}(1 + a)}{n^2} + 1$$

(B5)
hold. They are the real-space version of the fluctuation-dissipation theorem.

We already approximated the self-energy using a factorization of Eq. (B3). Our factorization is exact in the limit $3 \rightarrow 1^+$ so we don’t expect anything new from that equation. However, we can still use an approximate form for the response functions in the second identity Eq. (B2). Now our main point is that if the response functions satisfy the sum-rules at the two-particle level Eq. (B5), then there is a guarantee that the self-energy satisfies the sum-rule in Eq. (B8) relating one- and two-particle quantities.

As an example one can insert Eq. (11) inside Eq. (B2), which already contains the approximate form of the self-energy Eq. (9), to get an approximate form of the self-energy at a second level of approximation. We give the final form of this equation in Fourier space for practical use:

\begin{equation}
\Sigma_{\sigma}(k, \omega_n) \approx (Un + 4Vn) + \frac{T}{4} \sum_{\omega_{n'}} \int \frac{d\alpha}{\nu} \left\{ UU_{ss}(q) \chi_{ss}(q, \omega_{n'}) + U_{cc}(q) [U + 4V\gamma(q)] \chi_{cc}(q, \omega_{n'}) \right\} G_0(k + q, \omega_n + \omega_{n'}). \quad (B6)
\end{equation}

where $\gamma(q) = \sum_{\sigma} \cos(q_a, a)$. As we expect, the above formula for the self-energy Eq. (B6) satisfies the sum-rule in Eq. (B3). This, in fact, is a result of using Eqs. (19), (20), (21), and (22), which are another version of the fluctuation-dissipation theorem Eq. (B5).

We have to mention that we dropped out a term during the calculation which is given by

\begin{equation}
\Sigma_{\sigma HF}(1, 2) = -V \sum_a G_0(1, 1+a) \delta(1+a, 2). \quad (B7)
\end{equation}

One should include the correction term to the response function we already discussed in the last section to take care of presence the above term. This means that one should include both corrections in the self-energy and the response function (or ignore them from both) to have the sum-rule Eq. (B8).

Following the procedure established for the ordinary Hubbard model\cite{1}, one could also take into account transverse spin fluctuations and crossing symmetry to write a more general result.

\begin{itemize}
  \item[1] Y. M. Vilk, Liang Chen and A.-M.S. Tremblay, Phys. Rev. B 49, 13267 (1994); Y.M. Vilk, Liang Chen, and A.-M.S. Tremblay, Physica C 235-240, 2335 (1994).
  \item[2] Y. M. Vilk, and A. -M.S. Tremblay, J. Phys. I 7, 1309 (1997).
  \item[3] S. Moukouri, S. Allen, F. Lemay, B. Kyung, D. Poulin, Y.M. Vilk et A.-M. S. Tremblay, Phys. Rev. B 61, 7887 (2000).
  \item[4] B. Kyung, S. Allen, A.-M. S. Tremblay, Phys. Rev. B 64, 075116 (2001).
  \item[5] B. Kyung, J.S. Landry, D. Poulin, A.-M.S. Tremblay, Phys. Rev. Lett. 90, 090702 (2003).
  \item[6] B. Kyung, J.S. Landry and A.-M.S. Tremblay, Phys. Rev. B 68, 174502 (2003).
  \item[7] J. Kanamori, Prog. Theor. Phys. 30, 275 (1963); K. A. Bruckner and C. A. Levinson, Phys. Rev. 97, 2344 (1955); K. A. Bruckner and J. L. Gummel, Phys. Rev. 109, 1023 (1958); ibid 109, 1040 (1958).
  \item[8] K. S. Singwi, M. P. Tosi, R. H. Land and A. Sjölander, Phys. Rev. 176, 589 (1968).
  \item[9] Some of these higher-order correlation functions will be discussed more deeply in a future publication.
  \item[10] Kota Hanasaki, and Masatoshi Imada, cond-mat/0506240.
  \item[11] S. Onari, R. Arita, K. Kuroki and H. Aoki, Phys. Rev. B 70, 094523 (2004).
  \item[12] R. Pietig, R. Buila, and S. Blawid. Phys. Rev. Lett. 82, 4046 (1999).
  \item[13] M. Calandra, J. Merino, and R. H. Mckenzie, Phys. Rev. B. 66, 195102 (2002).
  \item[14] M. Vojta, R.E. Hetzel, R.M. Noack, Phys. Rev. B 60, R8417 (1999).
  \item[15] Vojta M, Hubsch A, Noack RM, Phys. Rev. B 63, 045105 (2001).
  \item[16] B. Fourcade and G. Sproken, Phys. Rev. B 29, 5096 (1984); L. M. del Bosch and L. M. Falicov, Phys. Rev. B 37, 6037 (1988).
  \item[17] M. Aichhorn, H.G. Evertz, W. von der Linden, and M. Potthoff, Phys. Rev. B 70, 235107 (2004).
  \item[18] A. Avella, F. Mancini, Euro. Phys. J. B 41, 149 (2004).
  \item[19] Y. Ohta, K. Tsutsui, W. Koshibae, and S. Maekawa, Phys. Rev. B 70, 13504 (1994).
  \item[20] X.Z. Yan Phys. Rev. B 48, 7140 (1993).
  \item[21] B M. Bartkowiak, J. A. Henderson, J. Oitmaa, P. E. de Brito, Phys. Rev. B 51, 14077 (1995).
  \item[22] P. G. J. van Dongen, Phys. Rev. B 49, 7904 (1994); P. G. J. van Dongen, Phys. Rev. B 50, 14016 (1994).
  \item[23] S. Onari, R. Arita, K. Kuroki, and H. Aoki, Phys. Rev. B 70, 094523 (2004).
25 J. Kishine, H. Namaizawa, Prog. Theor. Phys. 93, 519 (1995).
26 J. Callaway, D.P. Chen, D.G. Kanhere, and Qiming Li, Phys. Rev. B 42, 465 (1990) and Physica B 163, 127 (1990).
27 Subir Sachdev, Quantum Phase Transition (Cambridge University Press, 1999).
28 S. A. Kivelson, E. Fradkin, and V. J. Emery, Nature (London) 393, 550 (1998).
29 A. Neumayer and W. Metzner, Phys. Rev. B 67, 035112.
30 Y. Zhang and J. Callaway, Phys. Rev. B 39, 9397 (1989).
31 S. Allen, A.-M.S. Tremblay, Y.M. Vilk, in ”Theoretical Methods for Strongly Correlated Electrons”, David Sénéchal, André-Marie Tremblay and Claude Bourbonnais (eds.) CRM Series in Mathematical Physics, (Springer, New York, 2003), p.341.
32 Gordon Baym, Phys. Rev. 127, 1391 (1962).
33 L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics (Benjamin, Menlo Park, 1962).
34 P.C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959). This paper also contains numerous references to previous work.
35 Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids 56, 1769 (1995); Y.M. Vilk, and A.-M.S. Tremblay, Europhys. Lett. 33, 159 (1996).
36 P. Vashishta and K. S. Singwi, Phys. Rev. B 6, 875 (1972).
37 R. K. Moudgil, P. K. Ahluwalia and K. N. Pathak, Phys. Rev. B 52, 11945 (1995).
38 In one dimension, the momentum dependence of the interactions cannot be neglected. See for example, H. Nélisse, C. Bourbonnais, H. Touchette, Y.M. Vilk and A.-M.S. Tremblay, European Journal of Physics B 12, 351 (1999).
39 S. Roy, C. Brillon and A.-M.S. Tremblay (unpublished).
40 J. E. Hirsch, Phys Rev Lett. 53, 2327 (1984); H. Q. Lin and J. E. Hirsch, Phys. Rev. B 33, 8155, (1986).