Dual Boson approach with instantaneous interaction

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I. INTRODUCTION

The Hubbard model¹–⁴ describes interacting itinerant electrons. The Coulomb interaction between these electrons leads to correlations and makes this a many-body problem. When interaction and itinerancy are almost equally strong, the resulting electronic correlations make the system notoriously hard to study.

The Dynamical Mean-Field Theory (DMFT)⁵ is an important tool to describe correlated electrons. The main idea of the method is to use an auxiliary “impurity” model that consists of only a single site. This impurity model should contain the most important correlation effects of the full system. This idea is exact in the limit of infinite dimension, in finite dimensional systems it still serves as a useful approximation.

Extensions of DMFT have been developed⁶ to add the spatial correlations and non-local interactions that DMFT ignores. These extensions add additional correlation effects on top of DMFT, but they can also change the impurity model that is used as a starting point. To account for screening by the non-local Coulomb interaction, Extended DMFT (EDMFT)⁸–¹³ and its diagrammatic extensions⁷, introduce dynamic interactions into the impurity model. While the EDMFT still considers electronic correlations at the level of the local impurity problem, the DB theory¹⁴ and other EDMFT-based approaches additionally accounts for nonlocal correlation effects diagrammatically.

The introduction of dynamic interactions comes at a computational cost. For single-band systems, dynamic density-density type¹⁵ interactions can be incorporated into CT-QMC impurity solvers at moderate cost¹⁶,¹⁷. Other dynamic interactions are more difficult to handle.¹⁸,¹⁹ In Exact Diagonalization solvers, dynamic interactions lead to a very large Hilbert space and require discretization of the bosonic bath.²⁰ Moreover, the inclusion of dynamic interactions may lead to a violation of conservation laws.²¹

To address these situations, a simplification of the Dual Boson approach that does not require dynamic interactions in the impurity model has been introduced recently.²² We use the fact that the dynamic interactions in Dual Boson are a priori free parameters in the Hubbard-Stratonovich decoupling that leads to the impurity model. The dynamic interaction is usually determined using a set of self-consistency conditions, one for every frequency. By forcing the interaction to be instantaneous (independent of frequency), the number of free parameters is drastically reduced, with the benefit of having a simpler impurity model at the end.

So far, this method has not been systematically tested. In this work we aim to systematically test its performance in description of collective electronic instabilities of the two- and three-dimensional extended Hubbard model. We compare this instantaneous interaction Dual Boson approach with the traditional dynamic interaction Dual Boson approach and with the Dynamical Mean-Field which always keeps the interaction of the original Hubbard model. We also discuss the relationship with the two-particle self-consistent approach²³,²⁴ and the Moriya correction in DΓA²⁵, which are also based on self-consistently renormalizing an effective interaction.
II. MODEL AND METHOD

We consider the half-filled extended Hubbard model on the square and cubic lattice,

\[ H = - \sum_{i,j,\sigma} t_{ij} c_{ij\sigma}^\dagger c_{ij\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i,j} V_{ij} (n_i - \langle n_i \rangle) (n_j - \langle n_j \rangle), \]  

(1)

Here \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) are creation and annihilation operators for an electron on site \( i \) with spin \( \sigma \) and \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) is the corresponding number operator. The total electronic density on site \( i \) is equal to \( n_i = n_{i\uparrow} + n_{i\downarrow} \). The physical parameters of the model are the hopping amplitude \( t_{ij} \), the on-site Coulomb interaction \( U \), and the intersite Coulomb interaction \( V_{ij} \). We consider only nearest-neighbour hopping and interaction, \( t_{ij} = t \) and \( V_{ij} = V \) when \( i \) and \( j \) are nearest-neighbors and 0 otherwise.

For \( V = 0 \), this model is simply the Hubbard model. In this work, we consider the (extended) Hubbard model at half-filling, \( \langle n_i \rangle = 1 \). This is obtained by replacing setting \( \mu = U/2 \). We restrict ourselves to phases without explicit symmetry breaking. We do calculate the susceptibility associated with antiferromagnetic (AF) and charge density wave (CDW) phases to check for instabilities associated with antiferromagnetic (AF) and explicit symmetry breaking. We do calculate the susceptibility and we do not calculate dual self-energy.

This separation is made by introducing fermionic and bosonic hybridization functions \( \Delta, \Lambda \), where \( \rho \) is a bosonic channel, e.g., charge or \( S^z \).

\[ S_{\text{imp}} = - \sum_{\nu,\sigma} c_{\nu\sigma}^\dagger [i\nu + \mu - \Delta_\nu] c_{\nu\sigma} + U \sum_\omega n_{\omega\uparrow} n_{\omega\downarrow} + \frac{1}{2} \sum_{\rho,\omega} \Lambda_{\rho\omega} \rho_{\omega} \rho_{-\omega}. \]  

(4)

These hybridizations \( \Delta, \Lambda \) can be chosen freely. Below in Section II A we discuss how to make this choice. In general, the Dual Boson approach considers \( \Lambda \) to be a function of \( \omega \). In this work, we restrict ourselves to constant \( \Lambda \). In that case, the impurity action can simply be rewritten as

\[ S_{\text{imp}} = - \sum_{\nu,\sigma} c_{\nu\sigma}^\dagger [i\nu + \mu - \Delta_\nu] c_{\nu\sigma} + U' \sum_\omega n_{\omega\uparrow} n_{\omega\downarrow}. \]  

(5)

where \( U' = U + \Lambda_{\text{ch}} - \Lambda_{\text{sp}} \). For the impurity model to also be at half-filling, we take \( \mu' = U'/2 \). This choice of hybridization functions is useful, since the resulting form of the impurity action does not introduce higher-order terms in the Ward identities.

The spatial correlations in the dual part of the problem are addressed using diagrammatic methods. In this work, we concentrate on the correlation effects in the susceptibility and we do not calculate dual self-energy corrections. The following definition for the susceptibility \( X_{\nu,\omega} = -\langle \rho_\nu \rangle_{\omega} \) can be applied both to the charge channel, with \( \rho = n - \langle n \rangle \), and to the spin channel, with \( \rho = S^z - \langle S^z \rangle \). The Dual Boson expression is given by

\[ X_{\nu,\omega}^{-1} = \chi_{\nu,\omega}^{-1} + \Lambda_\omega - V_{\text{q}}, \]  

(6)

where

\[ \chi_{\nu,\omega} = \chi_\omega + \chi_\omega \Pi_{\text{q}\omega} \chi_\omega, \]  

(7)

and \( \chi_\omega = -\langle \rho_\nu \rangle_{\omega}^{\text{imp}} \) is the corresponding susceptibility of the impurity model. The non-local correlation effects are contained in \( \Pi \), the dual polarization operator. In this work, we use the ladder equation to calculate \( \Pi \).

The restriction to instantaneous interactions simply leads to the replacement of \( \Lambda_\omega \) by a constant \( \Lambda \) in Eq. (6).

Dynamical Mean-Field Theory usually deals with the Hubbard model, with \( V = 0 \). The DMFT susceptibility is obtained by setting \( \Lambda = 0 \) in Eq. (6). This formulation of the DMFT susceptibility is equivalent to more traditional ways of computing it. The extended Hubbard model’s intersite Coulomb interactions can be included in the DMFT susceptibility via Eq. (6) with \( \Lambda = 0 \), this essentially corresponds to an RPA-like treatment of these additional interactions, in which they do not alter the impurity or the single-particle properties.
A. Self-consistency condition

So far, we have not specified the interaction renormalization $\Lambda$. This is done by a self-consistency condition. We use the “lattice” self-consistency condition proposed for the self-consistent Dual Boson approach\textsuperscript{29}, except that here we only two free parameters $\Lambda^{\text{ch}}$, $\Lambda^{\text{sz}}$ instead of two dynamic functions of frequency. This means we only need one self-consistency per channel instead of having a self-consistency for every Matsubara frequency.

$$\sum_\omega \chi^{\text{ch}/\text{sz}}(\omega) = \sum_\omega X^{\text{ch}/\text{sz}}_{\text{loc}, \omega},$$  \hspace{1cm} (8)

where $X_{\text{loc}}$ is the local part of the lattice susceptibility, obtained as the average over momenta of $X_q$. As shown in Ref. 22, this choice of the self-consistency condition follows from the invariance of the initial lattice problem with respect to variation of introduced hybridization functions, and allows to fulfill the Pauli principle.

The sum over frequencies in the self-consistency condition corresponds to taking the equal-time component of the susceptibility\textsuperscript{30}, so we can write

$$\chi^{\text{ch}/\text{sz}}(\tau = 0) = X^{\text{ch}/\text{sz}}_{\text{loc}}(\tau = 0).$$  \hspace{1cm} (9)

The difference between the local, equal time charge and spin susceptibility determines the double occupancy $D = \langle n_1 n_2 \rangle$. The self-consistency condition used here assures that the double occupancy of the lattice susceptibility is equal to the one of the impurity model\textsuperscript{31}. On the other hand, the potential energies will be different since the lattice model and the impurity model have different interactions $U$ and $U'$. This type of inconsistency between impurity and lattice generally occurs in approximate methods based on DMFT\textsuperscript{21}. Note that the argument about potential energies applies to the Hubbard model ($V = 0$), for the extended Hubbard model there is no direct correspondence between the potential energy of the impurity and the lattice since the latter also contains intersite contributions.

Dual Boson calculations with dynamic interactions in the $S^z$ channel break the spin rotational symmetry of the impurity model if they do not have the same dynamic interaction in the $S^x$ and $S^y$ channels. There is no such rotational symmetry breaking in the current approach, since the impurity model has the rotationally invariant interaction $U'$. In the dual part of the calculations, it is sufficient to calculate only the $S^z$ channel since the $S^x$ and $S^y$ channel follow from rotational symmetry.

Appendix A describes analytical results for the self-consistency condition in several simplifying limits, these results carry over from the self-consistent Dual Boson approach with dynamic interactions\textsuperscript{29}.

The reader might wonder why the self-consistency condition is important in the first place. The relation between the original and the dual theory is exact for any choice of $\Delta$ and $\Lambda$. However, the dual theory is only solved approximately, perturbatively. The choice of $\Lambda$ becomes important in this approximate theory. In this sense, there is some similarity with the Fierz ambiguity\textsuperscript{32–34}, where the decomposition of $U$ into channels determines the computational outcome of approximate methods even though the exact system is unchanged by the choice of decomposition. The present situation can also be seen through the lense of decomposition, since the impurity part of the calculation depends only on the combination $U' = U + \Lambda^{\text{ch}} - \Lambda^{\text{sz}}$, whereas the dual part of the calculation and the transformation between dual and lattice quantities are affected by how $U'$ is decomposed into the charge and magnetic channel.

A corollary to this discussion is that the choice of self-consistency condition should be informed by the approximations made in the dual theory, since only these approximations make the self-consistency condition relevant. Presently, the approximations are the elimination of vertices beyond the two-particle level, the restriction to ladder diagrams and finally the choice of the density and magnetic channels for the ladder. Starting with the last point, the choice of channels for the ladder and subsequently for the susceptibility directly informs the choice of $\Lambda^{\text{ch}}$ and $\Lambda^{\text{sz}}$ as the self-consistent parameters (see, e.g., Ref. 35 for a recent discussion on the role of channels in the attractive Hubbard model). Diagrammatic Monte Carlo approaches to the dual theory\textsuperscript{36,37} do not restrict themselves to ladder diagrams and are therefore not restricted by the second and third point.

B. Implementation

Apart from the self-consistency condition and the effective interaction, our method follows the Dual Boson approach\textsuperscript{34} and its implementation\textsuperscript{27}. For the impurity model, we use a modified version of the open source CT-HYB solver\textsuperscript{38,39} based on the ALPS libraries\textsuperscript{40}.

The implementation of the Dual Boson approach consists of two computationally heavy parts, the impurity solver and the evaluation of the dual diagrams, both implemented in C++ and linked together by a lighter python interface. The self-consistency condition is based entirely on the impurity susceptibility $\chi$ and the local part of the lattice susceptibility $X_{\text{loc}}$. These are part of the usual output of the impurity solver and the dual program. This means that the self-consistency condition can be implemented in the python interface, the renormalized effective interaction $U' = U + \Lambda^{\text{ch}} - \Lambda^{\text{sz}}$ enters the impurity solver as a parameter and no other changes are needed.

We use an update formula with damping parameter $\xi$,

$$\Lambda_{\text{new}} = \Lambda_{\text{old}} + \xi \frac{X_{\text{loc}}(\tau = 0) - \chi(\tau = 0)}{X_{\text{loc}}(\tau = 0)}.$$

A smaller value of $\xi$ makes the self-consistency procedure more stable at the cost of slower convergence, we take $\xi \in [0.1, 1]$. Similar to the self-consistent procedure to determine $U(\omega)$ used in Ref. 31, we find that convergence
Consistency condition disallows phase transitions.

\( N \) still satisfying Eq. (11), but only when taking the limit \( d \rightarrow \infty \). This means that a phase transition can occur while the limit of infinite systems. In that case, we replace a phase transition to an antiferromagnetic phase shows up as a divergence in the corresponding susceptibility, at zero frequency and at a specific momentum \( q^* \) which describes the ordering pattern. For the half-filled Hubbard model under investigation, antiferromagnetic ordering with \( q_{\text{AF}}, 2d = (\pi, \pi) \) or \( q_{\text{AF}}, 3d = (\pi, \pi, \pi) \) is most important.

Since this susceptibility appears in the self-consistency condition, let us take at somewhat closer look at how phase transitions and the self-consistency condition interact in practice\(^{24}\). We have previously written the self-consistency condition as

\[
\sum_\omega \chi^{\text{sz}}_\omega = \frac{1}{N} \sum_\omega \sum_\mathbf{q} X^{\text{sz}}_{\mathbf{q},\omega}. \tag{11}
\]

A phase transition to an antiferromagnetic phase shows up as a divergence in \( X_{\mathbf{q},\omega=0} \). This also means that the right-hand side of Eq. (11) would diverge\(^{21}\). However, the left-hand side is the correlation function of a single site and always stays finite.

This seems to suggest that Eq. (11) does not allow any phase transition to occur. The complication lies in the momentum sum, \( \frac{1}{N} \sum_\mathbf{q} \). For a finite system, a divergence at any \( \mathbf{q} \)-point would indeed correspond to a divergence of the local susceptibility and this is ruled out by the self-consistency condition. This is physically correct in the sense that in a finite system at \( T > 0 \) the free energy depends smoothly on all parameters and there cannot be a phase transition.

In this technical sense, phase transitions only occur in the limit of infinite systems. In that case, we replace the average over a finite set of discrete momenta by an integral over the Brillouin Zone. If we assume that \( X \propto (\mathbf{q} - \mathbf{q}_{\text{AF}})^{-2} \) in momentum space, then the right-hand side is dominated by the surroundings of \( \mathbf{q}_{\text{AF}} \) and can be written in terms of \( \mathbf{q}' = \mathbf{q} - \mathbf{q}_{\text{AF}} \) as

\[
\int d\mathbf{q}' |q'|^{-2} \propto \int_0^d d|q'||q'|^{-d-1}|q'|^{-2} = \int_0^d d|q'||q'|^{-3}. \tag{12}
\]

Here \( d \) is the dimension and only the lower limit of the integral is dangerous. This expression is finite for \( d = 3 \). This means that a phase transition can occur while still satisfying Eq. (11), but only when taking the limit \( N \rightarrow \infty \). On the other hand, for \( d = 2 \), the integral is logarithmically divergent, so that enforcing the self-consistency condition disallows phase transitions.

Regarding the first point, we should point out that many mean-field based methods produce phase transitions in finite systems. In fact, the system size does not even enter traditional Curie-Weiss mean-field theory. The DMFT susceptibility of a finite system can be divergent and non-local extensions like Dual Fermion or Dual Boson do not automatically correct this issue. Here, it is enforced by the self-consistency condition. This situation is in some sense reminiscent of the difference between finite-size and quantum cluster approaches\(^{42}\): finite-size simulations only obtain a phase transition after extrapolating to infinite system size, quantum cluster approaches already find the transition at a finite system size. The former situation is technically correct, the latter is convenient in practical situations.

Regarding the second point, we recognize that the self-consistency condition serves to enforce the Mermin-Wagner theorem\(^{43}\) in a two-dimensional system, which says that there can be no spontaneous symmetry breaking of continuous symmetries in two-dimensional systems at finite temperature. For the Hubbard model, the spin rotational symmetry cannot be spontaneously broken. In particular, this means that there can be no antiferromagnetic state at finite temperature. On the other hand, at \( T = 0 \), the system is an antiferromagnetic insulator at any \( U > 0 \). Together, this means that at low temperature, the system features very strong and long-ranged antiferromagnetic correlations that are almost truly long-ranged ordered. A similar situation takes place in low-dimensional Heisenberg model, see Ref. \(^{44}\) and Refs. therein.

This situation, with long but not infinitely ranged correlations, is challenging to reproduces in (computational) approximations. According to Vilk and Tremblay\(^{24}\), a sufficient criterion for ensuring that an approximation satisfies the Mermin-Wagner theorem is to verify that the double occupancy \( D = \langle n_\uparrow n_\downarrow \rangle \) obtained from taking the local, equal-time part of the susceptibility stays within the physical range \([0, n^2/2]\). The self-consistency condition of the current method ensures that the double occupancy of the Hubbard model is equal to that of a reference impurity model that is solved exactly. The latter stays within the physical bounds, so that the former does as well and the method satisfies the Mermin-Wagner theorem.

The self-consistently determined interaction acts to suppress phase transitions, both in finite systems and in two-dimensional systems in the thermodynamic limit. At the same time, it risks ruling out phase transitions that are physically allowed, such as the charge-order phase transition in the two-dimensional extended Hubbard model, which is not forbidden by Mermin-Wagner since it corresponds to the spontaneous breaking of a discrete symmetry.

We can use Eq. (11) to make an estimate for the relevant scale of the interplay between self-consistency condition and phase transitions. The left-hand side of the equation is of order unity, so that\(^{45}\) \( |X_{\mathbf{q},\omega}| \leq \beta N \).
D. Exact properties and approximate solutions

Let us take a step further back to put these developments in the general context of consistency in approximate solutions to many-body problems and in particular to Hubbard-like models. The central point is that (many) exact statements can be made about the true, exact solution of the model, to name just a few: equivalence of thermodynamic quantities and response functions according to the Kubo formula; the Mermin-Wagner theorem; conserved quantities corresponding to symmetries and Goldstone modes arising when these symmetries are broken; sum rules and high-frequency asymptotics derived from commutation relations. These concepts are central to our understanding of condensed matter physics.

However, approximate solutions are not guaranteed to satisfy these exact properties. In fact, they will usually not satisfy all these constraints. This issue goes back to the seminal work of Baym and Kadanoff, who formulated functional constructions to ensure that diagrammatic approaches satisfy certain conservation laws. The correspondence between correlation and response functions played an important role in the development of the theories of the electron gas and of magnetism in itinerant electron systems.

In the context of (extensions of) DMFT, the subject of exact properties came up for the thermodynamic consistency of zero- and one-particle properties and the consistency between one- and two-particle quantities, in particular the Kubo relation between correlation and response and the high-frequency asymptote of the susceptibility. Simultaneously, charge conservation and Goldstone modes were investigated.

The conclusion of these investigations is that the DMFT approximate solution to the finite-dimensional Hubbard model satisfies many of the exact properties, but not all. More specifically, the charge response is consistent, the DMFT susceptibility satisfies global charge conservation and the lowest order terms in the high-frequency asymptotes of the Green’s function, (local) self-energy and the (momentum-resolved) susceptibility are consistent with exact relations. The DMFT functional is conserving in the sense of Baym and Kadanoff. On the other hand, the DMFT susceptibility violates the Mermin-Wagner theorem, the potential energy/double occupancy is inconsistent between the one- and two-particle level and exact relations for the moments of the lower Hubbard band spectral weigh function in the atomic limit are violated. As we have already seen, DMFT also predicts phase transitions in finite size system, which is inconsistent with fundamental thermodynamic considerations.

Clearly, even the elegant construction of DMFT is not sufficient to recover all exact relations and it is unlikely that any approximate method can. It is possible to enforce specific relations, although usually at a cost. The self-consistency condition employed here can be seen in this way: it enforces the Mermin-Wagner theorem. In this way, it is similar to the λ introduced by Moriya. A similar Moriya-λ correction plays a central role in ladder-DΓA. The λ of DΓA is partially related to the Λω of DB. Both enter the (inverse) susceptibility as in Eq. 6, but in DB Λ also enters into the impurity model as follows from the exact dual transformation whereas in DΓA λ correction is introduced by hand and is not included in the impurity model. We should point out that the instantaneous Λ proposed here is even more similar to the instantaneous λ of DΓA.

III. SQUARE LATTICE HUBBARD MODEL

We now turn to numerical investigation of the instantaneous DB. We study the square lattice Hubbard (V = 0) model with t = 1. We use a 32 × 32 discretization of momentum space.

A. Effective interaction

We start by investigating the effective interactions Λ, since these are the quantities that enter the impurity model. Figure 1 shows Λ in the small to moderate coupling regime. We observe that Λ depends strongly on the inverse temperature β = 1/T, that Λ^ch and Λ^sq have opposite sign and that Λ is proportional to U at small interaction strengths.

The limit of small U can be understood in terms of perturbation theory. For the calculation of the susceptibility at small U, we can neglect the self-energy and treat the interaction in the RPA fashion, as a geometric series. Appendix A 2 gives the details of this approach, which confirm the opposite sign and the proportionality with U.

The observation that the effective interaction depends strongly on temperature is a major difference with the two-particle self-consistent (TPSC) approach. There, as

![Figure 1. Effective interaction as a function of temperature and interaction strength.](image-url)
Figure 2. Inverse antiferromagnetic susceptibility \( X_{AF}^{-1}(q,\omega=0) \) in the square lattice Hubbard model at \( \beta t = 3 \). A phase transition to an antiferromagnetically ordered phase occurs when this inverse susceptibility is equal to zero (dashed black line).

shown in Fig. 2 of Ref. 24, the effective interaction is independent of temperature at high temperatures. Here, on the other hand, the interaction renormalization vanishes as the temperature is increased. Self-consistent Dual Boson has DMFT as a starting point, the renormalization of the interaction is needed to ensure that the DMFT susceptibility satisfies the (local) Pauli principle. The lowest-order violations of the Pauli principle occur in \( \tilde{\Pi}^{(3)} \). It turns out that the contribution from this diagram, which contains four non-local propagators, decays rather quickly as a function of temperature. In TPSC, the lowest-order violations of the Pauli principle come from \( G_0 U G_0 \). This diagram looks the same as \( \tilde{\Pi}^{(3)} \), with the difference that now the Green’s functions are the bare Green’s functions of the system, which have a finite local part and which are numerically much larger. The improved starting point of DMFT is sufficient to describe the high temperature limit at any \( U \).

One of the main points of the self-consistent Dual Boson approach is that the self-consistency condition enforces the Mermin-Wagner theorem in two dimensions. The absence of antiferromagnetism in the self-consistent Dual Boson approach is visualized in Fig. 2. DMFT is unstable towards antiferromagnetism after \( U = 6 \) when the inverse of the magnetic susceptibility changes sign. The self-consistency condition enforces a positive value for the DB results and thus pushes the inverse susceptibility away from zero. However, enforcing this condition is not easy, since close to an instability the system is very sensitive to small changes in the effective impurity interaction. This makes calculations at \( U \geq 6 \) extremely unstable.

We proceed with an in-depth look at \( U/t = 5, \beta t = 3 \), this is just before the antiferromagnetic susceptibility in DMFT diverges. We find \( U'/t \approx 5.54 \), a more than 10% increase of the effective interaction. This change in interaction is composed of \( \Lambda^{ch} \approx 0.41, \Lambda^{sz} \approx -0.13 \).

Looking at the local magnetic susceptibility shown in Fig. 3, we see a large inconsistency in DMFT between the impurity and local lattice susceptibility. In the self-consistent approach, this inconsistency is removed almost completely, even though the self-consistency only enforces equality between the frequency-averaged susceptibilities. Essentially, the problem in DMFT is that abs \( X^{sz} \) is too large, so that the double occupancy from \( X \) can even turn negative. The self-consistency condition solves this by reducing abs \( X^{sz} \). This reduction in the lattice quantity occurs even though abs \( \chi^{sz} \) is increased due to the larger effective impurity interaction. The larger effective impurity interaction also increases the self-energy, shown in Fig. 4 (see also Appendix B).

IV. CUBIC LATTICE HUBBARD MODEL

We now move to a three-dimensional system. Let us consider the situation at one specific set of parameters in
Figure 5. Analysis of the self-consistency condition at \( U = 4 \) and \( \beta = 2.5 \), for a cubic lattice.

Figure 6. Self-energy at \( U = 4 \) and \( \beta = 2.5 \), for a cubic lattice. The points correspond to the Matsubara frequencies \( \nu_n \), lines are guides to the eye.

detail, to get a feeling for how the self-consistency condition works. We study \( U/t = 4 \) and \( \beta t = 2.5 \). We find \( U'/t \approx 4.18 \), a roughly 5% change in the effective interaction. The channel decomposition of the effective interaction is \( \Lambda_{ch} \approx +0.12 \) and \( \Lambda_{sz} \approx -0.06 \). The difference in magnitude between the charge and spin renormalization shows that we have clearly left the weakly correlated regime.

The calculations shown here have been performed on a \( 10 \times 10 \times 10 \) cubic lattice. We have verified that using a \( 20 \times 20 \times 20 \) lattice leads to very similar results. This conforms to the observation that replacing the integral in Eq. (12) by a finite momentum average is a well-behaved operation. All other potential sources of finite size effects are similar to DMFT and not relevant in this parameter regime.

The self-consistency condition enforces equality between the frequency averages of \( X^{loc} \) and \( \chi \). In Fig. 5, we show the difference of these two susceptibilities as a function of frequency. There is an essential difference between finite and zero frequency, in both the charge and the spin channel. The contribution at zero frequency is compensated by the finite frequencies. The sign difference between the charge and spin channel in Fig. 5 corresponds to the sign difference between \( \Lambda_{ch} \) and \( \Lambda_{sz} \).

The self-consistency condition on the two-particle level feeds back to the single-particle level via the impurity model. In Fig. 6 we show the self-energy of the impurity model. We see an enhancement of the self-energy in the self-consistent DB approach. This enhancement originates in the larger effective interaction \( U' > U \).

Moving away from fixed \( U \), Figure 7 shows how the effective interaction and the potential and kinetic energy develop as a function of the interaction \( U' \). The effective interaction becomes more relevant at larger \( U \), leading to a reduction in the potential energy and an increase in the kinetic energy (note the minus sign in \( E_{kin} = -\frac{2}{\beta} \langle k \rangle \)).

V. EXTENDED HUBBARD MODEL

We now turn our attention to the extended Hubbard model with finite \( V \). We study this model on a cubic lattice with fixed local interaction \( U = 5 \) and fixed temperature \( \beta = 2.5 \). We use a \( 10 \times 10 \times 10 \) lattice. Figure 8 shows...
that screening by the nonlocal interaction \( V \) reduces the effective impurity interaction \( U' \), so that \( U' < U \). As expected, this increases the potential energy and decreases the kinetic energy. Even though it decreases, the impurity interaction is still repulsive for all cases shown here, \( U' > 0 \). Looking at the inverse susceptibility in the charge channel, we find that it approaches zero as \( V \) is increased. Linear extrapolation\(^{67} \) predicts the charge order transition to occur at \( V \approx 0.99 \). The arrow marks \( V = U/z = 0.83 \), the point where charge-order becomes favorable in terms of the potential energy\(^{68} \). The actual transition occurs later due to the interplay between potential and kinetic energy and entropy.

The extrapolation here is based on data up to \( V = 0.95 \). In principle, no true divergence is expected in a finite system. This has nothing to do with the Mermin-Wagner theorem, since the charge ordering is not associated with the breaking of a continuous symmetry. Instead, however, for finite-size lattices the self-consistency cycle becomes difficult to stabilize when the phase transition region is approached: small changes in the effective interaction \( U' \) will lead to big changes in the susceptibility \( X \).

We can compare our results obtained with the self-consistent instantaneous interaction with those of Ref.\(^{27} \), where a frequency dependent interaction was used and self-consistency was only done at the EDMFT level. Figure 9 shows the charge susceptibility for these two methods in the cubic and square lattice Hubbard model. The qualitative behavior of both methods is the same, quantitative differences are visible. The self-consistent approach approaches the phase transition already at smaller values of \( U \), that is, the inverse susceptibility is smaller close to the phase transition. The origin of this seems to be the enhanced charge susceptibility of the impurity model that originates in the reduced value of the effective interaction \( U' < U \), as was visible in Fig. 8. For the two-dimensional situation, the inverse susceptibility in the self-consistent DB solution is approximately linear in the regime accessible here. Based on the arguments of Eq. (11), the self-consistency condition comes into play only when \( X^{-1} \approx 1/L^2 \approx 10^{-3} \) for the \( L = 32 \) system studied here. For a much smaller \( L = 2 \) system (dotted line), it sets in earlier and the dotted line bends upwards at small \( V \). Therefore, the true CDW phase boundary can be obtained extrapolating the results for the inverse charge susceptibility for different size of the system.

VI. CONCLUSIONS AND DISCUSSION

We have presented the Dual Boson approach with instantaneous interaction. By construction, this approach produces a susceptibility that satisfies the charge and spin conservation requirement, and the Mermin-Wagner theorem. The instantaneous interaction assumption means that the method does not need an impurity solver that can handle retarded interactions, an important simplification that makes it more amenable to the simulation of multiband systems. We have illustrated the method in two- and three-dimensional systems and

\[ \text{Figure 8. The extended Hubbard model on the cubic lattice, for } U = 5 \text{ and } \beta = 2.5. \text{ Solid lines are guides to the eye, the dashed line in the bottom panel is a linear fit with intercept at } V \approx 0.99. \]

\[ \text{Figure 9. Comparison of the charge order transition in the square and cubic lattice. The square lattice simulations correspond to } \beta = 3, \text{ the cubic lattice with } \beta = 2.5, \text{ all simulations are at } U = 5. \text{ The curves labeled DB constant } \Lambda \text{ correspond to the method proposed in this work, reference results using the scheme of Ref. 27 are shown as non-sc DB. Arrows indicate } V = U/6 \text{ and } V = U/4. \]
have analyzed how the proposed self-consistency condition affects the appearance of ordered phases. In our method the instantaneous interaction of the impurity model is adjusted by the “lattice” self-consistency condition on the bosonic hybridization function. Surprisingly, this constant hybridization function almost completely washes out the difference between the local part of the frequency dependent lattice and impurity susceptibilities. Mean-field based approaches typically overestimate the tendency towards ordered phases, as is clearest in two-dimensional or finite systems where phase transitions are forbidden. Enforcing self-consistency on the two-particle level can cure this deficiency. Compared to DMFT, we find that the feedback of collective excitations leads to an enhanced effective interaction and to a more correlated impurity model, as is visible in the double occupancy, kinetic energy and self-energy of both two and three-dimensional systems.

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Appendix A: Analytical results

1. $U = 0, t = 0$ or $d = \infty$

In these three cases the more restrictive self-consistency condition\textsuperscript{28} $\chi_\omega = X_{\text{loc,}\omega}$ is fulfilled for all $\omega$ by the solution $\Lambda = 0$. This means that $\Lambda = 0$ is also satisfies the instantaneous self-consistency condition used in this work. This solution corresponds to the exact DMFT solution of the Hubbard model in these three cases.

2. small $U$

We consider the Hubbard model, so $V = 0$, and we look at the charge channel of the susceptibility. To lowest order in $U$, we can neglect self-energy corrections to the susceptibility and use geometric (RPA-like) equations to describe the impact of the interaction. The impurity model only knows about the impurity interaction $U'$ and not about $U$ and $\Lambda$ separately,

$$\chi^{-1}_\omega = \chi(U = 0)^{-1}_\omega \mp U', \quad (A1)$$

where the sign is $-$ for the charge channel and $+$ for the spin channel. The dual polarization operator $\Pi$ in the ladder approach is completely determined by the expectation values of the impurity model and by $t$ and $\Delta$, since these enter $\tilde{G}$. In particular, $\Pi$ only depends on $U'$ and not on $U$ and $\Lambda$ separately, and the same holds for $\mathcal{X}$, which is also given by a geometric expression (It is essentially equal to the DMFT susceptibility of a Hubbard model with interaction $U'$).

$$\mathcal{X}_\omega = \mathcal{X}(U = 0)^{-1}_\omega \mp U', \quad (A2)$$

The lattice susceptibility according to DB is then given by Eq. (6).

$$X^{-1}_\omega = \mathcal{X}^{-1}_\omega + \Lambda, \quad (A3)$$

where $\Lambda$ is the interaction in the same channel as the susceptibility. Combining these equations, for the charge susceptibility we find

$$\left(\chi^{\text{ch}}_\omega\right)^{-1} = \mathcal{X}(U = 0)^{-1}_\omega - U + \Lambda^{\text{ch}} \quad (A4)$$

$$= X(U = 0)^{-1}_\omega - U + \Lambda^{\text{sz}} \quad (A5)$$

where we have used that $\mathcal{X} = X$ and is independent of the channel at $U = 0$. Similarly, we find

$$\left(X^{\text{sz}}_\omega\right)^{-1} = X(U = 0)^{-1}_\omega + U + \Lambda^{\text{ch}} \quad (A6)$$

Thus, the self-consistency conditions at small $U$ read

$$\sum_\omega \frac{\chi(U = 0)_\omega}{1 - (U + \Lambda^{\text{sz}} - \Lambda^{\text{ch}})\chi(U = 0)_\omega} = \sum_{q,\omega} \frac{X(U = 0)_{q,\omega}}{1 - (U - \Lambda^{\text{sz}})X(U = 0)_{q,\omega}}, \quad (A7)$$

$$\sum_\omega \frac{\chi(U = 0)_\omega}{1 + (U + \Lambda^{\text{ch}} - \Lambda^{\text{sz}})\chi(U = 0)_\omega} = \sum_{q,\omega} \frac{X(U = 0)_{q,\omega}}{1 + (U + \Lambda^{\text{ch}})X(U = 0)_{q,\omega}}. \quad (A8)$$

These two equations can be solved numerically for $\Lambda^{\text{ch}}, \Lambda^{\text{sz}}$. Expanding the denominators and using the condi-
tion $\chi(U = 0) = \sum_{q^{\omega}} X(U = 0)$, we find

$$U' \sum_{\omega} \chi^2(U = 0)_{\omega} = \left(U' \pm \Lambda_{\text{ch/sx}}^0\right) \sum_{q^{\omega}} X^2(U = 0)_{q^{\omega}},$$

$$\Lambda_{\text{ch/sx}}^0 = \pm U \cdot C = \pm U \frac{1}{2 - C^{-1}}, \quad (A9)$$

where

$$C = \frac{\sum_{\omega} \chi^2(U = 0)_{\omega}}{\sum_{q^{\omega}} X^2(U = 0)_{q^{\omega}}} - 1. \quad (A10)$$

It is clear that $\Lambda_{\text{ch}} = -\Lambda_{\text{sx}}$ in the small $U$ regime described by these equations. In addition, both components of $\Lambda$ depend linearly on $U$. The magnitude of $\Lambda$ depends on $C$.

The temperature is implicitly contained in $\chi(U = 0)$ and $X(U = 0)$, which are Lindhardt bubble expressions, and in the sum over Matsubara frequencies. Figure 10 compares the perturbative formula with the numerical results of Fig. 1.

Particle-hole symmetry on hypercubic lattices implies that the change $U \to -U$ corresponds simply to the interchange of magnetic and density fluctuations, without any difference on the one-particle level. Under the interchange of $\Lambda_{\text{ch}}$ and $\Lambda_{\text{sx}}$, the expressions given here are clearly consistent with this symmetry.

**Appendix B: Self-energy asymptotics**

The general concept that enforcing some exact properties will break others is visible in the present instantaneous DB as well. An example is the high-frequency asymptote of the local self-energy of the paramagnetic Hubbard model,

$$\Sigma_{\nu}^{\text{lat}} \underset{\nu \to \infty}{=} \frac{U \langle n \rangle}{2} + \frac{U^2 \langle n \rangle^2}{4} \frac{1}{i\nu} + \ldots \quad (B1)$$

For the impurity model, with interaction $U' \neq U$, we find

$$\Sigma_{\nu}^{\text{imp}} \underset{\nu \to \infty}{=} \frac{U' \langle n \rangle}{2} + \frac{U'^2 \langle n \rangle^2}{4} \frac{1}{i\nu} + \ldots \quad (B2)$$

At high frequencies, where the denominator $1 + g \tilde{\Sigma}$ is equal to unity, the relation between dual and lattice self-energy is $\Sigma_{\nu}^{\text{lat}} = \Sigma_{\nu}^{\text{imp}} + \tilde{\Sigma}$. This means that the *exact* solution of the dual action should have

$$\Sigma_{\nu}^{\text{exact}} \underset{\nu \to \infty}{=} \left(U - U'\right) \langle n \rangle + \frac{U^2 \langle n \rangle^2}{4} \frac{1}{i\nu} + \ldots \quad (B3)$$

Let us see how this exact expression can arise in dual perturbation theory. We consider a situation where the difference $U' - U = \Lambda$ is small, so that dual perturbation theory is justified and we also consider $U'$ sufficiently small that the vertices can be simplified by doing perturbation theory in the impurity model.

The bare bosonic dual propagator simplifies in the Hubbard model with instantaneous impurity interaction, it is local\(^{199}\) and given by,

$$\tilde{X}_{q^{\omega}} = \left(\chi^{-1}_{\omega} + \Lambda\right)^{-1} - \chi_{\omega} \quad (B4)$$

$$\tilde{X}_{q^{\omega}} / \chi^2 = \frac{\Lambda}{1 + \Lambda \chi_{\omega}} \quad (B5)$$

$$\approx \Lambda = U' - U. \quad (B6)$$

Here, the last line is obtained since we are interested in small $\Lambda$. This shows that the number of bosonic propagators determines the order in $(U' - U)$.

We identify three basic diagrams that could be relevant for the asymptote: a “Hartree” and a “Fock” diagram both containing only two-fermion-one-boson vertices and a diagram with a single two-fermion-two-boson vertex $\gamma^{(2,2)}$. The first two of these diagrams vanish since they contain a local dual fermion propagator, which is zero by the fermionic self-consistency condition. It is the third diagram, shown in Fig. 11, that we are interested in here. To evaluate it, we need to find a simplified expression for the vertex. In dual boson, vertices involving the bosonic degree of freedom typically have a “trivial” contribution, as has been discussed at length for the fermion-boson vertex\(^{14,27,70}\). It essentially originates in the fact that the number of Wick contractions is reduced when going from $c^\dagger c$ to $n$. This also applies to $\gamma^{(2,2)}$, which has a trivial contribution

$$\gamma^{(2,2)}_{\delta_{\nu_{1}^{\nu_{2}}}^{\omega_{1}}^{\omega_{2}}} \times \chi_{\nu_{1}} \chi_{\omega_{2}} \sim g_{\nu_{1}} \delta_{\nu_{1}^{\omega_{2}}^{\omega_{1}}}^{\omega_{1}} g_{\nu_{1}}^{\nu_{1}} \nu_{1}^{\omega_{2}}^{\omega_{1}} \nu_{1}^{\omega_{1}} \nu_{1}^{\omega_{2}}^{\omega_{1}} + \omega_{1}. \quad (B7)$$

![Figure 11. Left: Self-energy diagram that contributes to the asymptote. Right: Diagram of trivial contribution to $\gamma^{2,2}$.](image)
Evaluating the self-energy with symmetry factor $\frac{1}{2}$, and combining Eqs. (B6) and (B7) gives

$$\tilde{\Sigma}_{\nu} = \frac{1}{2} \sum \tilde{X}_{\nu} \cdot \sigma^{(2,2)}_{v} \tilde{\Sigma}^{(2,2)}_{\omega} \approx \frac{1}{2} \sum_{\alpha \nu} (U' - U) g_{\alpha \nu}$$

(B8)

$$= (U' - U) \frac{4}{2}$$

exactly the desired expression for the first order term. Higher-order terms should appear in a similar fashion, although they become progressively harder to evaluate: multiple diagrams will contribute and the diagrams become more involved.

The interpretation of this result is two-fold. On the one hand, as long as $U' - U$ is not too large, deviations between the exact and numerical asymptotics of the self-energy will also stay small. On the other hand, it shows that a diagram that includes a three-particle vertex is already needed to recover only the lowest order term in the asymptotic expansion of the self-energy. This occurrence of three-particle vertices to achieve consistency is reminiscent of Refs. 21, 57, 71.
For clarity, we reintroduce the normalization of the frequency sum by the temperature here. It is worth observing that these relations occur on very different length and time scales: The Mermin-Wagner theorem and Goldstone modes are long wavelength, low frequency phenomena whereas the high-frequency asymptote of the self-energy is a local, high frequency phenomenon.

For the Hubbard model, \( \tilde{X}(0) \) is always local. The self-consistency condition \( \sum_q \tilde{X}(0) = 0 \) then automatically ensures that \( \tilde{X} = 0 \) everywhere and that Dual Boson reduces to Dual Fermion. The self-consistency condition used in this work does not require \( \sum_q X(0) = 0 \) and \( X \) is finite in the Hubbard model.