

**Effective Ising model for correlated systems with charge ordering**E. A. Stepanov,<sup>1,2</sup> A. Huber,<sup>3</sup> A. I. Lichtenstein,<sup>2,3</sup> and M. I. Katsnelson<sup>1,2</sup><sup>1</sup>*Radboud University, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands*<sup>2</sup>*Theoretical Physics and Applied Mathematics Department, Ural Federal University, Mira Street 19, 620002 Ekaterinburg, Russia*<sup>3</sup>*Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany*

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Collective electronic fluctuations in correlated materials give rise to various important phenomena, such as charge ordering, superconductivity, Mott insulating and magnetic phases, and plasmon and magnon modes. Unfortunately, the description of these correlation effects requires significant effort, since they almost entirely rely on strong local and nonlocal electron-electron interactions. Some collective phenomena, such as magnetism, can be sufficiently described by simple Heisenberg-like models that are formulated in terms of bosonic variables. This fact suggests that other many-body excitations can also be described by simple bosonic models in the spirit of Heisenberg theory. Here we derive an effective bosonic action for charge degrees of freedom for the extended Hubbard model and define a physical regime where the obtained action reduces to a classical Hamiltonian of an effective Ising model.

DOI: [10.1103/PhysRevB.99.115124](https://doi.org/10.1103/PhysRevB.99.115124)**I. INTRODUCTION**

Remarkably, the majority of studies of collective charge excitations in modern condensed matter theory is still limited to the random phase approximation (RPA) [1–3]. Although this approach fulfills the charge conservation law and provides a qualitatively good description of plasmonic modes, it is based on a perturbation expansion and, strictly speaking, is applicable only to systems with relatively small Coulomb interaction. A correct description of plasmons in the correlated regime of large electron-electron interactions requires consideration of additional diagrammatic contributions to the electronic self-energy and polarization operator that contain vertex corrections. Unfortunately, the latter implies the use of advanced numerical techniques, which in the case of realistic calculations is extremely time-consuming. Additional diagrammatic corrections often violate the charge conservation law [4,5], which affects the result for the plasmonic spectrum. Nevertheless, recently a new theory that allows a conserving description of plasmons beyond RPA was proposed in Ref. [6]. This approach is based on the Dual Boson (DB) theory [7,8] and considers the polarization operator in the two-particle ladder form written in terms of local three- and four-point vertex functions. A further extension of this method to the multiorbital case is challenging due to its complicated diagrammatic structure.

Another interesting feature of collective charge excitations in many realistic materials is a tendency of the systems to the charge ordering (CO), which is widely discussed in the literature starting from the discovery of the Verwey transition in magnetite  $\text{Fe}_3\text{O}_4$  [9–11]. Nowadays, there is a number of other materials, such as the rare-earth compound  $\text{Yb}_4\text{As}_3$  [12–14], transition metal  $\text{MX}_2$  [15–17] and rare-earth  $\text{R}_3\text{X}_4$  [18–20] chalcogenides ( $\text{M} = \text{V}, \text{Nb}, \text{Ta}$ ;  $\text{R} = \text{Eu}, \text{Sm}$ ;  $\text{X} = \text{S}, \text{Se}$ ), Magnéli phase  $\text{Ti}_4\text{O}_7$  [21–24], vanadium bronzes  $\text{Na}_x\text{V}_2\text{O}_5$  and  $\text{Li}_x\text{V}_2\text{O}_5$  (see Refs. [14,25], and references

therein), where the charge ordering has been observed. Since this phenomenon is based on the presence of strong local and nonlocal electron-electron interactions, the theoretical description of this issue also requires the use of very advanced approaches (see, e.g., Refs. [26,27]).

Recent theoretical investigations of charge correlation effects caused by the strong nonlocal Coulomb interaction indicate that the description of collective charge excitations in the correlated regime can be drastically simplified. Thus, the study of the charge ordering within the dynamical cluster approximation (DCA) [28], Dual Boson [29,30], and GW+EDMFT [4,31] approaches showed similar results for the phase boundary between the normal and CO phases at half filling. The fact that a much simpler GW+EDMFT theory performs in reasonable agreement with the more advanced DB approach and with almost exact DCA method suggests that collective charge fluctuations can be described via a simple theory, at least in a specific physical regime. Unfortunately, the use of the GW+EDMFT theory for description of charge excitations is not fully justified, since this approach suffers from the Fierz ambiguity when the charge and spin channels are considered simultaneously [32,33], and from the “HS-UV/V” decoupling problem [34,35]. In this regard, the simplified (DB – GW) [29,30] approximation of the DB theory, which does not consider vertex corrections and is free of the above-mentioned problems, seems more preferable. However, it provides much worse results than the DB [30] and GW+EDMFT [31] theories. Therefore, the problem of the efficient description of collective charge excitations in correlated materials is still open.

In the case when accurate quantum mechanical calculations are challenging, the initial quantum problem can be replaced by an appropriate classical one. This thermodynamical approach is widely used, for example, for a description of the ordering in alloys [36–41]. There, the total energy of the ground state is mapped onto an effective Ising Hamiltonian,

with parameters determined from *ab initio* calculations within the framework of the density functional theory [42–44]. However, to our knowledge, no attempts to extend this theory to the description of charge fluctuations in the correlated regime and to derive the pair interaction of the Ising model directly from the quantum problem have been reported yet. Additional impulse for investigation of this important problem is given by theoretical studies of magnetism in correlated electronic systems [45–49], where an effective classical Heisenberg model for the quantum problem was derived. Since magnetism is also a collective electronic property, one may expect that charge degrees of freedom can be treated in a similar way.

Motivated by the above discussions, we introduce here a new theory that describes charge excitations of the extended Hubbard model in terms of bosonic variables that are related to electronic charge degrees of freedom. The corresponding bosonic action of the model is derived with the use of the advanced ladder DB approach. Consequently, the charge susceptibility has a complicated diagrammatic structure that takes into account frequency dependent vertex corrections. We also observe that the dependence of local vertex functions on fermionic frequencies is directly connected to the value of the double occupancy of lattice sites. Moreover, we find that in a wide range of physical parameters, when the double occupancy is large, this dependence is negligible, and the expression for the charge susceptibility can be drastically simplified. Thus, the theory reduces to an improved version of the GW+EDMFT and DB – GW approaches, where the susceptibility takes a simple RPA+EDMFT form. The further application of the derived simple theory to the hole-doped extended Hubbard model shows almost perfect agreement of the obtained result for the phase boundary between the normal and CO phases with much more elaborate and time-consuming ladder DB and DCA [50] methods. Finally, it has been shown that in the case of well-developed collective charge fluctuations the initial quantum problem can be mapped onto an effective classical Ising Hamiltonian written in terms of pair interaction between charge densities. This formalism can be efficiently used for the calculation of finite-temperature thermodynamic properties of the system. For instance, we show that the effective Ising model predicts the transition temperature between the normal and charge ordered phases in a good agreement with the DCA result, although our calculations are performed in the unbroken symmetry phase.

## II. BOSONIC ACTION FOR ELECTRONIC CHARGE

Let us start with the following action of the extended Hubbard model written in the Matsubara frequency  $(\nu, \omega)$  and momentum  $(\mathbf{k}, \mathbf{q})$  space:

$$\mathcal{S} = - \sum_{\mathbf{k}, \nu} c_{\mathbf{k}\nu}^* [i\nu + \mu - \varepsilon_{\mathbf{k}}] c_{\mathbf{k}\nu} + \frac{1}{2} \sum_{\mathbf{q}, \omega} [U + V_{\mathbf{q}}] \rho_{\mathbf{q}\omega}^* \rho_{\mathbf{q}\omega}. \quad (1)$$

Here  $c_{\mathbf{k}\nu}^*$  ( $c_{\mathbf{k}\nu}$ ) are Grassmann variables corresponding to the creation (annihilation) of an electron.  $\varepsilon_{\mathbf{k}}$  is the Fourier transform of the hopping amplitude  $t_{ij}$ , which is considered here in the nearest neighbor approximation on a two-dimensional square lattice. The energy scale is  $4t = 1$ .  $U$  and  $V_{\mathbf{q}}$  are

local and nonlocal Coulomb interactions, respectively. Charge degrees of freedom are described here introducing the bosonic variable  $\rho_{\mathbf{q}\omega} = n_{\mathbf{q}\omega} - \langle n_{\mathbf{q}\omega} \rangle$  that describes variation of the electronic density  $n_{\mathbf{q}\omega} = \sum_{\mathbf{k}, \nu, \sigma} c_{\mathbf{k}\nu\sigma}^* c_{\mathbf{k}+\mathbf{q}, \nu+\omega, \sigma}$  from the average value. Hereinafter, spin labels  $\sigma = \uparrow, \downarrow$  are omitted.

An effective bosonic action for charge degrees of freedom can be derived following transformations, as presented in a recent work [49]. There, the lattice action Eq. (1) is divided into the local impurity problem of the extended dynamical mean-field theory (EDMFT) [51–55] and the remaining nonlocal part. To decouple the single-electronic and collective charge degrees of freedom, one can perform *dual* transformations of the nonlocal part of the lattice action that lead to a new problem written in the *dual* space [29,30]. The inverse transformation back to the initial “lattice” space after truncation of the interaction of the *dual* action at the two-particle level results in the following bosonic action for charge variables (for details see Ref. [49] and Appendix A):

$$\mathcal{S}_{\text{ch}} = -\frac{1}{2} \sum_{\mathbf{q}, \omega} \rho_{\mathbf{q}\omega}^* X_{\mathbf{q}\omega}^{-1} \rho_{\mathbf{q}\omega}. \quad (2)$$

Here, the charge susceptibility  $X_{\mathbf{q}\omega}$  in the conserving ladder DB approximation is given by the following relation [49]:

$$X_{\mathbf{q}\omega}^{-1} = [X_{\mathbf{q}\omega}^{\text{DMFT}}]^{-1} + \Lambda_{\omega} - V_{\mathbf{q}}, \quad (3)$$

where  $\Lambda_{\omega}$  is the local bosonic hybridization function of the impurity problem.  $X_{\mathbf{q}\omega}^{\text{DMFT}} = \sum_{\nu, \nu'} [X_{\mathbf{q}\omega}^{\text{DMFT}}]_{\nu\nu'}$  is the charge susceptibility in the DMFT form [56,57] written in terms of lattice Green’s functions  $G_{\mathbf{k}\nu}$  and two-particle irreducible (2PI) in the charge channel four-point vertices  $\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}}$  of the local impurity problem (see Appendix A):

$$[X_{\mathbf{q}\omega}^{\text{DMFT}}]_{\nu\nu'}^{-1} = [X_{\mathbf{q}\omega}^0]_{\nu\nu'}^{-1} + \bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}}. \quad (4)$$

Here,  $[X_{\mathbf{q}\omega}^0]_{\nu\nu'} = \sum_{\mathbf{k}} G_{\mathbf{k}+\mathbf{q}, \nu+\omega} G_{\mathbf{k}\nu} \delta_{\nu\nu'}$  is a generalized bare lattice susceptibility, and the inversion should be understood as a matrix operation in the fermionic frequency  $\nu, \nu'$  space. Note that in the ladder DB approximation the lattice Green’s function is dressed only in the local impurity self-energy and therefore coincides with the usual EDMFT expression [51–55]. Thus, the relation for the lattice susceptibility can be written as  $X_{\mathbf{q}\omega} = \sum_{\nu, \nu'} [X_{\mathbf{q}\omega}]_{\nu\nu'}$ , where

$$[X_{\mathbf{q}\omega}]_{\nu\nu'}^{-1} = [X_{\mathbf{q}\omega}^0]_{\nu\nu'}^{-1} - U_{\nu\nu'\omega}^{\text{eff}} - V_{\mathbf{q}}, \quad (5)$$

and we introduced an effective bare local Coulomb interaction

$$U_{\nu\nu'\omega}^{\text{eff}} = -\Lambda_{\omega} - \bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}}. \quad (6)$$

Note that the 2PI vertex function  $\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}}$  is defined here in the particle-hole channel.

A recent study of magnetism of correlated electrons [49] shows that if the system exhibits well-developed bosonic fluctuations, the corresponding local vertex functions mostly depend on bosonic frequency  $\omega$ , while their dependence on fermionic frequencies  $\nu, \nu'$  is negligible. Therefore, one can expect that in a physical regime where charge fluctuations are dominant the local 2PI vertex function in the charge channel can be approximated as  $\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}} \simeq \bar{\gamma}_{\omega}^{2\text{PI}}$ , and the charge susceptibility Eq. (3) takes the following simple form:

$$X_{\mathbf{q}\omega}^{-1} = X_{\mathbf{q}\omega}^{0-1} - (U_{\omega}^{\text{eff}} + V_{\mathbf{q}}). \quad (7)$$

Here,  $X_{\mathbf{q}\omega}^0 = \sum_{\nu\nu'} [X_{\mathbf{q}\omega}^0]_{\nu\nu'} = \sum_{\mathbf{k}\nu} G_{\mathbf{k}+\mathbf{q},\nu+\omega} G_{\mathbf{k}\nu}$  is the bare lattice susceptibility, and the effective bare local Coulomb interaction Eq. (6) transforms to  $U_{\omega}^{\text{eff}} = -\Lambda_{\omega} - \bar{\gamma}_{\omega}^{2\text{PI}}$ . As it is also shown in Ref. [49] and Appendix B, in the considered case of well-developed collective fluctuations the 2PI vertex function can be approximated as

$$\gamma_{\omega}^{2\text{PI}} \simeq \chi_{\omega}^{-1} - \chi_{\omega}^{0-1} \simeq -U - \Lambda_{\omega}, \quad (8)$$

where  $\chi_{\omega}$  and  $\chi_{\omega}^0$  are the full and bare local susceptibilities of the impurity problem, respectively. As a consequence, the effective bare local Coulomb interaction reduces to the actual value of the local Coulomb interaction  $U_{\omega}^{\text{eff}} \simeq U$ . Therefore, the expression in Eq. (7) is nothing more than the RPA susceptibility constructed on top of the EDMFT result for Green's functions. This simplified approximation is referred in the text to as the RPA+EDMFT approach.

It is worth noting that in the regime of strong charge fluctuations the local self-energy takes the same form as in GW approach [58–60] (see Ref. [49] and Appendix B). Hence, the simplified theory can be reduced to the GW method in the case when the nonlocal contribution to the self-energy is also considered. Thus, we show that it is indeed possible to describe strong charge excitations by a simple bosonic action Eq. (2) in terms of charge susceptibility Eq. (7) that does not contain vertex corrections.

### III. REGIME OF STRONG CHARGE FLUCTUATIONS

Now, let us define the physical regime where the presented above technique is applicable. In Ref. [49] collective excitations have been studied in the ordered (antiferromagnetic) phase, where the proximity of the local magnetic moment  $m$  to its maximum value served as a signature of well-developed spin fluctuations. Here, we are interested in a similar description of a more complicated case when collective charge excitations are present in the system already in the normal phase. Since in the latter case all lattice sites are described by the same local impurity problem, the corresponding signature of strong bosonic fluctuations can no longer be found among local single-particle observables that are identical for every lattice site. It is worth mentioning that, contrary to the magnetic phase where the ordering of single-particle quantities (local magnetizations) is realized, the CO phase on a lattice corresponds to the ordering of doublons (see, e.g., Refs. [61,62]) that are two-particle observables. Thus, the double-occupancy of the lattice site, which is defined as  $d = \langle n_{\uparrow} n_{\downarrow} \rangle$  with the maximum value  $d_{\text{max}} = 0.25$  in the normal phase, can be proposed as a fingerprint of the existence of strong charge fluctuations in the system.

The corresponding result for the double occupancy of the two-dimensional extended Hubbard model Eq. (1) on the square lattice is shown on the  $U$ - $V$  phase diagram in Fig. 1 and obtained using the DB approach [63] without the approximation of the four-point vertex function introduced above. The phase boundary (red dashed line) between the normal (colored) and CO (gray) phases is determined from the zeros of the inverse charge susceptibility  $X_{\mathbf{q}\omega}^{-1}$  (3) at  $\mathbf{q} = (\pi, \pi)$  and  $\omega = 0$  point similarly to Refs. [29,30]. As already mentioned in the Introduction, this result for the phase boundary is in a very good agreement with the DCA calculations performed in

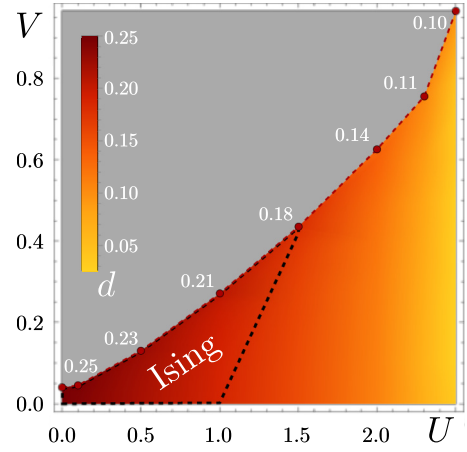


FIG. 1. Double occupancy of the extended Hubbard model shown on the  $U$ - $V$  phase diagram. Calculations are performed in the normal phase where the value of the double occupancy  $d$  is depicted by color. The gray part corresponds to the charge ordered phase. Values of the double occupancy at the phase boundary are explicitly mentioned. The area depicted by the black dashed line corresponds to the case of large value of the double occupancy  $d \gtrsim 70\% d_{\text{max}}$  and shows the regime where charge excitations can be described by an effective Ising model. Values of Coulomb interactions  $U$  and  $V$  are given in units of half of the bandwidth ( $W/2 = 4t = 1$ ). Therefore, the effective Ising model can be used for a broad range of values of the Coulomb interaction, which may even exceed half of the bandwidth. The inverse temperature is  $\beta = 50$ .

Ref. [28]. As expected, large charge fluctuations in the normal phase emerge in the region close to the phase transition to the ordered state. However, one can see that the strength of these fluctuations is not uniformly distributed along the phase boundary, since the value of  $d$  decreases with the increase of the local Coulomb interaction.

To clarify the connection between the value of the double occupancy and the strength of charge fluctuations, one can study an effective bare local Coulomb interaction  $U_{\nu\nu'\omega}^{\text{eff}}$  defined in Eq. (6). Figure 2 shows the ratio  $U_{\nu\nu'\omega}^{\text{eff}}/U$  between the effective and actual local Coulomb interactions as the function of fermionic frequency  $\nu$  at the  $\nu' = \omega = 0$  point. This result is obtained close to the phase boundary between the normal and CO phases shown in Fig. 1 for different values of the local Coulomb interaction  $U$  and, as a consequence, of the double occupancy  $d$ . The exact values of  $U$ ,  $V$ , and  $d$  for these calculations are specified in Table I. Here, one can immediately see that the effective Coulomb interaction

TABLE I. Double occupancy  $d$ , correction  $U'$  to the effective local Coulomb interaction  $U^{\text{eff}}$ , and static dielectric function  $\varepsilon$  obtained close to the phase boundary between the normal and CO phases for the given values of the local  $U$  and nonlocal  $V$  Coulomb interactions.

$U$	0.1	0.5	1.0	1.5	2.0	2.5
$V$	0.045	0.130	0.265	0.420	0.630	0.965
$d$	0.25	0.23	0.21	0.18	0.14	0.10
$U'$	-0.48	-0.68	-1.11	-1.81	-2.85	-5.24
$\varepsilon$	1.26	3.78	10.09	6.00	3.35	1.91

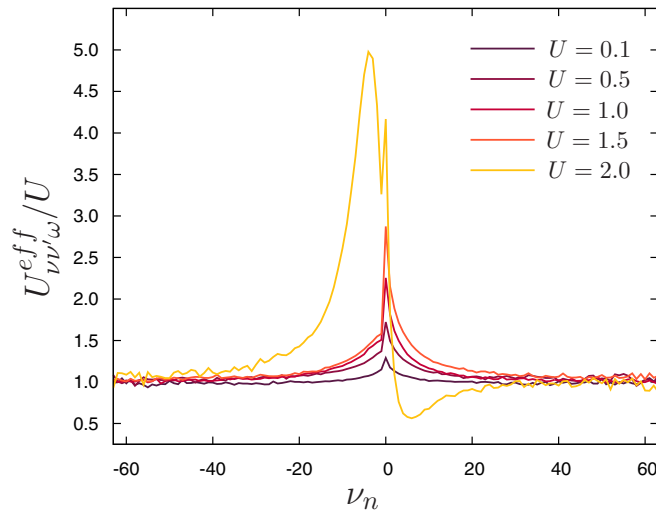


FIG. 2. Frequency dependence of the effective local Coulomb interaction  $U_{\nu\nu'\omega}^{\text{eff}}$  obtained for different values of  $U$  at the phase boundary between the normal and CO phases at the  $\nu' = 0$  and  $\omega = 0$  point for  $\beta = 50$ . As the double occupancy  $d$  is decreased, the dependence of the effective interaction  $U_{\nu\nu'\omega}^{\text{eff}}$  on fermionic frequency becomes larger.

at small values of  $U$  (large values of  $d$ ) is almost frequency independent. Decreasing the double occupancy, the frequency dependence of  $U^{\text{eff}}$  becomes crucial, and one can no longer approximate the local 2PI vertex function by neglecting its dependence on fermionic frequencies. Remarkably, the effective Coulomb interaction tends to the actual value of the local Coulomb interaction at large frequencies for every value of  $U$ , which is in perfect agreement with the theory presented above. A similar asymptotic behavior was reported for the 2PI vertex function of the DMFT impurity problem ( $\Lambda_\omega = 0$ ) in Ref. [64]. Thus, one can conclude that the presence of the bosonic hybridization function  $\Lambda_\omega$  in the local impurity problem changes local vertex functions. The presence of  $\Lambda_\omega$  in Eq. (3) restores the correct frequency behavior of the lattice susceptibility by canceling the bosonic hybridization from the vertex function in the effective local interaction. Therefore, the inclusion of the  $\Lambda_\omega$  in the theory has to be done consistently both in the local impurity problem and the lattice susceptibility Eq. (3); otherwise, it may lead to incorrect frequency behavior of bosonic quantities. Results for  $U_{\nu\nu'\omega}^{\text{eff}}/U$  for other values of  $\nu'$  and  $\omega$  can be found in Appendix A and show a similar connection of the double occupancy to the frequency dependence of the effective Coulomb interaction.

Let us now investigate the dependence of the effective local Coulomb interaction on the bosonic frequency  $\omega$ . As shown in Fig. 2, the use of the fermionic frequency independent approximation  $\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}} \simeq \bar{\gamma}_\omega^{2\text{PI}}$  for the 2PI vertex in the large double occupancy regime is now justified. Then, the effective Coulomb interaction  $U_\omega^{\text{eff}}$  can be extracted from the simplified expression for the charge susceptibility Eq. (7), where the left-hand side is substituted from Eq. (3). Since the leading contribution to the lattice susceptibility in this regime is given by the  $\mathbf{q} = (\pi, \pi)$  momentum, the corresponding effective

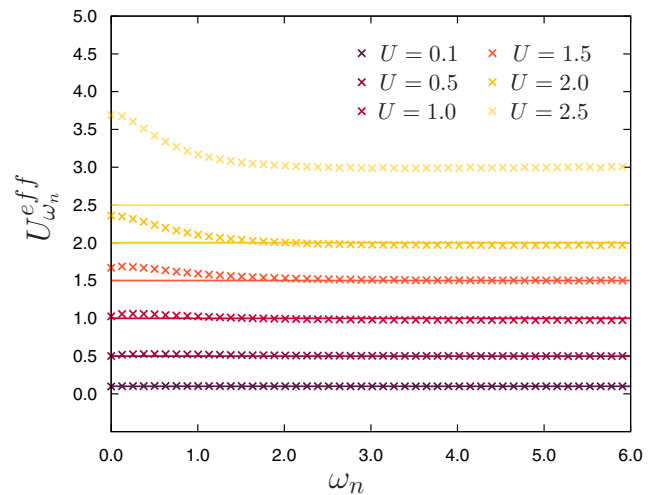


FIG. 3. Frequency dependence of the effective local Coulomb interaction  $U_\omega^{\text{eff}}$  obtained for  $\beta = 50$  close to the phase boundary between the normal and charge ordered phases for different values of the actual Coulomb interaction  $U$ . When the double occupancy is decreased, the difference between the effective and actual local Coulomb interactions becomes more notable.

interaction shown in Fig. 3 reads

$$U_\omega^{\text{eff}} = X_{(\pi,\pi),\omega}^{0-1} - [X_{(\pi,\pi),\omega}^{\text{DMFT}}]^{-1} - \Lambda_\omega. \quad (9)$$

Here, the result is obtained in the normal phase close to the CO for the same values of Coulomb interactions as in Fig. 2. It is worth mentioning that the above definition of the effective local Coulomb interaction is similar to the one of the two-particle self-consistent theory proposed by Vilk and Tremblay [65]. However, we use a more advanced ladder DB Eq. (3) for the lattice susceptibility, contrary to the RPA form with bare Green's functions considered in their work.

Remarkably, when the double occupancy is close to its maximum value, the effective Coulomb interaction  $U^{\text{eff}}$  does not depend on bosonic frequency either and again coincides with the actual Coulomb interaction. In the smaller  $d$  regime the bosonic frequency dependence appears and cannot be avoided for consideration anymore. Therefore, the large value of the double occupancy is indeed an indicator of a well-developed charge fluctuations. Taking into account results shown in Figs. 2 and 3, the value of the double occupancy for which the effective local interaction is frequency independent and coincides with the bare local Coulomb interaction  $U$  can be estimated as  $d \gtrsim 70\% d_{\text{max}}$ . As schematically shown in Fig. 1 by the black dashed line, the corresponding region where the use of a simple RPA+EDMFT approach is justified can be distinguished for the relatively broad range of Coulomb interactions. Surprisingly, the latter may even exceed half of the bandwidth.

#### IV. EXTENDED HUBBARD MODEL UPON DOPING

Calculation of phase boundaries became a standard test for the performance of the introduced theory [4,28–30,50]. To demonstrate the power of the derived above RPA+EDMFT approach in description of strong charge fluctuations, let us

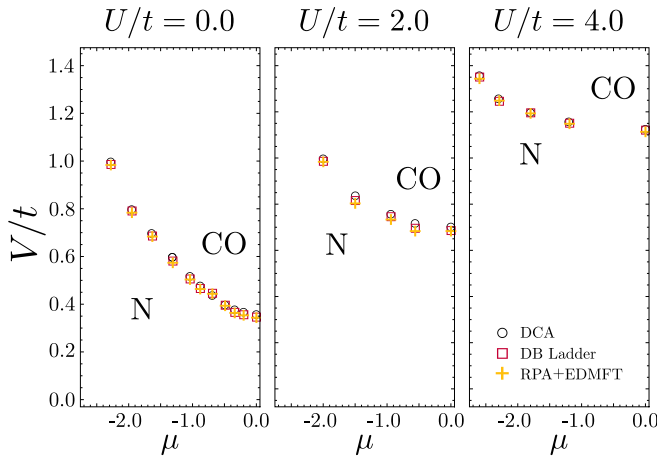


FIG. 4. Phase boundary between the normal (N) and charge-ordered (CO) phases of the hole-doped extended Hubbard model in the space of nearest-neighbor interaction  $V$  and chemical potential  $\mu$ . Calculations are performed for the Ladder DB and RPA+EDMFT approaches in the regime of large double occupancy where the use of the simplified approximation is justified. The DCA data is kindly provided by authors of the Ref. [50]. The local interaction is  $U = 0$  (left panel),  $U = 0.5$  (middle panel), and  $U = 1$  (right panel). The hopping amplitude is  $t = 0.25$ .  $\mu = 0$  corresponds to the half filling. All data are obtained for  $\beta = 12.5$  ( $T = 0.08$ ).

investigate the phase boundary between the normal and CO phases of the extended Hubbard model beyond the half filling. Recently, this issue has been addressed with the use of the dynamical cluster approximation [50] in the hole-doped case. DCA is a very advanced approach, which is based on a cluster dynamical mean field theory. Thus, the result obtained in Ref. [50] for the phase boundary can be considered as a benchmark. In the previous section we have distinguished the physical regime of applicability of the RPA+EDMFT approach at the half filling. This region is depicted by the black dashed line in Fig. 1. To study the performance of the RPA+EDMFT approach against more advanced ladder DB and DCA theories, we obtain the phase boundary in the same region of physical parameters upon the hole doping. The corresponding result is shown in Fig. 4 in the space of nearest-neighbor interaction  $V$  and chemical potential  $\mu$  for  $U = 0$  (left panel),  $U = 0.5$  (middle panel), and  $U = 1$  (right panel). The value of the chemical potential is counted from the half filling ( $\mu = 0$ ). The temperature  $T = 0.08$  ( $\beta = 12.5$ ) for numerical calculations is taken the same as in Ref. [50]. The RPA+EDMFT result (yellow pluses) for the phase boundary is obtained using Eq. (7) for the charge susceptibility, where the effective local interaction  $U_{\omega}^{\text{eff}}$  is replaced by the actual value of the Coulomb interaction  $U$  according to above discussions. The ladder DB result (red squares) is obtained using Eq. (3) as a single-shot calculation on top of the converged EDMFT solution. The DCA data (black circles) is kindly provided by the authors of Ref. [50].

Figure 4 shows that results for the phase boundary between the normal (N) and charge ordered (CO) phases almost perfectly coincide for all three theories for different values of local Coulomb interaction. Remarkably, the result of RPA+EDMFT is in a good agreement with more elaborate

methods even at large values of doping. Thus, results for the phase boundary have been compared up to 17%, 18%, and 20% of hole-doping for  $U = 0$ ,  $U = 0.5$ , and  $U = 1$ , respectively. This fact is even more surprising, since the RPA+EDMFT operates only with Green's functions of the single-site EDMFT solution of the problem, while the Dual Boson approach requires a calculation of local vertex functions to perform the diagrammatic extension of the EDMFT. The converged EDMFT solution for a one point in parameter space can be obtained, for example, within 20 iterations (20 min each) on a single node of the North-German Supercomputing Alliance (HLRN) cluster. At the same time, the simplest single shot ladder DB calculation requires additional iteration that is to be performed on the same cluster already on four nodes (each node contains 24 cores), which takes at least 60 min more for the one point.

Multiorbital version the Dual Boson theory is much more time-consuming, since it requires numerical calculation of vertex functions in the enlarged parameter space, and is not yet implemented. The extension of the DCA method to the multi-orbital case is even more complicated. An additional difficulty here corresponds to the fact that DCA calculations cannot be performed at reasonably low temperatures beyond the half filling due to the sign problem. For this reason, the comparison between three theories has been performed at  $\beta = 12.5$ , while previous DB calculations were done for much lower temperature  $\beta = 50$ . Therefore, the RPA+EDMFT appears to be a very appealing approach for the description of strong collective excitations in the multiorbital case, since it does not require complicated numerical efforts other than the EDMFT solution of the problem.

## V. EFFECTIVE ISING MODEL

In general, the existence of separate dynamics and a corresponding classical Hamiltonian for charge degrees of freedom is questionable. The possibility to introduce a classical problem for certain collective excitations is usually related to the existence of an adiabatic parameter that distinguishes these excitations from others that belong to different energy and timescales. Thus, in the case of spin fluctuations the adiabatic approximation is intuitive and implies that collective (spin) degrees of freedom are slower and have lower energy than single-particle (electronic) excitations [66]. Unfortunately, the corresponding adiabatic approximation for charge degrees of freedom does not exist. Therefore, it is very challenging to find a specific physical regime where the classical problem for charge degrees of freedom can still be introduced. As was recently obtained for spin fluctuations [49], the possibility of different energy and timescales separation lies in a nontrivial frequency behavior of local vertex functions. If the dependence of the local vertex on fermionic (single-particle) frequencies is negligibly small compared to the bosonic (collective) frequency dependence, then the separation of the corresponding bosonic excitation is justified.

Thus, in the regime of the large value of the double occupancy ( $d > 70\% d_{\text{max}}$ ), which is shown in Fig. 1 by the dashed black line, the quantum action Eq. (2) can be mapped onto an effective classical Hamiltonian, similarly to the case of collective spin fluctuations with the well-defined

local moment [49]. Note that in the case of charge degrees of freedom, the classical problem is given by the effective Ising Hamiltonian,

$$H_{\text{ch}} = - \sum_{\mathbf{q}} J_{\mathbf{q}} \sigma_{\mathbf{q}} \sigma_{-\mathbf{q}}, \quad (10)$$

written in terms of classical variables  $\sigma = \pm 1$ . An effective pair interaction  $J_{\mathbf{q}}$  between electronic densities can be defined from the nonlocal part of the inverse charge susceptibility at the zero bosonic frequency [48,49]. Additionally, quantum variables  $\rho_{\mathbf{q}\omega}^{(*)}$  that describe a deviation of the local electronic density from the average (half-filled) value have to be replaced in Eq. (2) as follows  $\rho_{\mathbf{q}\omega}^* \rho_{\mathbf{q}\omega} \rightarrow 2d \sigma_{\mathbf{q}} \sigma_{-\mathbf{q}}$ . To distinguish local and nonlocal contributions to the inverse susceptibility Eq. (3), one can again use an approximated version of the local 2PI vertex function in the charge channel. Since the latter does not depend on fermionic frequencies in the regime of well-developed charge fluctuations, the full four-point vertex  $\bar{\gamma}_{v\nu'\omega}$  of the impurity problem can also be approximated by the leading bosonic contribution. According to the Ref. [49] the latter corresponds to the full local charge susceptibility  $\chi_{\omega}$  that connects two three-point vertex functions  $\gamma_{v\omega}$  (for details see Appendix A):

$$\bar{\gamma}_{v\nu'\omega} \simeq -\gamma_{v\omega} \chi_{\omega} \gamma_{\nu'+\omega, -\omega} = \langle \text{---} \rangle, \quad (11)$$

Then, the relation Eq. (3) for the charge susceptibility reduces to

$$X_{\mathbf{q}\omega}^{-1} = \chi_{\omega}^{-1} + \Lambda_{\omega} - V_{\mathbf{q}} - \tilde{\Pi}_{\mathbf{q}\omega}^{(2)}, \quad (12)$$

where the second-order polarization operator reads

$$\tilde{\Pi}_{\mathbf{q}\omega}^{(2)} = \sum_{\mathbf{k}\nu} \gamma_{\nu+\omega, -\omega} \tilde{G}_{\mathbf{k}+\mathbf{q}, \nu+\omega} \tilde{G}_{\mathbf{k}\nu} \gamma_{\nu, \omega}, \quad (13)$$

and  $\tilde{G}_{\mathbf{k}\nu}$  is a nonlocal part of the lattice Green's function. Then, the effective pair interaction takes the following form:

$$\begin{aligned} J_{\mathbf{q}}/d &= -V_{\mathbf{q}} - \sum_{\mathbf{k}, \nu} \gamma_{\nu, 0} \tilde{G}_{\mathbf{k}+\mathbf{q}, \nu} \tilde{G}_{\mathbf{k}\nu} \gamma_{\nu, 0} \\ &= -V_{\mathbf{q}} - \langle \text{---} \rangle. \end{aligned} \quad (14)$$

Using an exact relation between the 2PI four-point and full three-point vertices, the latter can also be approximated as

$$\gamma_{v\omega} \simeq \chi_{\omega}^{-1} + \Lambda_{\omega} + U_{v\nu'\omega}^{\text{eff}} \simeq \chi_{\omega}^{0-1}, \quad (15)$$

as shown in Appendix B. Therefore, the result for the pair interaction Eq. (14) between electronic densities at first glance reduces to a similar expression for the exchange interaction derived for the magnetic system in Ref. [49]. However, the ‘‘correction,’’

$$U' = \chi_{\omega=0}^{-1} + \Lambda_{\omega=0}, \quad (16)$$

to the effective bare Coulomb interaction  $U^{\text{eff}}$  in Eq. (15) is larger than the local Coulomb interaction  $U$  as shown in Table I. This is not surprising, because the relatively large value of the inversed local charge susceptibility, which is defined as  $\chi_{\omega} = -\langle n_{\omega}^* n_{\omega} \rangle$ , when two electrons occupy the same lattice site is expected. Therefore, the term  $U'$  cannot

be neglected, contrary to the case of spin fluctuations at half-filling when the inversed local magnetic susceptibility  $\chi_{\omega=0}^{-1}$  is negligibly small [49]. Since the effective bare Coulomb interaction  $U^{\text{eff}}$  in the regime of large double occupancy coincides with the actual value of  $U$ , one can obtain a static approximation for the three-point vertex (see Appendix B),

$$\gamma_{v,0} \simeq \chi_{\omega=0}^{0-1} \simeq -\frac{U}{\varepsilon - 1} = -\tilde{U}, \quad (17)$$

where  $\varepsilon = U/\mathcal{W}_0$  is a static dielectric function defined via the renormalized local interaction  $\mathcal{W}_{\omega}$ . Therefore, the final expression for the pair interaction of the effective classical Ising model reads

$$J_{\mathbf{q}}/d = -V_{\mathbf{q}} - \sum_{\mathbf{k}, \nu} \tilde{U} \tilde{G}_{\mathbf{k}+\mathbf{q}, \nu} \tilde{G}_{\mathbf{k}\nu} \tilde{U}. \quad (18)$$

The effective Ising model can be used for modeling finite-temperature thermodynamic properties of the system, such as the electronic density, charge susceptibility, ground-state energy, and configurational structure of material [36–41]. All these observables make sense in the broken symmetry (CO) phase. These calculations are beyond the scope of the current paper. However, the Ising model also provides an analytical result for the transition temperature  $T_c$  between the normal and CO phases,

$$T_c = 2J/\ln(\sqrt{2} + 1), \quad (19)$$

where  $J = J_{\mathbf{q}=(\pi, \pi)}/4$  approximates the nearest-neighbor pair interaction. The result for the transition temperature can be compared to the one of Ref. [50] (Fig. 3). To this aim, we obtain the effective exchange interaction at  $U = 0.5$  for the same values of the nonlocal Coulomb interaction  $V = 0.19$  and  $V = 0.275$  used in Ref. [50]. Transition temperatures obtained within the DCA in these two cases are  $T_c = 0.103$  ( $\beta \simeq 9.69$ ) and  $T_c = 0.204$  ( $\beta \simeq 4.90$ ), respectively. Since we perform our calculations in the normal phase, the effective exchange interaction was obtained above the critical temperature at  $\beta = 8$  and  $\beta = 3$ , respectively. These temperatures still allow us to get reasonably large values of the double occupancy to justify the use of the effective Ising model. Estimated critical temperatures in our calculations are  $T_c = 0.114$  ( $J = 0.050$ ,  $d = 0.230$ ) and  $T_c = 0.190$  ( $J = 0.084$ ,  $d = 0.247$ ), respectively, which is in a good agreement with corresponding DCA results. Note that our calculations were performed in the unbroken symmetry phase. We believe that the agreement for the critical temperature is much better for calculations performed in the charge-ordered phase, where the value of the double occupancy is larger and collective fluctuations are much stronger.

## VI. CONCLUSION

In this work the bosonic action Eq. (2) for charge degrees of freedom of the extended Hubbard model Eq. (1) has been derived. It was found that local four-point vertex function of the impurity model is independent on fermionic frequencies in the regime of well-developed charge fluctuations. Remarkably, the latter can be efficiently determined looking at the deviation of the double occupancy from its maximum value. Thus, strong charge fluctuations are revealed in the case of

large double occupancy ( $d \gtrsim 70\% d_{\max}$ ), which corresponds to a broad range of values of Coulomb interaction. As a consequence, it was found that in this regime the dynamics of charge fluctuations can be described via a simplified RPA+EDMFT charge susceptibility Eq. (7) constructed from the EDMFT Green's functions. Moreover the effective local Coulomb interaction in this case coincides with the actual value of the bare Coulomb interaction. Remarkably, the RPA+EDMFT theory performs in a good agreement with more advanced methods even beyond the half filling. Thus, this simple approach correctly predicts the phase boundary between the normal and CO phases up to 20% of hole doping in a broad range of values of Coulomb interaction. The latter can even reaching the half of the bandwidth ( $U/t = 4$ ). Further, it was shown that in the regime of well-developed charge fluctuations, the initial quantum problem can be mapped onto an effective classical Ising model written in terms of a pair interaction between local electronic densities. This is a nontrivial result, since collective charge excitations cannot be separated from single electronic ones in the same way as it is usually done for spins, because the corresponding adiabatic approximation for charge degrees of freedom does not exist. Importantly, the expression for the pair interaction contains only single-particle quantities, which can be efficiently used in realistic multiband calculations. The predicted critical temperature of the effective Ising model is in a good agreement with the one of the DCA result, which allows to believe that this simple model can be efficiently used for calculation of finite-temperature thermodynamic properties of the system in the ordered phase. We further speculate that similar approximations are valid for realistic multiband systems that reveal strong charge fluctuations.

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#### APPENDIX A: BOSONIC ACTION FOR THE EXTENDED HUBBARD MODEL

Here we explicitly derive a bosonic problem for charge degrees of freedom of the extended Hubbard model. For this reason, one can divide the lattice action Eq. (1) into the local

impurity  $\mathcal{S}_{\text{imp}}$  and nonlocal  $\mathcal{S}_{\text{rem}}$  parts following the standard procedure of the DB theory [7,29]

$$\begin{aligned} \mathcal{S}_{\text{imp}} = & - \sum_{\nu, \sigma} c_{\nu\sigma}^* [i\nu + \mu - \Delta_\nu] c_{\nu\sigma} + U \sum_{\omega} n_{\omega\uparrow}^* n_{\omega\downarrow} \\ & + \frac{1}{2} \sum_{\omega} \Lambda_\omega \rho_\omega^* \rho_\omega, \end{aligned} \quad (\text{A1})$$

$$\begin{aligned} \mathcal{S}_{\text{rem}} = & - \sum_{\mathbf{k}, \nu, \sigma} c_{\mathbf{k}\nu\sigma}^* [\Delta_\nu - \varepsilon_{\mathbf{k}}] c_{\mathbf{k}\nu\sigma} + \frac{1}{2} \sum_{\mathbf{q}, \omega} [V_{\mathbf{q}} - \Lambda_\omega] \rho_{\mathbf{q}\omega}^* \rho_{\mathbf{q}\omega} \\ & + \sum_{\mathbf{q}, \omega} j_{\mathbf{q}\omega}^* \rho_{\mathbf{q}\omega}, \end{aligned} \quad (\text{A2})$$

where we introduced fermionic  $\Delta_\nu$  and bosonic  $\Lambda_\omega$  hybridization functions, and sources  $j_{\mathbf{q}\omega}$  for bosonic variables. The partition function of our problem is given by the following relation:

$$\mathcal{Z} = \int D[c^*, c] e^{-\mathcal{S}}, \quad (\text{A3})$$

where the action  $\mathcal{S}$  is given by Eq. (1). Using the Hubbard–Stratonovich transformation of the reminder term  $\mathcal{S}_{\text{rem}}$ , one can introduce *dual* fermionic  $f^*$ ,  $f$ , and bosonic variables  $\phi$  as follows:

$$\begin{aligned} & e^{\sum_{\mathbf{k}, \nu, \sigma} c_{\mathbf{k}\nu\sigma}^* [\Delta_\nu - \varepsilon_{\mathbf{k}}] c_{\mathbf{k}\nu\sigma}} \\ & = D_f \int D[f] e^{-\sum_{\mathbf{k}, \nu, \sigma} (f_{\mathbf{k}\nu\sigma}^* [\Delta_\nu - \varepsilon_{\mathbf{k}}]^{-1} f_{\mathbf{k}\nu\sigma} + c_{\mathbf{k}\nu\sigma}^* f_{\mathbf{k}\nu\sigma} + f_{\mathbf{k}\nu\sigma}^* c_{\mathbf{k}\nu\sigma})}, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} & e^{\frac{1}{2} \sum_{\mathbf{q}, \omega} \rho_{\mathbf{q}\omega}^* [\Lambda_\omega - V_{\mathbf{q}}] \rho_{\mathbf{q}\omega}} \\ & = D_\phi \int D[\phi] e^{-\left(\frac{1}{2} \sum_{\mathbf{q}, \omega} \phi_{\mathbf{q}\omega}^* [\Lambda_\omega - V_{\mathbf{q}}]^{-1} \phi_{\mathbf{q}\omega} + \phi_{\mathbf{q}\omega}^* \rho_{\mathbf{q}\omega}\right)}, \end{aligned} \quad (\text{A5})$$

where terms  $D_f = \det[\Delta_\nu - \varepsilon_{\mathbf{k}}]$  and  $D_\phi^{-1} = \sqrt{\det[\Lambda_\omega - V_{\mathbf{q}}]}$  can be neglected when calculating expectation values. Rescaling fermionic and bosonic fields on corresponding Green's functions of the impurity problem as  $f_{\mathbf{k}\nu}^* \rightarrow f_{\mathbf{k}\nu}^{(*)} g_{\nu}^{-1}$  and  $\phi_{\mathbf{q}\omega} \rightarrow \phi_{\mathbf{q}\omega} \chi_\omega^{-1}$ , and shifting bosonic variables, the nonlocal part of the action transforms to

$$\begin{aligned} \mathcal{S}_{\text{DB}} = & - \sum_{\mathbf{k}, \nu, \sigma} f_{\mathbf{k}\nu\sigma}^* g_{\nu\sigma}^{-1} [\varepsilon_{\mathbf{k}} - \Delta_\nu]^{-1} g_{\nu\sigma}^{-1} f_{\mathbf{k}\nu\sigma} \\ & + \sum_{\mathbf{k}, \nu, \sigma} [c_{\mathbf{k}\nu\sigma}^* g_{\nu\sigma}^{-1} f_{\mathbf{k}\nu\sigma} + f_{\mathbf{k}\nu\sigma}^* g_{\nu\sigma}^{-1} c_{\mathbf{k}\nu\sigma}] \\ & + \sum_{\mathbf{q}, \omega} \phi_{\mathbf{q}\omega} \chi_\omega^{-1} \rho_{\mathbf{q}\omega} - \frac{1}{2} \sum_{\mathbf{q}, \omega} (\phi_{\mathbf{q}\omega}^* - j_{\mathbf{q}\omega}^* \chi_\omega) \\ & \times \chi_\omega^{-1} [V_{\mathbf{q}} - \Lambda_\omega]^{-1} \chi_\omega^{-1} (\phi_{\mathbf{q}\omega} - \chi_\omega j_{\mathbf{q}\omega}). \end{aligned} \quad (\text{A6})$$

Integrating out initial degrees of freedom with respect to the impurity action Eq. (A1), one gets [7]

$$\begin{aligned} & \int D[c] e^{-\sum_i \mathcal{S}_{\text{imp}}^{(i)} - \sum_{\mathbf{k}, \nu, \sigma} [c_{\mathbf{k}\nu\sigma}^* g_{\nu\sigma}^{-1} f_{\mathbf{k}\nu\sigma} + f_{\mathbf{k}\nu\sigma}^* g_{\nu\sigma}^{-1} c_{\mathbf{k}\nu\sigma}] - \sum_{\mathbf{q}, \omega} \phi_{\mathbf{q}\omega}^* \chi_\omega^{-1} \rho_{\mathbf{q}\omega}} \\ & = \mathcal{Z}_{\text{imp}} \times e^{-\sum_{\mathbf{k}, \nu, \sigma} f_{\mathbf{k}\nu\sigma}^* g_{\nu\sigma}^{-1} f_{\mathbf{k}\nu\sigma} - \frac{1}{2} \sum_{\mathbf{q}, \omega} \phi_{\mathbf{q}\omega}^* \chi_\omega^{-1} \phi_{\mathbf{q}\omega} - \tilde{W}[f, \phi]}, \end{aligned} \quad (\text{A7})$$

where  $\mathcal{Z}_{\text{imp}}$  is a partition function of the impurity problem. Here, the interaction  $\tilde{W}[f, \phi]$  is presented as an infinite series

of full vertex functions of the local impurity problem Eq. (A1) [7,8]. The lowest order interaction terms are

$$\begin{aligned} \tilde{W}[f, \phi] = & \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \sum_{v, v', \omega} \sum_{\sigma(\ell)} \left( \phi_{\mathbf{q}\omega}^* \gamma_{v\omega} f_{\mathbf{k}v\sigma}^* f_{\mathbf{k}+\mathbf{q}, v+\omega, \sigma} \right. \\ & \left. - \frac{1}{4} \bar{\gamma}_{vv'\omega} f_{\mathbf{k}v\sigma}^* f_{\mathbf{k}+\mathbf{q}, v+\omega, \sigma'} f_{\mathbf{k}'+\mathbf{q}, v'+\omega, \sigma''} f_{\mathbf{k}'v'\sigma'''} \right), \end{aligned} \quad (\text{A8})$$

where the full three- and four-point vertex functions are defined as

$$\begin{aligned} \gamma_{v\omega} = & \langle c_{v\sigma} c_{v+\omega, \sigma}^* \rho_{\omega} \rangle_{\text{imp}} \chi_{\omega}^{-1} g_{v\sigma}^{-1} g_{v+\omega, \sigma}^{-1}, \\ \bar{\gamma}_{vv'\omega} = & \langle c_{v\sigma} c_{v+\omega, \sigma'}^* c_{v'+\omega, \sigma''} c_{v'\sigma'''}^* \rangle_{\text{c}} \text{imp} g_{v\sigma}^{-1} g_{v+\omega, \sigma'}^{-1} g_{v'+\omega, \sigma''}^{-1} g_{v'\sigma'''}^{-1}. \end{aligned} \quad (\text{A9})$$

Note that the four-point vertex  $\bar{\gamma}_{vv'\omega}$  is defined here in the particle-hole channel.

Therefore, the initial lattice problem transforms to the following *dual* action

$$\begin{aligned} \tilde{S} = & - \sum_{\mathbf{k}, v, \sigma} f_{\mathbf{k}v\sigma}^* g_{v\sigma}^{-1} [\varepsilon_{\mathbf{k}} - \Delta_v]^{-1} g_{v\sigma}^{-1} f_{\mathbf{k}v\sigma} + \sum_{\mathbf{k}, v} f_{\mathbf{k}v\sigma}^* g_{v\sigma}^{-1} f_{\mathbf{k}v\sigma} \\ & + \frac{1}{2} \sum_{\mathbf{q}, \omega} \phi_{\mathbf{q}\omega}^* \chi_{\omega}^{-1} \phi_{\mathbf{q}\omega} + \tilde{W}[f, \phi] - \frac{1}{2} \sum_{\mathbf{q}, \omega} (\phi_{\mathbf{q}\omega}^* - j_{\mathbf{q}\omega}^* \chi_{\omega}) \\ & \times \chi_{\omega}^{-1} [V_{\mathbf{q}} - \Lambda_{\omega}]^{-1} \chi_{\omega}^{-1} (\phi_{\mathbf{q}\omega} - \chi_{\omega} j_{\mathbf{q}\omega}). \end{aligned} \quad (\text{A10})$$

To come back to the original bosonic variables, one can perform the third Hubbard-Stratonovich transformation as

$$\begin{aligned} & e^{\frac{1}{2} \sum_{\mathbf{q}, \omega} (\phi_{\mathbf{q}\omega}^* - j_{\mathbf{q}\omega}^* \chi_{\omega}) \chi_{\omega}^{-1} [V_{\mathbf{q}} - \Lambda_{\omega}]^{-1} \chi_{\omega}^{-1} (\phi_{\mathbf{q}\omega} - \chi_{\omega} j_{\mathbf{q}\omega})} \\ & = D_{\bar{\rho}} \int D[\bar{\rho}] e^{-\sum_{\mathbf{q}, \omega} (\frac{1}{2} T \bar{\rho}_{\mathbf{q}\omega} [V_{\mathbf{q}} - \Lambda_{\omega}] \bar{\rho}_{\mathbf{q}\omega} - \phi_{\mathbf{q}\omega} \chi_{\omega}^{-1} \bar{\rho}_{-\mathbf{q}, -\omega} + j_{\mathbf{q}\omega} \bar{\rho}_{-\mathbf{q}, -\omega})}. \end{aligned} \quad (\text{A11})$$

Comparing this expression to Eq. (A2), one can see that sources  $j_{\mathbf{q}\omega}^*$  introduced for the initial degrees of freedom  $\rho_{\mathbf{q}\omega}$  are also the sources for new bosonic fields  $\bar{\rho}_{\mathbf{q}\omega}$ . Therefore, fields  $\bar{\rho}_{\mathbf{q}\omega}$  indeed represent initial degrees of freedom and have the same physical meaning as original *composite* bosonic variables  $\rho_{\mathbf{q}\omega} = \sum_{\mathbf{k}v\sigma} c_{\mathbf{k}v\sigma}^* c_{\mathbf{k}+\mathbf{q}, v+\omega, \sigma} - \langle n_{\mathbf{q}\omega} \rangle$  of the lattice problem Eq. (1). Nevertheless,  $\bar{\rho}_{\mathbf{q}\omega}$  can now be treated as *elementary* bosonic fields that have a well-defined propagator, since they are introduced as a decoupling fields of dual degrees of freedom  $\phi_{\mathbf{q}\omega}$  and, therefore, independent on fermionic variables  $c_{\mathbf{k}v\sigma}^*$  ( $c_{\mathbf{k}v\sigma}$ ). Taking sources to zero and replacing  $\bar{\rho}_{\mathbf{q}\omega}$  by  $\rho_{\mathbf{q}\omega}$ , dual bosonic fields can be integrated out as [49]

$$\begin{aligned} & \int D[\phi] e^{-\frac{1}{2} \sum_{\mathbf{q}, \omega} \phi_{\mathbf{q}\omega}^* \chi_{\omega}^{-1} \phi_{\mathbf{q}\omega} - \phi_{\mathbf{q}\omega}^* \chi_{\omega}^{-1} \rho_{\mathbf{q}\omega} - \tilde{W}[f, \phi]} \\ & = \mathcal{Z}_{\phi} \times e^{\frac{1}{2} \sum_{\mathbf{q}, \omega} \rho_{\mathbf{q}\omega}^* \chi_{\omega}^{-1} \rho_{\mathbf{q}\omega} - W[f, \rho]}, \end{aligned} \quad (\text{A12})$$

where  $\mathcal{Z}_{\phi}$  is a partition function of the Gaussian part of the bosonic action. Here, we restrict ourselves to the lowest order interaction terms of  $\tilde{W}[f, \phi]$  shown in Eq. (A8). Then, the integration of dual bosonic fields in Eq. (A12) simplifies and  $W[f, \rho]$  keeps an efficient dual form of  $\tilde{W}[f, \phi]$  Eq. (A8) with

replacement of bosonic variables  $\phi \rightarrow \rho$

$$\begin{aligned} W[f, \rho] = & \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \sum_{v, v', \omega} \sum_{\sigma(\ell')} (\rho_{\mathbf{q}\omega}^* \gamma_{v\omega} f_{\mathbf{k}v\sigma}^* f_{\mathbf{k}+\mathbf{q}, v+\omega, \sigma} \\ & - [\bar{\gamma}_{vv'\omega} + \gamma_{v\omega} \chi_{\omega} \gamma_{v'+\omega, -\omega}] f_{\mathbf{k}v\sigma}^* f_{\mathbf{k}+\mathbf{q}, v+\omega, \sigma} \\ & \times f_{\mathbf{k}'+\mathbf{q}, v'+\omega, \sigma'}^* f_{\mathbf{k}'v'\sigma'}). \end{aligned} \quad (\text{A13})$$

As can be seen in Ref. [49], the four-point vertex becomes irreducible with respect to the full local bosonic propagator  $\chi_{\omega}$ , while the three-point vertex  $\gamma_{v\omega}$  remains invariant. Therefore, the problem transforms to the following action of an effective *s-d* model:

$$\mathcal{S}_{s-d} = - \sum_{\mathbf{k}, v, \sigma} f_{\mathbf{k}v\sigma}^* \tilde{G}_0^{-1} f_{\mathbf{k}v\sigma} - \frac{1}{2} \sum_{\mathbf{q}, \omega} \rho_{\mathbf{q}\omega}^* X_{\text{E}}^{-1} \rho_{\mathbf{q}\omega} + W[f, \rho], \quad (\text{A14})$$

where

$$X_{\text{E}} = [\chi_{\omega}^{-1} + \Lambda_{\omega} - V_{\mathbf{q}}]^{-1} \quad (\text{A15})$$

is the EDMFT susceptibility and  $\tilde{G}_0$  is a nonlocal part of the EDMFT Green's function. When the main contribution to the four-point vertex is given by the reducible contribution with respect to the full local bosonic propagator, i.e.,

$$\bar{\gamma}_{vv'\omega} \simeq -\gamma_{v\omega} \chi_{\omega} \gamma_{v'+\omega, -\omega} = \text{Diagram}, \quad (\text{A16})$$

the interaction part of the action Eq. (A14) takes the most simple form that contains only the three-point vertex function,

$$W'[f, \rho] \simeq \sum_{\mathbf{k}, \mathbf{q}} \sum_{v, \omega} \rho_{\mathbf{q}\omega}^* \gamma_{v\omega} f_{\mathbf{k}v\sigma}^* f_{\mathbf{k}+\mathbf{q}, v+\omega, \sigma}. \quad (\text{A17})$$

According to derivations presented in Ref. [49], one can integrate out *dual* fermionic degrees of freedom using the ladder approximation and obtain an effective problem written in terms of bosonic degrees of freedom only

$$\mathcal{S} = -\frac{1}{2} \sum_{\mathbf{q}, \omega} \rho_{\mathbf{q}\omega}^* X_{\text{q}\omega}^{-1} \rho_{\mathbf{q}\omega}, \quad (\text{A18})$$

where the expression for the lattice susceptibility reads

$$[X_{\text{q}\omega}^{\text{ladd}}]^{-1} = [X_{\text{q}\omega}^{\text{DMFT}}]^{-1} + \Lambda_{\omega} - V_{\mathbf{q}}. \quad (\text{A19})$$

Here,

$$\hat{X}_{\text{q}\omega}^{\text{DMFT}} = \text{Tr} \{ \hat{X}_{\text{q}\omega}^0 [I + \hat{\gamma}_{\omega}^{2\text{PI}} \hat{X}_{\text{q}\omega}^0]^{-1} \} \quad (\text{A20})$$

is the DMFT-like [56,57] susceptibility written in terms of lattice Green's functions, and 2PI vertex functions of impurity model defined as

$$\hat{\gamma}_{\omega}^{2\text{PI}} = \hat{\gamma}_{\omega} [I - \hat{\chi}_{\omega}^0 \hat{\gamma}_{\omega}]^{-1}. \quad (\text{A21})$$

Here, multiplication and inversion should be understood as a standard matrix operations in the space of fermionic frequencies  $v, v'$ .  $I$  is the identity matrix in the same space, and the trace is taken over the external fermionic indices. For simplicity, we omit fermionic indices wherever they are not crucial for understanding. Matrix elements of the bare



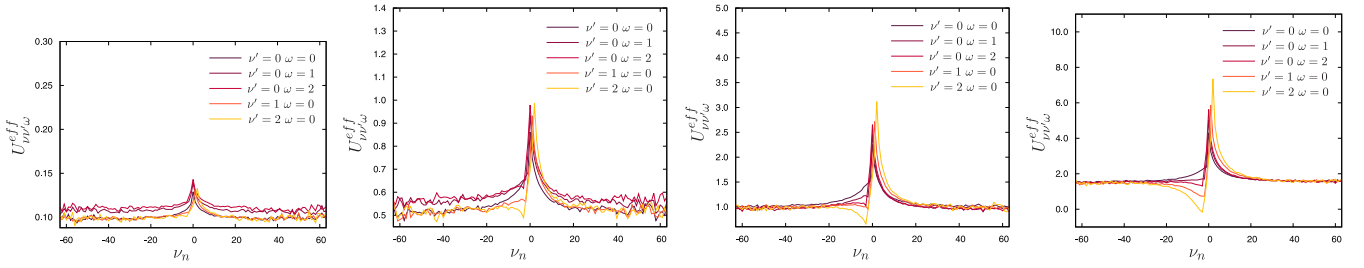


FIG. 5. Frequency dependence of the effective local Coulomb interaction  $U_{\nu\nu'\omega}^{\text{eff}}$  obtained for different values of the actual Coulomb interaction  $U = 0.1, 0.5, 1.0, 1.5$  (from left to right) in the normal phase close to the charge ordering for different values of fermionic  $\nu'$  and bosonic  $\omega$  frequencies for  $\beta = 50$ . The dependence of the effective interaction on fermionic frequency becomes larger at larger Coulomb interaction.

lattice  $\hat{X}_{\mathbf{q}\omega}^0$  and local impurity  $\hat{\chi}_{\omega}^0$  charge susceptibilities are defined as

$$X_{\mathbf{q}\omega; \nu\nu'}^0 = \sum_{\mathbf{k}, \sigma} G_{\mathbf{k}+\mathbf{q}, \nu+\omega, \sigma} G_{\mathbf{k}\nu\sigma} \delta_{\nu\nu'}, \quad (\text{A22})$$

$$\chi_{\omega; \nu\nu'}^0 = \sum_{\sigma} g_{\nu+\omega, \sigma} g_{\nu\sigma} \delta_{\nu\nu'}. \quad (\text{A23})$$

Matrix elements  $\bar{\gamma}_{\nu\nu'\omega}$  of the four-point vertex function  $\hat{\gamma}_{\omega}$  are defined in Eq. (A9).

Therefore, the charge susceptibility Eq. (A19) in the ladder approximation can be rewritten as

$$X_{\mathbf{q}\omega}^{\text{ladd}} = \text{Tr} \left\{ \hat{X}_{\mathbf{q}\omega}^0 [I - (I V_{\mathbf{q}} + \hat{U}_{\omega}^{\text{eff}}) \hat{X}_{\mathbf{q}\omega}^0]^{-1} \right\}, \quad (\text{A24})$$

where we introduced an effective bare local interaction,

$$U_{\nu\nu'\omega}^{\text{eff}} = -\Lambda_{\omega} - \bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}}, \quad (\text{A25})$$

shown in Fig. 5 for different values of fermionic  $\nu'$  and bosonic  $\omega$  frequencies.

Another simplified expression for the charge susceptibility can be obtained after expanding the simplified form of interaction  $W[f, \rho]$  given by Eq. (A17) up to the second order with respect to bosonic fields  $\rho$  in the expression for the partition function of the action Eq. (A14). This results in

$$[X_{\mathbf{q}\omega}^{(2)}]^{-1} = -V_{\mathbf{q}} + \Lambda_{\omega} + \chi_{\omega}^{-1} - \tilde{\Pi}_{\mathbf{q}\omega}^{(2)}, \quad (\text{A26})$$

where

$$\tilde{\Pi}_{\mathbf{q}\omega}^{(2)} = \sum_{\mathbf{k}, \nu, \sigma} \gamma_{\nu+\omega, -\omega} \tilde{G}_{\mathbf{k}+\mathbf{q}, \nu+\omega\sigma} \tilde{G}_{\mathbf{k}\nu\sigma} \gamma_{\nu, \omega} \quad (\text{A27})$$

is the second-order polarization operator and  $\tilde{G}_{\mathbf{k}\nu}$  is a nonlocal part of the lattice (EDMFT) Green's function. As discussed in the main text, this expression can be transformed to a pair interaction of the classical Ising model.

## APPENDIX B: VERTEX APPROXIMATION

According to discussions presented in the main text, the expression for the 2PI four-point vertex function can be approximated as  $\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}} \simeq \bar{\gamma}_{\omega}^{2\text{PI}}$  when its dependence on fermionic

frequencies is negligible. Then, using the exact relation for the local impurity susceptibility

$$\chi_{\omega} = \text{Tr} \left\{ \hat{\chi}_{\omega}^0 - \hat{\chi}_{\omega}^0 \hat{\gamma}_{\omega} \hat{\chi}_{\omega}^0 \right\} = \text{Tr} \left\{ \hat{\chi}_{\omega}^0 [I + \hat{\gamma}_{\omega}^{2\text{PI}} \hat{\chi}_{\omega}^0]^{-1} \right\} \quad (\text{B1})$$

and assuming that the 2PI vertex does not depend on fermionic frequencies, one gets

$$\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}} \simeq \bar{\gamma}_{\omega}^{2\text{PI}} = \chi_{\omega}^{-1} - \chi_{\omega}^{0-1}. \quad (\text{B2})$$

As shown in Ref. [49], in the case of well-developed collective fluctuations the four-point function is described by the bosonic frequency and three-point vertex function that enters the exact Hedin equation [58] for the self-energy and polarization operator of the impurity problem is close to unity. As a consequence, the local self-energy and polarization operator take the same form as in GW approach [58–60]. Thus, the polarization operator of the impurity problem can be approximated as  $\Pi_{\omega} \simeq \chi_{\omega}^0$  neglecting the vertex function. Using the exact relation for the local charge susceptibility of the impurity problem, one gets the following relation:

$$\chi_{\omega}^{-1} = \Pi_{\omega}^{-1} - (U + \Lambda_{\omega}) \simeq \chi_{\omega}^{0-1} - (U + \Lambda_{\omega}). \quad (\text{B3})$$

Therefore, in the regime of strong charge fluctuations the 2PI vertex function can be approximated as  $\bar{\gamma}_{\nu\nu'\omega}^{2\text{PI}} \simeq -U - \Lambda_{\omega}$ .

The three-point vertex can also be approximated using the exact relation between three- and four-point vertex functions, and the simplified form of the 2PI vertex [49],

$$\gamma_{\nu\omega} \simeq \gamma_{\omega} = \chi_{\omega}^{-1} - \bar{\gamma}_{\omega}^{2\text{PI}} = \chi_{\omega}^{-1} + \Lambda_{\omega} + U_{\omega}^{\text{eff}}, \quad (\text{B4})$$

where  $U_{\omega}^{\text{eff}} = -\Lambda_{\omega} - \bar{\gamma}_{\omega}^{2\text{PI}}$ . Taking into account that in the regime of well-developed charge fluctuations the effective interaction coincides with the actual value of the bare local Coulomb interaction  $U_{\omega}^{\text{eff}} \simeq U$ , one can further write

$$\gamma_{\omega} \simeq \chi_{\omega}^{-1} + \Lambda_{\omega} + U = \Pi_{\omega}^{-1} = \frac{U \mathcal{W}_{\omega}}{\mathcal{W}_{\omega} - U} = \frac{U}{1 - \varepsilon_{\omega}}, \quad (\text{B5})$$

where we introduced the renormalized local Coulomb interaction  $\mathcal{W}_{\omega} = U/(1 - \Pi_{\omega}U)$  that is connected to the bare Coulomb interaction via the dielectric function  $\varepsilon_{\omega} = U/\mathcal{W}_{\omega}$ .

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