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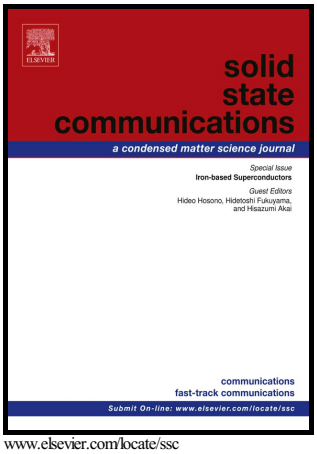

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Competition between spin and charge order in a one-dimensional lattice

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Abstract

In this paper, we study the presence of competing instabilities in one-dimensional (1D) extended Hubbard model (EHM). Using the extended two-particle self-consistent approximation (ETPSC), we derive the density and interaction dependent crossover diagram for spin and charge density wave fluctuations at arbitrary wave number. We determine the phase transitions of the system by means of spin and charge susceptibilities. We draw the phase diagram which separates different phases of the model for several effective particle densities.

Keywords: A. One-dimensional lattice; B. TPSC approach; D. Spin and charge susceptibilities; D. Phase diagram

1. INTRODUCTION

In the context of strongly correlated electron systems, single-band Hubbard model with on-site interaction U and hopping amplitude t is the simplest model of correlated electrons [1]. Inter-band hopping terms are ignored and referred to multi-band Hamiltonians[2]. Competing orders, due to the different particle interactions, in these type of systems are also quite common. For example, in high-temperature (hT_c) superconductors and some organic materials, the screening is not perfect so the site-site interactions play a considerable role, in such cases the Extended Hubbard model is also more useful. This Hamiltonian takes into account a nearest-neighbor interaction of strength V [3, 4]. This model has also been used to understand the behavior of quasi-one-dimensional materials including conductive polymers such as polyacetylene [5], organic-charge transfer materials such as $TTF-TCNQ$ or $(TMTSF)_2PF_6$ [6], carbon nanotubes [7] and Quantum wires[8]. In the present paper, we have used the extended version of the two-particle self-consistent (TPSC) approach that allows one to treat the extended Hubbard model. The ETPSC approach is a semi-analytical, non-perturbative and non-diagrammatic approach, at non-zero temperatures, which works best from weak to intermediate values of coupling (U and V less than the bandwidth $W = 2zt = 4dt$ with $z = 2$, the number of nearest neighbors, in $d = 1$)[9, 10]. The large-U limit of the model is referred to as the t-J model which is derivable by means of a canonical transformation as an expansion in t/U. People have calculated the boson and electron Green's functions of this model based on a diagrammatic, variational-derivative discription at [11]. Representation of Hamiltonian by X operators and then using the functional derivative approach is another powerful method to investigate the ground state propersites

of a system. In this direction people have calculated Bose-like Green's functions of t-J and Hubbard models [12, 13], which describes strongly interacting magnons and doublons. Similar works based on the functional derivative approach, following Kadanoff and Baym, have done earlier for Heisenberg and s-d models [14]. In the extended version of the TPSC approach, one includes not only a near-neighbor interaction V, but also some functional derivative term of pair correlation functions. The accuracy of this approach has been checked by comparing with Quantum Monte Carlo (QMC) simulations for a two-dimensional lattice [15, 16]. The use of functional derivative approach to find the physical quantities of different systems, suitable for computational and/or analytical purposes has also investigated in various conditions. The generating functional of different Green's functions for Hubbard model and single-impurity Anderson model has found based on an iterative solution at [17]. In this direction the Legendre transformation is another useful approach to find the variational-derivative equations for Hubbard and single-impurity Anderson models [18]. People have used the TPSC and ETPSC approach to investigate the associated effects due to charge and spin competition on honeycomb [19] and triangular[20] lattices, respectively. Unlike Parquet re-summations, Fluctuation-exchange (FLEX) and Random Phase approximation (RPA), this method satisfies not only conservation laws, but also the Pauli principle, Mermin-Wagner theorem and sum rules for spin and charge fluctuations. These fluctuations govern the spin and charge susceptibilities in ETPSC and are similar to those appearing in RPA. Longitudinal spin susceptibility of a Heisenberg ferromagnet in RPA-type form, based on a diagrammatic technique in terms of variational derivative functional equations is followed at [21]. Susceptibilities in ETPSC are momentum and frequency dependent and are computed self-consistently in such a way that local sum rules are satisfied. Note that this approach was developed to study the single band Hubbard model [22, 23]. The competition between charge and spin orders has also been studied in two [24], three [25] and higher dimensions [26]. The one dimensional case has been studied at various fillings [27, 28]. Depending on the strengths of the interactions, the ground state phase diagram of the one-dimensional EHM undergoes different phases. For repulsive on-site interactions U which are sufficiently large compared to the inter-site repulsion V, specifically, for $U > 2V$, the ground state is a spin density wave (SDW) phase. For $2V > U$, the ground state has charge density wave (CDW) order. In one-dimensional case, there have seen a first order spin density wave to charge density wave transition at $U = 2V$ line [38]. In this work, we present the ETPSC formalism, which focuses on finding a set of closed equations for irreducible spin and charge vertices. At last, we present the numerical results for spin and charge response functions and $U - V - T$ phase diagrams. In order to determine the phase diagram of this system, we calculate self-consistently two thermodynamical quantities to the renormalized classical regime for charge and spin fluctuations at three fillings, $n = 0.5, 1$ and 1.25. It is particularly worth noting that, at the renormalized classical regime, spin and/or charge fluctuations are large and correlation length becomes greater than the thermal de Broglie wavelength.

2. THEORY AND METHOD

We have used the Extended Hubbard model to describe a many fermion system, on a one-dimensional lattice. This one band Hamiltonian just consider nearest neighbour hopping with intra-site and inter-site Coulombic interactions of U and V , respectively

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

where μ is the chemical potential and $c_{i\sigma}$ is the annihilation operator for electrons with spin $\sigma =\uparrow, \downarrow$, at site i and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. The parameter n is the particle number per site and in this case that we are dealing with non-magnetic states $\langle n_{\downarrow}(\mathbf{r}) \rangle = \langle n_{\uparrow}(\mathbf{r}) \rangle = n/2$. Extended TPSC is a non-perturbative approach which is based on the two-particle Green's function formalism and allows one to treat the EHM.

One of the most important steps in this method is to correctly find the Heisenberg equation of motion, and after a comparison between it and Dyson's equation [9, 29], we are able to find an explicit expression for the self-energy Σ,

$$\Sigma_{\sigma}(1,2) = -U \langle T_{\tau} n_{\tilde{\sigma}}(1) c_{\sigma}(1) c^{\dagger}_{\sigma}(\bar{3}) \rangle G^{-1}_{\sigma}(\bar{3},2) - V \sum_{a,\sigma'} \langle T_{\tau} n_{\tilde{\sigma}'}(1+a) c_{\sigma}(1) c^{\dagger}_{\sigma}(\bar{3}) \rangle G^{-1}_{\sigma}(\bar{3},2) \tag{2}$$

where summation on a runs over the nearest-neighbour sites of site 1. In the above formula, numbers with over-bar mean a summation (integration) over the corresponding spatial dimensions (including imaginary time), and $\tilde{\sigma} = -\sigma$. By the definition of pair correlation function $g_{\sigma,\sigma'}(i,j)$, Eq. (3), we can find a more effective form of self-energy, Eq. (2),

$$g_{\sigma,\sigma'}(i,j) \equiv \frac{\langle n_{\sigma}(i) n_{\sigma'}(j) \rangle - \delta(i,j)\delta_{\sigma\sigma'} \langle n_{\sigma}(i) \rangle}{\langle n_{\sigma}(i) \rangle \langle n_{\sigma'}(j) \rangle} \tag{3}$$

For electrons with spin, this quantity is proportional to probability of finding one electron with spin σ' on site j, when another electron with spin σ is held on site i. Note that if $g_{\sigma,\sigma'}(i,j) = 1$ one can recover the RPA approximation, $g_{\sigma\sigma}(0) = 0$ according to Pauli principle. Based on the previous definition and the definition of Green's function and Wick's theorem [30] we reached to a more practical form for the Σ_{σ},

$$\Sigma_{\sigma}(1,2) = U G_{\tilde{\sigma}}(1,1^{+}) \delta(1,2) g_{\sigma\tilde{\sigma}}(1,1) + V \sum_{a,\sigma'} G_{\sigma'}(1+a, 1+a^{+}) \delta(1,2) g_{\sigma\sigma'}(1,1+a) \tag{4}$$

In this equation, if time at 1 is τ_1 then at 1^{+} becomes $\tau_1 + \epsilon$ in the limit of $\epsilon \to 0$. The pair correlation function corresponding to U term is associated with electrons in the same site but with

different spins, obviously it is different for nearest-neighbour electrons. By including of pair correlation functions, the corresponding expression for the self-energy is beyond the Hartree-Fock approximation. In order to find the response (four-point) functions, first we need to find an expression for the functional derivative of the Green's function with respect to the weak external field,

$$\chi_{\sigma\sigma'}(1,2;3,4) \equiv -\frac{\delta G_\sigma(1,2)}{\delta \phi_{\sigma'}(3,4)} \tag{5}$$

At equation (5), after the use of Dyson's equation ($G_\sigma^{-1}(1,2) = G_\sigma^{(0)-1}(1,2) - \phi_\sigma(1,2) - \Sigma_\sigma(1,2)$), and the identity $G_{\sigma'}(1,\bar{1})G_\sigma^{-1}(\bar{1},2) = \delta(1-2)\delta_{\sigma'\sigma}$ we have to find an expression for the functional derivative of the self-energy, Eq. (4) with respect to the Green's function, (irreducible vertex) $\delta\Sigma_\sigma/\delta G_{\sigma'}$. According to the equation (4), to find the irreducible vertex, first we need to know the functional derivative of the pair correlation function with respect to the Green's function.

Based on the ETPSC formalism, we are able to evaluate an explicit expression for the functional derivative of the pair correlation functions. One way, of course, is to simply ignore all these terms, as it is done earlier based on the Singwi approach [31] to the electron gas [32]. In the ETPSC approach we replace the unknown functional derivative terms by functional derivatives with respect to the density as $\frac{\delta g_{\sigma\sigma'}(1,2)}{\delta G_{\sigma''}(3,4)} \approx \frac{\delta g_{\sigma\sigma'}(1,2)}{\delta n_{\sigma''}(3)}\delta(3,4)$ where $n_\sigma(1) = G_\sigma(1,1)$. To evaluate this type of functional derivative, point 3 must coincide with either 2 or 1, then we have a simpler equation to evaluate

$$\frac{\delta g_{\sigma\sigma'}(1,2)}{\delta n_{\sigma''}(3)} \approx \frac{\delta g_{\sigma\sigma'}(1,2)}{\delta n_{\sigma''}(1)}\frac{\delta n_{\sigma''}(1)}{\delta n_{\sigma''}(3)} + \frac{\delta g_{\sigma\sigma'}(1,2)}{\delta n_{\sigma''}(2)}\frac{\delta n_{\sigma''}(2)}{\delta n_{\sigma''}(3)} \tag{6}$$

These unknown functional derivative terms enter the spin (11) and charge (12) vertices. More simplifications are based on the particle-hole (PH) symmetry [16]. Placement of this approximation in Eq. (5), for the irreducible vertex $\delta\Sigma_\sigma/\delta G_{\sigma'}$, will lead to an explicit expression for the response (four-point) function $\chi_{\sigma\sigma'}(1,2;3,4)$. After this step and reducing the four-particle response function to two-particle, we are ready to find the dynamic correlation functions for the density and magnetization, they are given by the following definition for susceptibilities,

$$\chi_{cc,ss}(1;2) \equiv \sum_{\sigma\sigma'}(\sigma\sigma')\chi_{\sigma\sigma'}(1;2) \tag{7}$$

$$\chi_{cc,ss}(1;2) = 2[\chi_{\sigma\sigma}(1;2) \pm \chi_{\sigma\bar{\sigma}}(1;2)], \tag{8}$$

To obtain the response functions of the system, we set the external potential equal to zero. The final factored form of charge and spin susceptibilities in Fourier-Matsubara space are given by

$$\chi_{cc,ss}(\mathbf{q},\omega) = \frac{\chi^0(\mathbf{q},\omega)}{1 \pm \frac{\chi^0(\mathbf{q},\omega)}{2}U_{cc,ss}(\mathbf{q})}, \tag{9}$$

In the above equation, $\chi^0(\mathbf{q},\omega)$ is the non-interacting (free) response function,

$$\chi^0(\mathbf{q},\omega_n)=\int_{BZ}\frac{d\mathbf{p}}{\nu}\frac{f^0(\mathbf{p}+\frac{\mathbf{q}}{2})-f^0(\mathbf{p}-\frac{\mathbf{q}}{2})}{i\omega_n-\epsilon_{\mathbf{p}+\mathbf{q}/2}+\epsilon_{\mathbf{p}-\mathbf{q}/2}}. \tag{10}$$

and $\omega_n = (2n+1)\pi T$ is the fermionic Matsubara frequency. In the TPSC approach, in order to meet the charge and spin sum rules we introduce two independent effective interactions, $U_{cc}(\mathbf{q})$ for the charge channel and $U_{ss}(\mathbf{q})$ for the spin channel, given by

$$U_{ss}=Ug_{\sigma\tilde{\sigma}}-4V\Big\{g_{ss}(1,1+a)\gamma(\mathbf{q})+n\frac{\delta g_{s\sigma}(1,1+a)}{\delta m(1)}\Big\}, \tag{11}$$

$$U_{cc}=U\Big[g_{\sigma\tilde{\sigma}}(1,1)+n\frac{\delta g_{\sigma\tilde{\sigma}}(1,1)}{\delta n(1)}\Big]+4V\Big\{g_{cc}(1,1+a)\gamma(\mathbf{q})+n\frac{g_{s\sigma}(1,1+a)}{\delta n(1)}[1+\gamma(\mathbf{q})]\Big\}. \tag{12}$$

where, $f^0(\mathbf{q})=1/[1+exp((\epsilon_{\mathbf{q}}-\mu_0)/T)]$ is the free momentum distribution function, $\epsilon_{\mathbf{q}}=-2t\cos(qa)$ is the free particle dispersion relation and $\gamma(\mathbf{q})=\cos(qa)$, all associated to a one dimensional lattice. The extension of above relations to square [16], triangle [20] and cubic lattices is straightforward. We must find some equal expressions for the functional derivatives of the pair correlation functions at Eqs. (11-12). In order to do that, we use the PH symmetry to obtain the following equations:

$$\frac{\delta g_{s\sigma}(1,2)}{\delta n(1)}=\frac{\delta g_{s\sigma}(1,2)}{\delta m(1)}=\big[1-g_{cc}(1,2)\big] \tag{13}$$

$$\frac{\delta g_{\uparrow\downarrow}(1,1)}{\delta n(1)}=2\big[1-g_{\uparrow\downarrow}(1,2)\big] \tag{14}$$

These equations are valid just when PH symmetry is satisfied. In the case of square lattice, this validity has been checked by comparison with QMC calculations even in the absence of PH symmetry [16]. Note that, pair correlation functions are related to instantaneous structure factors by

$$g_{cc}(\mathbf{r}_j)=1+\frac{1}{n}\int_{BZ}\frac{d\mathbf{q}}{\nu}\big[S_{cc}(\mathbf{q})-1\big]exp(i\mathbf{q}.\mathbf{r}_j) \tag{15}$$

$$g_{ss}(\mathbf{r}_j)=\frac{1}{n}\int_{BZ}\frac{d\mathbf{q}}{\nu}\big[S_{ss}(\mathbf{q})-1\big]exp(i\mathbf{q}.\mathbf{r}_j) \tag{16}$$

where $S_{ss,cc}(\mathbf{q})=S_{\sigma\sigma}(\mathbf{q})\mp S_{\sigma\tilde{\sigma}}(\mathbf{q})$ are the instantaneous spin and charge structure factors. These quantities relate to the corresponding response functions by the fluctuation-dissipation theorem. In another word, self-consistency in this method is established by connecting the static structure factors to the response functions through the fluctuation-dissipation theorem,

$$S_{cc,ss}(\mathbf{q})=\frac{T}{n}\sum_{\omega_n}\chi_{cc,ss}(\mathbf{q},\omega_n) \tag{17}$$

3. Numerical results

In this section, we present our simulation results by substitution the above equations for pair correlation functions and functional derivatives in expressions for irreducible local field vertices, U_{cc} and U_{ss}. A quantity which gives information about the evolution of the charge/spin excitations in the system is the corresponding charge/spin susceptibility. Our first result is the non-interacting (Lindhard function) case as Fig. 1 for different values of density $n = 0.75, 1, 1.5$ and 1.75 at $T = 0.4$.

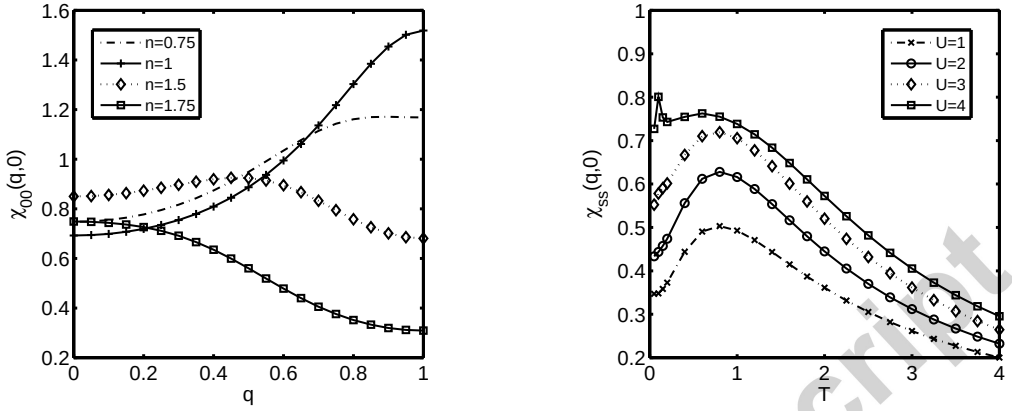

Figure 1: The free response function (left plane) for different densities at $n = 0.75, 1, 1.5$ and 1.75 for $T = 0.4$ and static spin susceptibilities χ_{ss} (right plane) at $n = 0.5$ and $V = 1$ for $U = 4, 3, 2$ and 1 as a function of temperature at $q = \pi/a$.

Note that we are working in units where $k_B = t = \hbar = 1$. The largest response is for $n = 1$, with a symmetric structure (in the range $-1 < q < 1$) like the others. At higher values of density, there is a deep minimum at $q = 1$, this is the main reason for the absence of spin or charge ordering. In the presence of interactions, the interacting response functions are strongly modified, as shown for the typical values of $U = 4$ and $V = 1$. The shape of the non-interacting susceptibility, Eq. (10) is mostly determined by the non-interacting dispersion relation $\gamma(\mathbf{q})$.

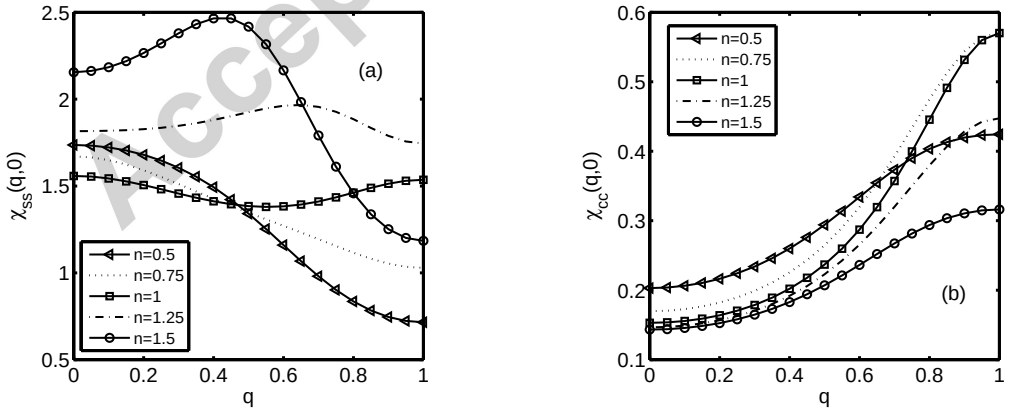

Figure 2: The spin (a) and charge (b) response function, at fixed value of $U = 3.5, V = 1, T = 0.4$ and different values of the densities $n = 0.5, 0.75, 1, 1.25$ and 1.5.

Temperature evolution of χ_{ss} for weak and intermediate coupling at $n = 0.5$ is presented in Fig. 1. As it is clear the position of the maximum does not strongly depend on the U interactions and located around $T = 0.8$. This implicates that the energy necessary to have spin excitations are somehow independent of the charge. The situation is different at half filling case [35]. In Fig. 2 we show the spin and charge response functions for the values of q correspond to the first Brillouin zone and $T = 0.4$. Note that since our response functions are symmetric with respect to q, we have just considered half of the Brillouin zone. In the ETPSC approach, the presence of V term at the Hubbard Hamiltonian, introduces a wave vector dependent vertex as in Eqs. (11,12). According to Fig. 2(a), spin fluctuations correspond to different fillings have maxima at various values of q. For the values of density less than unity, spin fluctuations are very small than the other n's. The height of the peaks increases when V is reduced, hence nearest-neighbour repulsion does not favor spin order. This situation is different at Fig. 2(b), for charge response function. In this figure, all characteristic curves have maxima at the end of the Brillouin zone for all densities. By comparison between Figs. 2(a) and 2(b) one noticed that CDW fluctuations are suppressed in favor of SDW fluctuations for these values of U and V. This scenario is different for the other values of interactions. The dominant role that is played by on-site inetration U is examined in a symmetrical Hubbard model at $T = 0K$ in the $d = \infty$ limit. In this study the key quantities of the system like density of states (DOS), internal energy and paramagnetic susceptibilty are abtained as a fucntion of U. Based on the calculations, the system would be in the formation of local moments or in the strong Kondo scattering region, which indicates the occurrence of a structural rearrengment [36].

The importance of the functional derivative terms and accuracy of their evaluation have significant consequences on the final results. We also emphasize that all these low-temperature behaviors are non-perturbative. The high-temperature behavior where the quantities vary smoothly can be understood perturbatively.

Phase diagrams

We now turn to the corresponding phase diagrams (in the $U - V$ parameter space) of this system. The results of this section are good examples of what is happening in a correlated matter, and that what important role is played by the electronic interactions. Basic assumptions and formalizations of the ETPSC approach in the case of attractive Hubbard model (negative values of interactions) could be followed along the lines of [33, 34]. The phase transition is between two competing states of matter which are different in symmetry, and away from the phase transition one of the two states wins the contest. These ordering competitions are not long ranged, according to the Mermin-Wagner theorem. Either the charge or the spin correlations grow exponentially at some characteristic wave vector q, that suggests which long-range order will likely be stabilized at zero temperature. Since our approach is not valid deep in the renormalized classical regime, one cannot be sure that the zero-temperature phase will be precisely what suggested by the behavior at T_x. In each curve the crossover temperature

at which we may have order is different compared to the others. The corresponding wave vectors and crossover temperatures T_x at which either spin or charge diverged, are obtained from the conditions $\chi_{ss}(q,0)/\chi_0(q,0) = 10$ or $\chi_{cc}(q,0)/\chi_0(q,0) = 10$. In the case of non-interacting neighbours ($V = 0$), just Lindhard function $\chi_0(q,0)$ is responsible in determining of the dominant q. In the present case that V interactions are considered, this scenario changes, since it introduces a wave vector dependence to the vertices, as in Eqs. (11,12). Figures. (3 and 4) show the corresponding phase diagrams of the system at $n = 0.5, 1$ and 1.25.

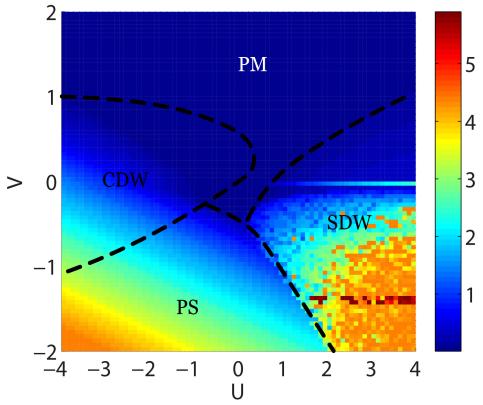

Figure 3: (Color online) Value of the crossover temperature T_x to the renormalized classical regime as a function of U and V at filling $n = 0.5$. The wave vector and spin or charge character of the growing correlations is indicated by initials: Spin density waves (SDW), phase separation, or $\mathbf{q} = 0$ charge instability (PS), charge density waves (CDW) and paramagnetic (PM) region. The color scale appears on the right of the plot. Regions where either U or V are negative are shown for illustrative purposes only.

In each characteristic curve, there are separated regions by dotted line, which clarify four different fluctuating regimes. Spin-density wave (SDW), charge-density wave (CDW), paramagnetic (PM), and phase separation (PS), regimes. There have seen a non-direct transition at half filling case, near the $U = 2V$ line between the CDW and the SDW states[37]. In the weak to intermediate-coupling region, some kind of spin-charge separation is present. This behavior is more obvious for half filling and $n = 1.25$ cases. If one goes away from the $U = 2V$ line towards larger V at $U < 0$, spin degrees of freedom are canceled and leaves us a CDW degree of freedom, as shown in [38].

The PS regime is defined by the growth of charge response function at $q = \omega = 0$, in this regime the negative values of U and V favor charge instabilities at zero wave vector. Indeed, at negative values of interactions, superconducting fluctuations will be competing. Since superconductivity has not been considered here, the results should be taken as just indicative of what might happen in the spin or charge sectors. The PM region is somewhere that neither the spin nor charge response functions can satisfy the above mentioned criteria even at very low temperature ($T = 0.01$). In other words, even at low temperatures, each local or long range order in this region, is suppressed. The portion of PM region in Fig.(3) for $n = 0.5$ is larger than other densities and this state of matter occurs mostly at

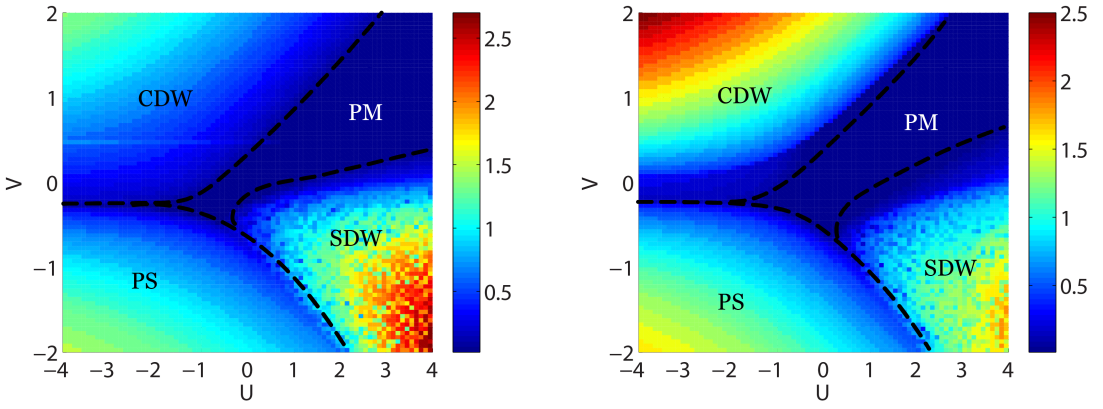

Figure 4: (Color online) Crossover temperature T_x to the renormalized classical regime as a function of U and V at filling $n = 1$ (left panel) and $n = 1.25$ (right panel)

positive values of U and V. At small and positive values of V toward the negative ones, SDW phase is the dominant degree of freedom. By increasing of n charge density wave area grows and occurs at higher values of T_x.

4. conclusion

To summarize, in this paper, we have studied the ground state behavior of the one-dimensional extended Hubbard model using the extended Two-particle self-consistent approach. This model describes a system of correlated electrons with on-site repulsion U, the inter-site electron-electron interaction V and hopping amplitude t. With the assumption that the interaction terms U and V are less that the lattice bandwidth W, we find the ground state phase diagrams of this system. In this direction, spin and charge degrees of freedom play an important role. We used the particle-hole symmetry to estimate the functional derivatives of the pair-correlation function in the local field charge and spin vertices. Our results show that spin and charge degrees of freedom are arranged in the form of SDW, CDW and PS phases. At the paramagnetic phase, there is no divergence in susceptibilities. Localization of single charges on different sites occur in the region where SDW correlations are strongest, namely $U \geq -2V \geq 0$. At negative values of U and V we have PS region, and for $-2V \leq U \leq 0$, CDW is the dominant phase, therefore in these two regions charge instabilities are favored. The methodology of the present paper can be applied to systems with different structures and/or longer-range interactions, as it is under study.

5. ACKNOWLEDGMENT

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