# 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, Sjölander (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 quantify how 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 Coulombic 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 Coulombic 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 twoparticle self-consistent approach<sup>1,2</sup> (TPSC) to study the extended Hubbard model, which includes nearest-neighbor repulsion in addition to the usual on-site repulsion. This model is interesting in its own right, independent of the abovementioned theoretical question. Indeed, the extended Hubbard model allows one to study materials where competition between charge and spin order manifest themselves. In hightemperature 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<sup>1-6</sup> (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. 2. In particular, TPSC conserves spin and charge, satisfies the Pauli principle (two parallel spin electrons cannot occupy the same site), the Mermin-Wagner theorem in two dimensions, the local-moment and local-charge sum rules, does not assume a Migdal theorem, and it includes Kanamori-Brückner<sup>7</sup> screening. Although it is limited to interaction strengths less than the bandwidth, TPSC is a nonperturbative approach. Indeed, perturbative approaches are either crossing symmetric (satisfy the Pauli principle), like parquet resummations, or they are conserving (in the Baym-Kadanoff spirit), like the fluctuation exchange approximation,<sup>8,9</sup> but they are not both crossing symmetric and conserving. The TPSC approach is a close relative to the Singwi, Tosi, Land, Sjölander (STLS) method<sup>10</sup> used in the electron gas problem. The STLS approximation was first introduced to describe the structure functions of an electron liquid where it provided much better results than 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 a 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 onebody 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 different point of view on the STLS method by comparing it to the TPSC approach. As we will show in more detail, 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 nonlocal potentials, it is more accurate to use local or nonlocal factorization, respectively, 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.<sup>11</sup> 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 be obtained by quantum Monte Carlo (QMC) simulations. We will carefully analyze the approximations involved in the method and discuss other possibilities for improvement.

We now discuss 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 superexchange  $4t^2/U$  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 socalled 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 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<sup>12</sup> that uses a new correlator-projection method. The relevant theoretical literature for these compounds focuses on the square lattice<sup>9,13,14</sup> and on ladders for the quarter-filled case.<sup>15,16</sup> The competition between charge and spin orders has also been studied in one-, $^{17-19}$  two-, $^{20-22}$  three-, $^{23}$  and higher dimensions<sup>24</sup> at various fillings. The combined effect of charge fluctuations in addition to the usual spin fluctuation in favoring one type or another of unconventional superconductivity has also been studied using this model.<sup>25-2</sup>

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. 28 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. III 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 obtain various results on the influence of the nearest-neighbor interaction V on spin and charge fluctuations.

## **II. THEORY**

We first introduce the extended Hubbard Hamiltonian,

$$H = -t \sum_{\langle \mathbf{ij} \rangle \sigma} \sigma(c^{\dagger}_{\mathbf{i\sigma}}c_{\mathbf{j\sigma}} + c^{\dagger}_{\mathbf{j\sigma}}c_{\mathbf{i\sigma}}) + U \sum_{\mathbf{i}} n_{\mathbf{i\uparrow}} n_{\mathbf{i\downarrow}} + V \sum_{\langle \mathbf{ij} \rangle \sigma \sigma'} \sigma \sigma' n_{\mathbf{i\sigma}} n_{\mathbf{j\sigma'}} - \mu \sum_{\mathbf{i}} n_{i}, \qquad (1)$$

where  $c_{i\sigma}(c_{i\sigma}^{\dagger})$  are annihilation (creation) operators for elec-

trons 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 noninteracting 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<sup>29</sup> and then return to the approach that is more usual with the STLS approximation,<sup>10</sup> 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 she or he is more familiar with.

Before we proceed, let us mention that the final equations that we derive and then use in the rest of this paper have a clear physical meaning that can be described as follows. Equations (14) and (15) are the spin  $\chi_{ss}$  and charge  $\chi_{cc}$  susceptibilities, respectively. They have a RPA-like form, with the usual noninteracting susceptibility  $\chi_0$  Eq. (20), but with renormalized values of the spin  $U_{ss}$  and charge  $U_{cc}$  irreducible vertices instead of the bare U. These quantities, appearing in Eqs. (16) for  $U_{ss}$  and (17) for  $U_{ch}$ , depend on equaltime correlation functions, so-called pair-correlation functions. These equal-time correlators can in turn be obtained either from the Pauli principle, Eq. (25) in one case or, in the other cases, self-consistently from the starting susceptibilities by using the fluctuation-dissipation theorem. Indeed, note that Eqs. (18) or (19), (21), and (22) relate the pair-correlation functions to the spin and charge structure factors  $S_{cc}$  and  $S_{cc}$  that are themselves related to the susceptibilities through the fluctuation-dissipation theorem in Eq. (24). In summary, the spin and charge static structure factors can be determined through the fluctuation-dissipation theorem from the response functions that include four unknown constants. Three of these unknown are pair-correlation functions that are related to Fourier transforms of the static structure factors and thus can be found self-consistently with the help of the fluctuation-dissipation theorem, while the last constant can be found by the Pauli principle. A formula for an improved self-energy is derived in Appendix B. We now proceed with the detailed derivations. They can be skipped if one is interested only in the results that appear in Sec. III.

#### A. Functional derivative approach

Following the functional methods of the Schwinger school,<sup>30–32</sup> we begin with the generating function  $\ln Z[\phi_{\sigma}]$  with source fields  $\phi_{\sigma}$  in the grand canonical ensemble

$$Z[\phi_{\sigma}] = -\operatorname{Tr}[e^{-\beta H}T_{\tau}S(\beta)], \qquad (2)$$

where  $\beta = 1/T$  and *T* is the temperature, while *S* is defined as follows:

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$$\ln S(\boldsymbol{\beta}) = -\sum_{\mathbf{i},\mathbf{j},\sigma} \int_{0}^{\boldsymbol{\beta}} d\tau d\tau' c_{\mathbf{i}\sigma}^{\dagger}(\tau) c_{\mathbf{j}\sigma}(\tau') \phi_{\sigma}(\mathbf{i},\mathbf{j},\tau,\tau'), \quad (3)$$

where  $T_{\tau}$  is the time-ordering operator, and  $\tau$  is the imaginary time. The Green function can be calculated from the first functional derivative of the generating function  $Z[\phi_{\sigma}]$  as follows:

$$G_{\sigma}(1,2) = -\frac{\delta \ln Z[\phi_{\sigma}]}{\delta \phi_{\sigma}(2,1)} = \frac{\operatorname{Tr}[e^{-\beta H}T_{\tau}S(\beta)c_{\sigma}^{\dagger}(2)c_{\sigma}(1)]}{\operatorname{Tr}[e^{-\beta H}T_{\tau}S(\beta)]}$$
(4)

where we have introduced the shorthand 1 to stand for both the site position and the corresponding imaginary time, as in the equation

$$G_{\sigma}(1,2) = -\langle T_{\tau}c_{1\sigma}(\tau_1)c_{2\sigma}^{\dagger}(\tau_2)\rangle = -\langle T_{\tau}c_{\sigma}(1)c_{\sigma}^{\dagger}(2)\rangle, \quad (5)$$

where the angular brackets represent a thermal average in the canonical ensemble.

The equation of motion for the Green function has the following form,<sup>2,29,31</sup>:

$$G_0^{-1}(1,\bar{2})G_{\sigma}(\bar{2},3) = \delta(1,3) + \Sigma_{\sigma}(1,\bar{2})G_{\sigma}(\bar{2},3) + \phi_{\sigma}(1,\bar{2})G_{\sigma}(\bar{2},3),$$
(6)

where  $G_0^{-1}(1,2) = \left[\frac{\partial}{\partial \tau} - \epsilon(1,2)\right] \delta(1,2)$  is the noninteracting Green function,  $\Sigma_{\sigma}$  is the self-energy, and the bar is a shorthand for  $\Sigma_i \int d\tau$ . The above equation is nothing more than the Dyson equation that can be obtained by the diagrammatic technique. It can also be written in the form

$$G_{\sigma}^{-1}(1,2) = G_0^{-1}(1,2) - \phi_{\sigma}(1,2) - \Sigma_{\sigma}(1,2), \tag{7}$$

with the self-energy

$$\Sigma_{\sigma}(1,2) = -U\langle T_{\tau}c_{\tilde{\sigma}}^{\dagger}(1)c_{\tilde{\sigma}}(1)c_{\sigma}(1)c_{\sigma}^{\dagger}(\bar{3})\rangle G_{\sigma}^{-1}(\bar{3},2)$$
$$-V\sum_{\sigma',a} \langle T_{\tau}c_{\sigma'}^{\dagger}(1+a)$$
$$\times c_{\sigma'}(1+a)c_{\sigma}(1)c_{\sigma}^{\dagger}(\bar{3})\rangle G_{\sigma}^{-1}(\bar{3},2), \qquad (8)$$

where  $\tilde{\sigma} = -\sigma$  and the summation on *a* runs over the nearestneighbor sites of the site 1 (the imaginary time is the same at 1+*a* and at 1). One needs an approximation to deal with the above two-body density operator. By analogy with the factorization pioneered by Singwi *et al.*<sup>10</sup> we write

$$\begin{split} \Sigma_{\sigma}(1,2) &\cong UG_{\tilde{\sigma}}(1,1^{+})G_{\sigma}(1,3)G_{\sigma}^{-1}(3,2)g_{\sigma\tilde{\sigma}}(1,1) \\ &+ V\sum_{\sigma',a} G_{\sigma'}(1+a,1) \\ &+ a^{+})G_{\sigma}(1,\bar{3})G_{\sigma}^{-1}(\bar{3},2)g_{\sigma\sigma'}(1,1+a) \\ &= U\delta(1,2)G_{\tilde{\sigma}}(1,1^{+})g_{\sigma\tilde{\sigma}}(1,1) + V\delta(1,2) \\ &\times \sum_{\sigma',a} G_{\sigma'}(1+a,1+a^{+})g_{\sigma\sigma'}(1,1+a), \quad (9) \end{split}$$

where  $g_{\sigma\sigma'}(i,j)$  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,

$$g_{\sigma\sigma'}(1,2) \equiv \frac{\langle T_{\tau}c_{\sigma}^{\dagger}(1)c_{\sigma}(1)c_{\sigma'}^{\dagger}(2)c_{\sigma'}(2)\rangle - \delta(1,2)\delta_{\sigma,\sigma'}\langle T_{\tau}c_{\sigma}^{\dagger}(1)c_{\sigma}(1)\rangle}{\langle T_{\tau}c_{\sigma'}^{\dagger}(1)c_{\sigma}(1)\rangle\langle T_{\tau}c_{\sigma'}^{\dagger}(2)c_{\sigma'}(2)\rangle} \equiv \frac{\langle n_{\sigma}(1)n_{\sigma'}(2)\rangle - \delta(1,2)\delta_{\sigma,\sigma'}\langle n_{\sigma}(1)\rangle}{\langle n_{\sigma}(1)\rangle\langle n_{\sigma'}(2)\rangle}, \quad (10)$$

where  $\langle n_{\sigma}(1)n_{\sigma'}(2)\rangle$  is the density-density correlation function. In this last formula it is assumed that  $\tau_1 = \tau_2$ . With this procedure, the four-point function  $\langle T_{c}c_{\sigma}^{\dagger}(1)c_{\sigma}(1)c_{\sigma}(1)c_{\sigma}^{\dagger}(\bar{3})\rangle$ appearing in the definition of the self-energy Eq. (8) is factorized à la Hartree-Fock everywhere,<sup>29</sup> except when the point  $\bar{3}$  is equal to 1<sup>+</sup>, in which case there is no approximation involved. The Fock contribution from the *V* term is discussed in Appendix A. It gives a very small contribution in the regime studied in the present paper. We caution the reader that the above-mentioned factorization is not exactly the one 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  $G_{\sigma}(1,\bar{3})G_{\sigma'}^{-1}(\bar{3},2) = \delta_{\sigma\sigma'}\delta(1,2)$  and using the Dyson equation, Eq. (7), we obtain the exact result

$$\Pi_{\sigma\sigma'}(1,2;3,3) \equiv -\frac{\delta G_{\sigma}(1,2)}{\delta \phi_{\sigma'}(3,3)} = G_{\sigma}(1,\bar{4}) \frac{\delta G_{\sigma}^{-1}(\bar{4},\bar{5})}{\delta \phi_{\sigma'}(3,3)} G_{\sigma}(\bar{5},2)$$
$$= -\delta_{\sigma\sigma'} G_{\sigma}(1,3) G_{\sigma}(3,2)$$
$$-\sum_{\sigma''} G_{\sigma}(1,\bar{4}) \frac{\delta \Sigma_{\sigma}(\bar{4},\bar{5})}{\delta G_{\sigma''}(\bar{6},\bar{7})} \frac{\delta G_{\sigma''}(\bar{6},\bar{7})}{\delta \phi_{\sigma'}(3,3)} G_{\sigma}(\bar{5},2).$$
(11)

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) by

$$\frac{\delta \Sigma_{\sigma}(4,5)}{\delta G_{\sigma''}(6,7)} = U \delta_{\tilde{\sigma}\sigma''} \delta(4,5) \,\delta(4,6) \,\delta(5,7) g_{\sigma\tilde{\sigma}}(4,4) + V \sum_{a} \,\delta(4,5) \,\delta(4+a,6) \,\delta(5+a,7) g_{\sigma\sigma''}(4,4+a) + U \delta(4,5) G_{\tilde{\sigma}}(4,4^{+}) \frac{\delta g_{\sigma\tilde{\sigma}}(4,4)}{\delta G_{\sigma''}(6,7)} + V \delta(4,5) \sum_{\sigma''' a} G_{\sigma'''}(4,4^{+}) \frac{\delta g_{\sigma\sigma'''}(4,4+a)}{\delta G_{\sigma''}(6,7)}.$$
(12)

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 Refs. 1 and 29 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 functionals, 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 (less than a few percent) as long as |8V| is small compared to the bandwidth. Their contribution becomes more significant as Vincreases. 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

$$\Pi_{cc,ss}(1,2;3,3) \equiv \sum_{\sigma\sigma'} (\sigma\sigma')\Pi_{\sigma\sigma'}(1,2;3,3) = 2[\Pi_{\sigma\sigma}(1,2;3,3) \pm \Pi_{\sigma\bar{\sigma}}(1,2;3,3)] = -2G_{\sigma}(1,3)G_{\sigma}(3,2) \\ -2UG_{\sigma}(1,\bar{4})G_{\sigma}(\bar{4},2)g_{\sigma\bar{\sigma}}(\bar{4},\bar{4}) \left[ \frac{\delta G_{\sigma}(\bar{4},\bar{4}^{+})}{\delta\phi_{\bar{\sigma}}(3,3)} \pm \frac{\delta G_{\sigma}(\bar{4},\bar{4}^{+})}{\delta\phi_{\sigma}(3,3)} \right] - 2VG_{\sigma}(1,\bar{4})G_{\sigma}(\bar{4},2)\sum_{\sigma',a} g_{\sigma\sigma'}(\bar{4},\bar{4}+a) \\ \times \left[ \frac{\delta G_{\sigma}(\bar{4}+a,\bar{4}+a^{+})}{\delta\phi_{\bar{\sigma}}(3,3)} \pm \frac{\delta G_{\sigma}(\bar{4}+a,\bar{4}+a^{+})}{\delta\phi_{\sigma}(3,3)} \right] - 2UG_{\sigma}(1,\bar{4})G_{\sigma}(\bar{4},2)G_{\bar{\sigma}}(\bar{4},\bar{4}) \left[ \frac{\delta g_{\sigma\bar{\sigma}}(\bar{4},\bar{4})}{\delta\phi_{\sigma}(3,3)} \pm \frac{\delta G_{\sigma}(\bar{4}+a,\bar{4}+a^{+})}{\delta\phi_{\bar{\sigma}}(3,3)} \right],$$
(13)

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 the zero source field.<sup>1,2</sup> For the plus sign (corresponding to the charge response function), we assume that the functional derivative of the pair correlation function with 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:

$$\chi_{ss}(\mathbf{q},\omega_n) = \frac{\chi^0(\mathbf{q},\omega_n)}{1 - \frac{\chi^0(\mathbf{q},\omega_n)}{2}U_{ss}(\mathbf{q})},$$
(14)

$$\chi_{cc}(\mathbf{q},\omega_n) = \frac{\chi^0(\mathbf{q},\omega_n)}{1 + \frac{\chi^0(\mathbf{q},\omega_n)}{2}U_{cc}(\mathbf{q})},$$
(15)

where

$$U_{ss}(\mathbf{q}) = Ug_{\sigma\bar{\sigma}}(0) - 4Vg_{ss}(a)\sum_{\alpha} \cos(q_{\alpha}a), \qquad (16)$$

$$U_{cc}(\mathbf{q}) = U[g_{\sigma\tilde{\sigma}}(0) + ng'_{\sigma\tilde{\sigma}}(0)] + 4Vg_{cc}(a)\sum_{\alpha} \cos(q_{\alpha}a),$$
(17)

and  $\omega_n = 2\pi nT$  is the Matsubara frequency. One can easily see the similarity of the above equations with those in Refs. 1 and 2 and also find out how these equations can be extended to a system with longer range interactions 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

$$g_{cc,ss} \equiv \sum_{\sigma\sigma'} (\sigma\sigma') n_{\sigma} n_{\sigma'} g_{\sigma\sigma'} / n^2, \qquad (18)$$

or simply

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$$g_{cc,ss}(\mathbf{r}) = [g_{\sigma\sigma}(\mathbf{r}) \pm g_{\sigma\tilde{\sigma}}(\mathbf{r})]/2$$
(19)

for a spin-unpolarized system, with  $|\mathbf{r}|=0$  or *a*.  $\chi^0(\mathbf{q}, \omega_n)$  is the response function for noninteracting electrons given by

$$\chi^{0}(\mathbf{q},\omega_{n}) = \int_{BZ} \frac{d\mathbf{p}}{\nu} \frac{f^{0}\left(\mathbf{p} + \frac{\mathbf{q}}{2}\right) - f^{0}\left(\mathbf{p} - \frac{\mathbf{q}}{2}\right)}{i\omega_{n} - \epsilon_{\mathbf{p}+\mathbf{q}/2} + \epsilon_{\mathbf{p}-\mathbf{q}/2}}.$$
 (20)

In the above formula  $\nu$  is the volume of the Brillouin zone (BZ),  $f^0(\mathbf{q})=1/\{1+\exp[(\epsilon_q-\mu)/T]\}\)$  is the Fermi-Dirac distribution function, and  $\epsilon_q=-2t\Sigma_\alpha\cos(q_\alpha a)$  is the noninteracting particle dispersion relation. At this level of approximation, the self-energy is a constant,<sup>29</sup> so it can be absorbed in the chemical potential. The situation is different when the Fock-like term is included (see Appendix B).

The pair-correlation functions are related to the static structure factors by

$$g_{cc}(\mathbf{r}) = 1 + \frac{1}{n} \int_{BZ} \frac{d\mathbf{q}}{\nu} [S_{cc}(\mathbf{q}) - 1] \exp(i\mathbf{q} \cdot \mathbf{r}), \qquad (21)$$

$$g_{ss}(\mathbf{r}) = \frac{1}{n} \int_{BZ} \frac{d\mathbf{q}}{\nu} [S_{ss}(\mathbf{q}) - 1] \exp(i\mathbf{q} \cdot \mathbf{r}), \qquad (22)$$

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

$$\sum_{\mathbf{l}} e^{i\mathbf{p}\cdot\mathbf{r}_{\mathbf{l}}} \equiv \nu \delta(\mathbf{p}), \quad \int_{BZ} \frac{d\mathbf{p}}{\nu} e^{i\mathbf{p}\cdot\mathbf{r}_{\mathbf{l}}} \equiv \delta_{\mathbf{r}_{\mathbf{l}},0}.$$
(23)

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

$$S_{\sigma\sigma'}(\mathbf{q}) = \frac{T}{\sqrt{n_{\sigma}n_{\sigma'}}} \sum_{\omega_n} \chi_{\sigma\sigma'}(\mathbf{q}, \omega_n).$$
(24)

The above equations [Eqs. (15)–(24)] form eight relations containing nine unknowns. The extra unknown can be fixed using the Pauli principle, namely,

$$g_{\sigma\sigma}(0) = 0$$
 or  $g_{cc}(0) = -g_{ss}(0)$ . (25)

To conclude, note that the RPA approximation on the nearest-neighbor interaction V can be simply recovered by setting  $g_{cc}(1)=1$  and  $g_{ss}(1)=0$ , which means that the RPA does not give any extra correction to the spin response function of the extended Hubbard model. This is a consequence of the fact that the different spin components (spin parallel and antiparallel) of the off-site interaction are identical in the original Hamiltonian. We will see that this is in contradiction with QMC calculations. Finally, at this level of approximation, the self-energy Eq. (9) is a constant. As in the original

TPSC approach,<sup>3,29,33</sup> we can perform a second step to improve our approximation for the self-energy. This is discussed in Appendix A.

## B. Wigner distribution function approach

In this section, we present the approach for obtaining the structure factors that parallels that of STLS.<sup>10</sup> It is based on the equation of motion for the Wigner distribution function. We just show the calculation for the ordinary Hubbard model (V=0) in order to shorten the length of the equations. This will suffice to demonstrate the difference between TPSC and STLS.

The one- and two-body Wigner distribution function (OBWDF and TBWDF) are defined by

$$f_{i\sigma}(\mathbf{p},\tau) = \sum_{\mathbf{l}} e^{i\mathbf{p}\cdot\mathbf{r}_{\mathbf{l}}} \langle c^{\dagger}_{\mathbf{i}+\mathbf{l}/2,\sigma} c_{\mathbf{i}-\mathbf{l}/2,\sigma} \rangle, \qquad (26)$$

$$f_{\mathbf{i}\mathbf{i}'\sigma\sigma'}(\mathbf{p},\mathbf{p}',\tau) = \sum_{\mathbf{l},\mathbf{l}'} e^{i\mathbf{p}\cdot\mathbf{r}_{\mathbf{l}}} e^{i\mathbf{p}'\cdot\mathbf{r}_{\mathbf{l}'}} \\ \times \langle c^{\dagger}_{\mathbf{i}+\mathbf{l}'2,\sigma}c_{\mathbf{i}-\mathbf{l}'2,\sigma}c^{\dagger}_{\mathbf{i}'+\mathbf{l}'/2,\sigma'}c_{\mathbf{i}'-\mathbf{l}'/2,\sigma'} \rangle.$$

$$(27)$$

One should notice that the operators in the above equations act on some lattice sites that do not exist in the real system. Knowing that the Winger distribution functions (WDFs) are not real physical functions, we define them in this manner for the sake of simplicity in the notation. One can also define the WDFs in terms of operators that 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

$$n_{\mathbf{i}\sigma}(\tau) = \int_{BZ} \frac{d\mathbf{p}}{\nu} f_{\mathbf{i}\sigma}(\mathbf{p}, \tau), \qquad (28)$$

with the same definitions of Fourier transforms as above, Eq. (23).

We first need to write the equation of motion for the operator  $c_{i,\sigma}$  to obtain the equation of motion for the OBWDF later on. In the presence of a one-body external potential  $V_{i,\sigma}^{ext}$ , this equation, after a bit of algebra, can be written as

$$-\frac{\partial c_{\mathbf{i},\sigma}}{\partial \tau} = [H, c_{\mathbf{i},\sigma}] = -t \delta_{\mathbf{i}}^{2}(c_{\mathbf{i},\sigma}) + Uc_{\mathbf{i},\sigma}c_{\mathbf{i},\tilde{\sigma}}^{\dagger}c_{\mathbf{i},\tilde{\sigma}} + V_{\mathbf{i},\sigma}^{ext}c_{\mathbf{i},\sigma},$$
(29)

where  $\delta_{\mathbf{i}}^2 c_{\mathbf{i},\sigma} = \sum_{\langle \mathbf{j} \rangle_{\mathbf{i}}} c_{\mathbf{j},\sigma}$ , and  $\langle \mathbf{j} \rangle_{\mathbf{i}}$  means that the sum runs over all nearest-neighbors of site  $\mathbf{i}$ . Using the above equation, one can write the equation of motion for the OBWDF,

$$-\frac{\partial f_{\mathbf{i},\sigma}(\mathbf{p},\tau)}{\partial \tau} = -2it\sum_{\alpha} \sin(q_{\alpha})(\delta_{\mathbf{i}})_{\alpha}f_{\mathbf{i},\sigma}(\mathbf{p},\tau) - \sum_{\mathbf{l}} \int_{BZ} \frac{d\mathbf{p}_{1}}{\nu} e^{i(\mathbf{p}-\mathbf{p}_{1})\cdot\mathbf{r}_{\mathbf{l}}} (V_{\mathbf{i}+\mathbf{l}/2,\sigma}^{ext} - V_{\mathbf{i}-\mathbf{l}/2,\sigma}^{ext}) f_{\mathbf{i},\sigma}(\mathbf{p}_{1},\tau) - U\sum_{\mathbf{l},\mathbf{i}'} \int_{BZ} \frac{d\mathbf{p}_{1}}{\nu} \int_{BZ} \frac{d\mathbf{p}_{2}}{\nu} e^{i(\mathbf{p}-\mathbf{p}_{1})\cdot\mathbf{r}_{\mathbf{l}}} (\delta_{\mathbf{i}-\mathbf{i}',\mathbf{l}/2} - \delta_{\mathbf{i}-\mathbf{i}',-\mathbf{l}/2}) f_{\mathbf{i}\mathbf{i}'\sigma\tilde{\sigma}}(\mathbf{p}_{1},\mathbf{p}_{2},\tau).$$
(30)

To derive the first term on the right-hand side of the above equation, we used the following identity, which we prove in one dimension only (for the sake of simplicity of notation):

$$\delta_{\mathbf{i}}^{2}(c_{i+l/2,\sigma}^{\dagger})c_{i-l/2,\sigma} - c_{i+l/2,\sigma}^{\dagger}\delta_{\mathbf{i}}^{2}(c_{i-l/2,\sigma}) = c_{i+l/2+1,\sigma}^{\dagger}c_{i-l/2,\sigma} - c_{i+l/2,\sigma}^{\dagger}c_{i-l/2-1,\sigma} + c_{i+l/2-1,\sigma}^{\dagger}c_{i-l/2,\sigma} - c_{i+l/2,\sigma}^{\dagger}c_{i-l/2+1,\sigma} = \delta_{\mathbf{i}}(c_{i+l/2+1/2,\sigma}^{\dagger}c_{i-l/2-1/2,\sigma}) - \delta_{\mathbf{i}}(c_{i+l/2-1/2,\sigma}^{\dagger}c_{i-l/2+1/2,\sigma}) = \delta_{\mathbf{i}}\delta_{2l}(c_{i+l/2,\sigma}^{\dagger}c_{i-l/2,\sigma}), \quad (31)$$

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

The TBWDF appears in the equation of motion for the OBWDF Eq. (30), 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:

$$f_{\mathbf{i}\mathbf{i}'\sigma\tilde{\sigma}}(\mathbf{p},\mathbf{p}',\tau) \approx f_{\mathbf{i}\sigma}(\mathbf{p},\tau)f_{\mathbf{i}'\tilde{\sigma}}(\mathbf{p}',\tau)g_{\sigma\tilde{\sigma}}(\mathbf{i}',\mathbf{i}',\tau) \quad (32)$$

$$\approx f_{\sigma}(\mathbf{p}) f_{\bar{\sigma}}(\mathbf{p}') g_{\sigma\bar{\sigma}}(0) + f_{\sigma}(\mathbf{p}) f_{\mathbf{i}'\bar{\sigma}}(\mathbf{p}',\tau) g_{\sigma\bar{\sigma}}(0) + \overline{f}_{\mathbf{i}\sigma}(\mathbf{p},\tau) f_{\bar{\sigma}}(\mathbf{p}') g_{\sigma\bar{\sigma}}(0) + f_{\sigma}(\mathbf{p}) f_{\bar{\sigma}}(\mathbf{p}') \sum_{\mathbf{i},\sigma'} \frac{\partial g_{\sigma\bar{\sigma}}(\mathbf{i}',\mathbf{i}',\tau)}{\partial n_{\mathbf{j},\sigma'}(\tau)} \overline{n}_{\mathbf{j},\sigma'}(\tau),$$
(33)

where we define  $f_{i\sigma}(\mathbf{p}, \tau) \cong f_{\sigma}(\mathbf{p}) + \overline{f}_{i\sigma}(\mathbf{p}, \tau)$ , with  $\overline{f}_{i\sigma}(\mathbf{p}, \tau)$  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  $g_{\sigma\overline{\sigma}}(\mathbf{i}', \mathbf{i}', \tau)$ , which means that  $\overline{f}_{i\sigma}(\mathbf{p}, \tau)$  and  $\overline{n}_{\mathbf{j},\sigma'}(\tau)$  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. (30). The functional dependence of  $g_{\sigma\overline{\sigma}}(\mathbf{i},\mathbf{i}',\tau)$  on  $n_{\mathbf{j},\sigma'}(\tau)$ again appears in the above equation. We use the well-known local approximation  $\partial g_{\sigma\overline{\sigma}}(\mathbf{i},\mathbf{i},\tau)/\partial n_{\mathbf{j},\sigma'}(\tau) = \delta_{\mathbf{i},\mathbf{j}}\partial g_{\sigma\overline{\sigma}}(\mathbf{0})/\partial n_{\sigma'}$ where  $n_{\sigma}$  is the average number of particles per site with spin  $\sigma$ . The final nonzero contribution from the above approximation for the TBWDF to the equation of the motion finally takes the following form:

$$\begin{aligned} K_{\mathbf{i}\mathbf{i}'\sigma\sigma'}(\mathbf{p},\mathbf{p}',\tau) &= f_{\sigma}(\mathbf{p})\overline{f}_{\mathbf{i}'\tilde{\sigma}}(\mathbf{p}',\omega)g_{\sigma\tilde{\sigma}}(0) \\ &+ f_{\sigma}(\mathbf{p})f_{\tilde{\sigma}}(\mathbf{p}')\sum_{\sigma'}\frac{\partial g_{\sigma\tilde{\sigma}}(0)}{\partial n_{\sigma'}}\overline{n}_{\mathbf{i}',\sigma'}(\tau). \end{aligned}$$
(34)

The exact form of  $f_{\sigma}(\mathbf{p})$  is not known, but in first approximation it is reasonable to replace it by the Fermi-Dirac func-

tion  $f^0_{\sigma}(\mathbf{p})$ . The final equation for  $\overline{f}_{i\sigma}(\mathbf{p}, \tau)$  in Fourier space can finally be written as

$$\begin{bmatrix} \omega_n - 4t \sum_{\alpha} \sin\left(\frac{q_{\alpha}}{2}\right) \sin(p_{\alpha}) \end{bmatrix} \overline{f}_{\sigma}(\mathbf{q}, \mathbf{p}, \omega_n) = \begin{bmatrix} f_{\sigma}^0 \left(\mathbf{p} + \frac{\mathbf{q}}{2}\right) \\ -f_{\sigma}^0 \left(\mathbf{p} - \frac{\mathbf{q}}{2}\right) \end{bmatrix} V_{\sigma}^{ext}(\mathbf{q}, \omega_n) \\ + U \sum_{\mathbf{l}} \int_{BZ} \frac{d\mathbf{p}_1}{\nu} \int_{BZ} \frac{d\mathbf{p}_2}{\nu} e^{i(\mathbf{p} - \mathbf{p}_1) \cdot \mathbf{r}_{\mathbf{l}}} [e^{i\mathbf{q}/2 \cdot \mathbf{r}_{\mathbf{l}}} \\ -e^{-i\mathbf{q}/2 \cdot \mathbf{r}_{\mathbf{l}}}] K_{\sigma\sigma'}(\mathbf{q}, \mathbf{p}_1, \mathbf{p}_2, \omega_n).$$
(35)

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

$$\bar{n}_{\sigma}(\mathbf{q},\omega_{n}) = \chi_{\sigma}^{0}(\mathbf{q},\omega_{n})V_{\sigma}^{ext}(\mathbf{q},\omega_{n}) + U\chi_{\sigma}^{0}(\mathbf{q},\omega_{n}) \\ \times \left[\bar{n}_{\tilde{\sigma}}(\mathbf{q},\omega_{n})g_{\sigma\tilde{\sigma}}(0) + n_{\sigma}\sum_{\sigma'}\frac{\partial g_{\sigma\tilde{\sigma}}(0)}{\partial n_{\sigma'}}\bar{n}_{\sigma'}(\mathbf{q},\omega_{n})\right],$$
(36)

where  $\chi^0_{\sigma}(\mathbf{q},\omega)$  is given by

$$\chi_{\sigma}^{0}(\mathbf{q},\omega_{n}) = \int_{BZ} \frac{d\mathbf{p}}{\nu} \frac{f_{\sigma}^{0}\left(\mathbf{p}+\frac{\mathbf{q}}{2}\right) - f_{\sigma}^{0}\left(\mathbf{p}-\frac{\mathbf{q}}{2}\right)}{i\omega_{n}+\epsilon_{\mathbf{p}+\mathbf{q}/2}-\epsilon_{\mathbf{p}-\mathbf{q}/2}}.$$
 (37)

One can invert the equation for the change in density, Eq. (36), in order to obtain the density in terms of the external potential to extract the susceptibility,

$$\overline{n}_{\sigma}(\mathbf{q},\omega_n) = \chi_{cc}(\mathbf{q},\omega_n) V_{cc}^{ext}(\mathbf{q},\omega_n) + \chi_{ss}(\mathbf{q},\omega_n) V_{ss}^{ext}(\mathbf{q},\omega_n),$$

where  $V_{cc,ss}^{ext}(\mathbf{q},\omega_n) = [V_{\sigma}^{ext}(\mathbf{q},\omega_n) \pm V_{\tilde{\sigma}}^{ext}(\mathbf{q},\omega_n)]/2$ , and the coefficients of the external potential are the response functions, which are given by following formula:

$$\chi_{cc,ss}(\mathbf{q},\omega_n) = \frac{\chi^0(\mathbf{q},\omega_n)}{1 \mp \frac{U_{cc,ss}}{2}\chi^0(\mathbf{q},\omega_n)},$$
(38)

where  $\chi^0(\mathbf{q}, \omega_n) = 2[\chi^0_{\sigma}(\mathbf{q}, \omega_n) + \chi^0_{\widetilde{\sigma}}(\mathbf{q}, \omega_n)], \quad U_{ss} = Ug_{\sigma\widetilde{\sigma}}(0),$ and  $U_{cc} = U[g_{\sigma\widetilde{\sigma}}(0) + n\partial g_{\sigma\widetilde{\sigma}}(0)/\partial n].$  Equation (38) is the same as Eqs. (14) and (15) 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.<sup>34</sup> The authors add an extra unknown multiplier constant and fix it by the compressibility sum rule. If they had used the Pauli principle instead 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

$$f_{\mathbf{i}\mathbf{i}'\sigma\tilde{\sigma}}(\mathbf{p},\mathbf{p}',\tau) \approx f_{\mathbf{i}\sigma}(\mathbf{p},\tau)f_{\mathbf{i}'\tilde{\sigma}}(\mathbf{p}',\tau)g_{\sigma\tilde{\sigma}}(\mathbf{i},\mathbf{i}',\tau).$$
(39)

This should be contrasted with the TPSC factorization appearing in Eq. (32), 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  $\mathbf{p}$  and  $\mathbf{p}'$  leads to the exact result

$$\langle n_{\mathbf{i}\sigma}(\tau)n_{\mathbf{i}'\sigma'}(\tau)\rangle = \langle n_{\mathbf{i}\sigma}(\tau)\rangle\langle n_{\mathbf{i}'\sigma'}(\tau)\rangle g_{\sigma\tilde{\sigma}}(\mathbf{i},\mathbf{i}',\tau).$$
(40)

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  $f_{ii'\sigma\bar{\sigma}}(\mathbf{p},\mathbf{p}',\tau)$  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 can be seen in Eq. (29). The factorization that appears correct, as judged by comparisons with the QMC, is the one that takes the role of the potential into account. In the case of the simple Hubbard model, the potential is local in time and space, so one needs a local factorization to model the interaction terms as best as possible.

The formal STLS approximation can be obtained by replacing the above STLS factorization, Eq. (39), in the equation of motion, Eq. (30), and then by repeating the same steps as above. We must also ignore the functional derivative of the pair-correlation function with respect to density to recover the simplest result. The final forms of the response functions are given by

$$\chi_{cc,ss}(\mathbf{q},\omega_n) = \frac{\chi^0(\mathbf{q},\omega_n)}{1 \mp \frac{U}{2} [1 - G_{\sigma\tilde{\sigma}}(\mathbf{q},\omega_n)] \chi^0(\mathbf{q},\omega_n)}, \quad (41)$$

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

$$G_{\sigma\tilde{\sigma}}(\mathbf{q},\omega_n) = -\frac{2}{n} \int_{BZ} \frac{d\mathbf{k}}{\nu} S_{\sigma\tilde{\sigma}}(\mathbf{k}-\mathbf{q}) \frac{\chi_{\sigma}^0(\mathbf{q},\mathbf{k},\omega_n)}{\chi_{\sigma}^0(\mathbf{q},\omega_n)}, \quad (42)$$

where  $\chi_{\sigma}^{0}(\mathbf{q}, \mathbf{k}, \omega_{n})$  is the inhomogeneous free response function

$$\chi_{\sigma}^{0}(\mathbf{q},\mathbf{k},\omega_{n}) = \int_{BZ} \frac{d\mathbf{p}}{\nu} \frac{f_{\sigma}^{0}\left(\mathbf{p}+\frac{\mathbf{k}}{2}\right) - f_{\sigma}^{0}\left(\mathbf{p}-\frac{\mathbf{k}}{2}\right)}{\omega_{n}+\epsilon_{\mathbf{p}+\mathbf{q}/2}-\epsilon_{\mathbf{p}-\mathbf{q}/2}}.$$
 (43)

The local field factor in the STLS approximation can be obtained by taking the following limit:<sup>35</sup>

$$G_{\sigma\tilde{\sigma}}^{\text{STLS}}(\mathbf{q}) = \lim_{\omega_n \to \infty} G_{\sigma\tilde{\sigma}}(\mathbf{q}, \omega_n) = -\frac{2}{n} \int_{BZ} \frac{d\mathbf{k}}{\nu} S_{\sigma\tilde{\sigma}}(\mathbf{k})$$
$$-\mathbf{q} \frac{\sum_{\alpha} \sin\left(\frac{q_{\alpha}}{2}\right) \sin\left(\frac{k_{\alpha}}{2}\right)}{\sum_{\alpha} \sin^2\left(\frac{q_{\alpha}}{2}\right)}. \tag{44}$$

This integral can be simplified using  $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{q}$  so that the final result appears as  $\mathbf{q}$  independent,

$$G_{\sigma\bar{\sigma}}^{\text{STLS}} = -\frac{2}{nD} \int_{BZ} \frac{d\mathbf{k}}{\nu} S_{\sigma\bar{\sigma}}(\mathbf{k}) \sum_{\alpha} \cos\left(\frac{k_{\alpha}}{2}\right).$$
(45)

## **III. NUMERICAL RESULTS**

We now present our numerical results obtained from Eqs. (15)–(24). 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 the TPSC with other approaches and understand the source of the differences, and 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. We take the TPSC results represented by the solid lines in Fig. 1 (spin on top, charge on the bottom) as our reference. Indeed, it was shown in great detail before<sup>1,2</sup> that the TPSC values for the spin and charge structure factors agree very closely with QMC calculations that are essentially exact within small statistical uncertainties. However, TPSC is a weak to intermediate coupling method, so it eventually fails for U > 8t. Nevertheless, if one is not too close to phase transitions, TPSC results for the spin structure factor are still excellent at U=8t, while the results for the charge structure factor begin to deviate from QMC because of the approximation involved in the evaluation of the functional derivative. The STLS results, represented by the long-dashed line in Fig. 1, deviate substantially from TPSC. The inaccuracy of the STLS method for the Hubbard model comes from the fact that the potential is local, so one should use the local pair-correlation function to correct the factorization in the equation of motion instead of the nonlocal factoring used in the STLS approach, as dis-



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.

cussed in Sec. II C. In addition, since both charge and spin structure factors for STLS are larger than for TPSC, it is clear that STLS does not satisfy the Pauli principle  $\langle n_{\sigma}^2 \rangle$  $=\langle n_{\sigma}\rangle$  [or  $g_{\sigma\sigma}(0)=0$ ], a key requirement for electrons on a lattice at large density, where the probability of having two electrons on the same site is large in the absence of interactions. For the charge structure factor, one 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. (39),  $U_{cc}$ =  $U[g_{\sigma\tilde{\sigma}}(0) + n\partial g_{\sigma\tilde{\sigma}}(0)/\partial n]$ . We call LA0, represented by the dot-dashed line in Fig. 1, the approximation that neglects completely  $n\partial g_{\alpha\tilde{\alpha}}(0)/\partial n$ . The difference between STLS and LA0 is very small. However, the difference between TPSC, LA, and 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 with 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  $g_{\sigma\bar{\sigma}}(0)$  to obtain the static spin structure factor. Could this quantity be determined from the compressibility sum rule instead of from the sum rule relating  $g_{\sigma\bar{\sigma}}(0)$  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=0case, compared with QMC results of Ref. 28. Both short and long wavelength 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



FIG. 2. The inverse of the spin part of the static response function at specific momenta and V=0, U=4, and n=1 as a function of temperature. Symbols are QMC results extracted from Ref. 28.

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  $g_{\sigma\tilde{\sigma}}(0)$  in the effective interaction, corrects the result properly over the entire Brillouin zone.<sup>36</sup> 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 wavelength 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.<sup>37</sup> 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  $g_{\alpha\tilde{\alpha}}(0)$  is determined by an integral over all wave vectors [Eqs. (22) and (24)] 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. 28 as a benchmark. 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. For the charge structure factor, 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



FIG. 3. The staggered static structure factors as a function of temperature for U=4, n=1, and V=0, 0.5, and 1. The dots are the QMC results of Ref. 28, while lines are our results. The upper and lower curves (dots) are related to the spin and charge components, respectively.

writing down Eqs. (14) and (15) are not too important when 8V is less than the bandwidth W (which is 8t here) in the case of the spin fluctuations, and when 16V is less than the bandwidth in the case of the charge fluctuations. The effect of V is important since a 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 at around  $V \approx 1.25$ , while in our case it persists to a higher value  $V \approx 2$ . This is a result of the fact that  $|g_{ss}(a)|$ decreases with increasing V and their combination inside  $U_{ss}$ , Eq. (16), does not grow fast enough to cancel the U term contribution, which is responsible for the divergence in  $\chi_{ss}$ . Based on the same argument one can realize the main reason for the failure of the approximation in  $\chi_{cc}$  at higher value of V. The functional derivative terms become important to take these effects 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 temperature for the same parameters as the previous figure. All features are similar to what was mentioned in Fig. 3. However, the zero-frequency contribution is most affected by U and V, so the limitations of the theory are more apparent in Fig. 4 than in Fig. 3, since in the latter case the zero frequency staggered susceptibility is only one of the contributions entering the structure factor, as can be seen from the fluctuation-dissipation theorem in Eq. (24).

The comparisons between our approach and QMC calculations hold all the way down to the beginning of the renormalized classical regime, namely, down to the temperature below which the correlation functions begin to increase exponentially with the correlation length. Below that crossover temperature (discussed further in the following subsection), finite-size effects should become important in QMC. Further-



FIG. 4. The staggered static charge and spin susceptibilities as a function of temperature using the same parameters and symbols as in Fig. 3.

more, our approach is in the  $N=\infty$  universality class,<sup>38</sup> while the actual universality class for this problem is N=3. Hence, one expects deviations when one is too far below the crossover temperature.

# C. The effect of V: Crossover temperature and incommensurability

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  $g_{\sigma\bar{\sigma}}(0)$  and  $g_{cc,ss}(a)$  as a function of temperature for V



FIG. 5. The variation of  $g_{\sigma\bar{\sigma}}(0)$  and  $g_{cc,ss}(a)$  as a function of temperature for U=4, n=1, and V=0, 0.5, and 1.



FIG. 6. The charge and spin components of the structure factors at T=0.5, n=1, U=4, and V=-0.5, 0, and 0.5. The upper and lower

curves correspond to the spin and charge components, respectively.

=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 at 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  $g_{ss}(a)$  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 twodimensional 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.<sup>1,2</sup> 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 Vwithin our present approximation, even at very low temperature. We observe that as we increase the V, the staggered spin fluctuations are depressed since  $g_{\sigma\bar{\sigma}}(0)$  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=0.5, for V=-0.5, 0, and 0.5. Both functions show a peak at around  $q_x = \pi$  and  $q_y = \pi$ , a sign of the tendency toward staggered ordering. It is obvious from the figure that antiferromagnetic fluctuations are 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.

To illustrate how the incommensurability evolves with temperature and density, we plot the spin component of static



FIG. 7. The spin component of the static structure factor at U = 4, V=0, and n=0.8, for T=0.4, 0.2, and 0.1.

structure factor in Figs. 7 and 8. It is clear from Fig. 7 that the incommensurability shows up at a crossover temperature that depends on the density and on V. The position of the peak changes with temperature and also with V (not shown). In principle, there is a maximum deviation from  $(\pi, \pi)$  for the position of the peak, depending on the density and on V [the maximum incommensurability for V=0 is  $(0.74\pi, \pi)$ ].<sup>1</sup> This is qualitatively the behavior observed in neutron scattering measurements,<sup>39</sup> although one has to take into account the details of lattice structure to get more quantitative results. In Fig. 8 we show the density dependence of the incommensurability in the spin component of the static structure factor. The effect of V (not shown for clarity) appears as a suppression (positive V) or enhancement (negative V) of the peak.



FIG. 8. The spin component of the static structure factor at U = 4, V=0, and T=0.1, for n=0.8, 0.7, 0.6, and 0.5.



FIG. 9. The density dependence of the magnitude of the wave vector where the maximum of the spin structure factor appears at U=4 and T=0.5, for V=0.2, 0, and -0.2. The plateau at  $\sqrt{2}$  corresonds to the commensurate case  $\mathbf{q} = (\pi, \pi)$ .

The position of the maxima also moves to the left (positive V) or right (negative V).

To illustrate how the interaction V influences the incommensurability, we show in Fig. 9 the density dependence of the magnitude of the wave vector where is located the maximum in the spin structure factor when U=4, T=0.5, and V varies: V=0.2, 0, and -0.2. The plateau at  $|q_{max}| = \sqrt{2\pi/a}$ corresponds to the commensurate case  $\mathbf{q}_{max} = (\pi, \pi)$ . When V=0, the incommensurability depends only on the noninteracting susceptibility  $\chi_0$ , since the interaction has no wave vector dependence. This is clearly not the case for  $V \neq 0$ because of the cosine dependence of the effective interaction in Eq. (16). Positive V makes the spin fluctuations incommensurate, closer to half-filling with a maximum spin susceptibility that remains on the zone boundary for small V. Below a critical density the wave vector of the incommensurability decreases until it reaches  $|\mathbf{q}_{max}| = \pi/a$ . It stays at this value down to a very low V-dependent doping, where it generally begins to decrease. Incommensurability in general is also affected by details of the Fermi surface.<sup>40</sup>

In Fig. 10 we show the crossover temperature as a function of filling factor for V=-0.4, -0.2, 0, 0.2, and 0.4. At this temperature, the antiferromagnetic correlation length  $\xi$  begins to increase exponentially. This temperature is not precisely defined; however, as soon as the correlation length is large compared with the lattice spacing, the rise is rather sharp. Since the ratio  $\chi_{ss}(q_x,q_y,0)/\chi_0(q_x,q_y,0)$  scales as  $\xi^2$ at its peak (see Ref. 38 for more details), we identify the crossover temperature as that temperature where the ratio reaches a value of 100, corresponding to a correlation length  $\xi$  of order 10. 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 tempera-



FIG. 10. The crossover temperature as a function of filling factor for U=4 and V=-0.4, -0.2, 0, 0.2, and 0.4. Positive V reduces the strength of antiferromagnetic fluctuations while negative V has the opposite trend.

ture. When the ratio is taken as larger, the rounding occurs over a narrower range of densities. This can also be checked by standard finite-size scaling arguments. In general, there are quantum critical points at zero temperature where the exponential regime ends.<sup>41</sup> In Fig. 10, 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 nearestneighbor sites, and our method is quite accurate as long at |8V| < 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. Figure 11 corrects this by presenting the peak position (x or y component) 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. 10. 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 noninteracting susceptibility, but when V is finite there is also an 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 < 0and decreased when V > 0, concomitant with the tendency to increase or decrease the antiferromagnetic crossover temperature at half-filling.

# **IV. CONCLUSION AND SUMMARY**

We generalized the TPSC approach to the extended Hubbard model that contains nearest-neighbor repulsion V in ad-



FIG. 11. Magnitude of the wave vector where is located the maximum of the spin structure factor at the crossover temperature as a function of filling for U=4 and V=-0.4, -0.2, 0, 0.2, and 0.4.

dition to the usual on-site U term. That nonperturbative 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 approximations 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  $g_{\sigma\tilde{\sigma}}(0)$  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 simulations show that for 8V < 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, TPSC (Refs. 1 and 2) was the first method to obtain quantitative estimates for the crossover temperature to the renormalized-classical regime where spin fluctuations grow exponentially, diverging only at zero temperature, in agreement with the Mermin-Wagner theorem in two dimensions. Mean-field estimates are incorrect by hundreds of percent. The quantitative estimates obtained from TPSC were extremely useful in practice to study the pseudogap phenomenon in electron-doped cuprates near optimal doping.42,43 Incommensurability is also an aspect of the problem that can be addressed with TPSC that is beyond the reach of QMC, for example, because of finite-size effects. The extension of TPSC derived in the present paper was applied to quantify the effect of the near-neighbor interaction V. We found that when V > 0, its effect is to decrease both the crossover temperature and the range of dopings over which this crossover occurs. In addition, the crossover to 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 nonperturbative and quantitative estimates can be obtained. They are beyond the reach of standard methods such as 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: ANOTHER POSSIBILITY FOR FACTORIZATION

Here we would like to return to Eq. (8) in order to mention the Fock-type factorization of the V term, which can be introduced as follows:

$$\Sigma'_{\sigma}(1,2) = -V \sum_{a} G_{\sigma}(1,1+a) \,\delta(1+a,2) g_{xx}(1,1+a),$$
(A1)

where  $\Sigma'_{\sigma}(1,2)$  is the extra contribution to the self-energy in Eq. (9) ( $\Sigma'$  here does not mean the real part of the self-energy), and  $g_{xx}(a)$  is a new pair-correlation function, defined as

$$g_{xx}(a) = \frac{\langle T_{\tau} c_{\sigma}^{\dagger}(1+a) c_{\sigma}(1+a) c_{\sigma}^{\dagger}(1) c_{\sigma}(1) \rangle}{G_{\sigma}(1,1+a^{\dagger}) G_{\sigma}(1+a,1^{\dagger})}.$$
 (A2)

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

$$g_{xx}(a) = \frac{g_{\sigma\sigma}(a)n_{\sigma}^{2}}{G_{\sigma}(1, 1+a^{+})G_{\sigma}(1+a, 1^{+})}.$$
 (A3)

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

$$G_{\sigma}(1+a,1^{+}) = \int \frac{d\mathbf{q}}{\nu} e^{i\mathbf{q}\cdot\mathbf{a}} n_{\sigma}(\mathbf{q}) = \int \frac{d\mathbf{q}}{\nu} [\cos(\mathbf{q}\cdot\mathbf{a}) + i\sin(\mathbf{q}\cdot\mathbf{a})] n_{\sigma}(\mathbf{q}) = n_{c}(a) + in_{s}(a),$$
(A4)

where  $n_{\sigma}(\mathbf{q})$  is the momentum distribution  $\langle c_{\mathbf{q}\sigma}^{\dagger}c_{\mathbf{q}\sigma}\rangle$ . The extra contribution to the approximate self-energy is obtained by substituting Eq. (A4) and Eq. (A3) in Eq. (A1). The final form in Fourier space is

$$\Sigma_{\sigma}'(\mathbf{q}) = -2V n_{\sigma}^2 g_{\sigma\sigma}(a) \frac{n_c(a) [\cos(q_x a) + \cos(q_y a)] + n_s(a) [\sin(q_x a) + \sin(q_y a)]}{n_c(a)^2 + n_s(a)^2}.$$
 (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 final contribution of the above equation renormalizes the hopping term as follows:

$$t' = t + \frac{2V n_{\sigma}^2 g_{\sigma\sigma}(a)}{n_c(a)}.$$
 (A6)

The effect of this renormalization for positive V is merely a depression in the structure functions. The effect is opposit 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 nonzero 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 the presence of stripes in the system.<sup>44,45</sup>

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

$$\frac{\delta \Sigma'_{\sigma}(4,5)}{\delta G_{\sigma''}(6,7)} = -V \delta_{\sigma\sigma''} \sum_{a} \delta(4+a,5) \,\delta(4,6) \,\delta(4+a,7) g_{xx}(4,4) + a) - V \sum_{a} G_{\sigma}(4,4+a) \,\delta(4+a,5) \frac{\delta g_{xx}(4,4+a)}{\delta G_{\sigma''}(6,7)} .$$
(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:

$$\chi'_{\sigma\sigma}(1,2) = VG_{\sigma}(1,\bar{3})G_{\sigma}(\bar{3}+a,1)\frac{\delta G_{\sigma}(\bar{3},\bar{3}+a)}{\delta\phi_{\sigma}(2,2)}g_{xx}(\bar{3},\bar{3}+a).$$
(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. Equation (11) for parallel spins is our basic equation for this task. We replace  $1 \rightarrow 3$ ,  $2 \rightarrow 3+a$ , and  $3 \rightarrow 1$ , then multiply both sides of the equation by  $VG_{\sigma}(1,3)G_{\sigma}(3+a,1)g_{xx}(3,3+a)$ , finally performing a sum over the internal index 3. Using also Eq. (12) and the simplest approximation for the functional derivative that has Uas coefficient, the final result is given by the following equation:

$$\begin{split} \chi'_{\sigma\sigma}(1,2) &= \chi^{1V(2)}_{\sigma\sigma}(1,2) + Ug_{\sigma\tilde{\sigma}}(0)\chi^{1V(2)}_{\sigma\sigma}(1,\bar{4})\chi_{\tilde{\sigma}\sigma}(\bar{4},2) \\ &+ V\sum_{a,\sigma'} g_{\sigma\sigma'}(a)\chi^{1V(2)}_{\sigma\sigma}(1,\bar{4}+a)\chi_{\sigma'\sigma}(\bar{4}+a,2) \\ &+ Un_{\tilde{\sigma}}\sum_{\sigma'} \frac{\delta g_{\sigma\tilde{\sigma}}(0)}{\delta n_{\sigma'}}\chi^{1V(2)}_{\sigma\sigma}(1,\bar{4})\chi_{\sigma'\sigma}(\bar{4},2), \quad (A9) \end{split}$$

where  $\chi_{\sigma\sigma}^{1V(2)}(1,2)$  is

$$\chi_{\sigma\sigma}^{1V(2)}(\mathbf{q},\omega_n) = Vg_{xx}(a)G_{\sigma}(1,\bar{3})G_{\sigma}(\bar{3},2)G_{\sigma}(1,\bar{3}+a)G_{\sigma}(\bar{3}+a,2)$$
(A10)

while 1*V* 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  $\chi'_{\sigma\sigma}(1,2)$ . Equation (A9) and (13) after equating labels 1 and 2 [in Eq. (13)] form a set of coupled equations which in principle can be solved. Here we

tor and also as a separate factor in all terms; thus, 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:

$$\chi_{\sigma\sigma}^{1V(2)}(\mathbf{q},\omega_n) = g_{xx}(a) \int \frac{d\mathbf{k}}{\nu} \int \frac{d\mathbf{k}'}{\nu} \frac{f_{\sigma}\left(\mathbf{k} + \frac{\mathbf{q}}{2}\right) - f_{\sigma}\left(\mathbf{k} - \frac{\mathbf{q}}{2}\right)}{i\omega_n - (\boldsymbol{\epsilon}_{\mathbf{k}+\mathbf{q}/2} - \boldsymbol{\epsilon}_{\mathbf{k}-\mathbf{q}/2})} \frac{f_{\sigma}\left(\mathbf{k}' + \frac{\mathbf{q}}{2}\right) - f_{\sigma}\left(\mathbf{k}' - \frac{\mathbf{q}}{2}\right)}{i\omega_n - (\boldsymbol{\epsilon}_{\mathbf{k}'+\mathbf{q}/2} - \boldsymbol{\epsilon}_{\mathbf{k}'-\mathbf{q}/2})} \mathbf{V}(|\mathbf{k} - \mathbf{k}'|), \tag{A11}$$

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

$$\chi_{\sigma\sigma'}^{1V(1)}(\mathbf{q},\omega_n) = g_{\sigma\sigma'}(a)V(q)\chi_{\sigma\sigma}^0(\mathbf{q},\omega_n)^2.$$
(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.<sup>2,3,29,33</sup> This improved self-energy leads to one-particle spectral functions that compare extremely well with QMC in the case of the usual Hubbard model.<sup>3</sup> 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

$$\Sigma_{\sigma}(1,\overline{2})G_{\sigma}(\overline{2},3) = -U\langle T_{\tau}c_{\overline{\sigma}}^{\dagger}(1)c_{\overline{\sigma}}(1)c_{\sigma}(1)c_{\sigma}^{\dagger}(3)\rangle$$
$$-V\sum_{\sigma',a}\langle T_{\tau}c_{\sigma'}^{\dagger}(1+a)c_{\sigma'}(1+a)c_{\sigma}(1)c_{\sigma}^{\dagger}(3)\rangle$$
(B1)

$$= -U\left[\frac{\delta G_{\sigma}(1,3)}{\delta \phi_{\tilde{\sigma}}(1^{++},1^{+})} - G_{\tilde{\sigma}}(1,1^{+})G_{\sigma}(1,3)\right] \\ -V\sum_{\sigma',a}\left[\frac{\delta G_{\sigma}(1,3)}{\delta \phi_{\sigma'}(1+a^{++},1+a^{+})} - G_{\sigma'}(1+a,1+a^{+})G_{\sigma}(1,3)\right].$$
(B2)

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

$$\Sigma_{\sigma}(1,\bar{2})G_{\sigma}(\bar{2},1^{+}) = Un_{\sigma}n_{\tilde{\sigma}}g_{\sigma\tilde{\sigma}}(0) + 2Vn^{2}g_{cc}(a)$$
(B3)

$$= U[\chi_{\sigma\tilde{\sigma}}(1,1) + n_{\sigma}n_{\tilde{\sigma}}] + 2V[\chi_{cc}(1,1+a) + n^2], \quad (B4)$$

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

$$g_{\sigma\tilde{\sigma}}(0) = \frac{\chi_{\sigma\tilde{\sigma}}(1,1)}{n_{\sigma}n_{\tilde{\sigma}}} + 1,$$
$$g_{cc}(a) = \frac{\chi_{cc}(1,1+a)}{n^2} + 1$$
(B5)

hold. They are the real-space version of the fluctuationdissipation theorem.

We already approximated the self-energy using a factorization of Eq. (B1). Our factorization is exact in the limit 3  $\rightarrow 1^+$ , so we donot 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. (B3) 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,

$$\Sigma_{\sigma}(\mathbf{k},\omega_{n}) \approx (Un_{\tilde{\sigma}} + 4Vn) + \frac{T}{4} \sum_{\omega_{n'}} \int \frac{d\mathbf{q}}{\nu} \{UU_{ss}(\mathbf{q})\chi_{ss}(\mathbf{q},\omega_{n'}) + U_{cc}(\mathbf{q})[U + 4V\gamma(\mathbf{q})]\chi_{cc}(\mathbf{q},\omega_{n'})\}G_{0}(\mathbf{k} + \mathbf{q},\omega_{n'}) + \omega_{n'}\},$$
(B6)

where  $\gamma(\mathbf{q}) = \sum_{\alpha} \cos(q_{\alpha}a)$ . As we expect, the above formula for the self-energy Eq. (B6) satisfies the sum-rule in Eq. (B1). This, in fact, is a result of using Eqs. (21)–(24), 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

$$\Sigma'_{\sigma HF}(1,2) = -V \sum_{a} G_{\sigma}(1,1+a) \,\delta(1+a,2). \tag{B7}$$

One should include this correction term in the response function we already discussed in the previous section to take care of the presence of 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 satisfy the sum rule, Eq. (B3).

Following the procedure established for the ordinary Hubbard model,<sup>3,29</sup> one could also take into account transverse spin fluctuations and crossing symmetry to write a more general result.

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