Dynamical mean-field theory for bosons

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\textbf{Abstract.} We discuss the recently developed bosonic dynamical mean-field theory (B-DMFT) framework, which maps a bosonic lattice model onto the self-consistent solution of a bosonic impurity model with coupling to a reservoir of normal and condensed bosons. The effective impurity action is derived in several ways: (i) as an approximation to the kinetic energy functional of the lattice problem, (ii) using a cavity approach and (iii) using an effective medium approach based on adding a one-loop correction to the self-consistently defined condensate. To solve the impurity problem, we use a continuous-time Monte Carlo algorithm based on the sampling of a perturbation expansion in the hybridization functions and the condensate wave function. As applications of the formalism, we present finite-temperature B-DMFT phase diagrams for the bosonic Hubbard model on a three-dimensional (3D) cubic and a 2D square lattice, the condensate order parameter as a function of chemical potential, critical exponents for the condensate, the approach to the weakly interacting Bose gas regime for weak repulsions and the kinetic energy as a function of temperature.
1. Introduction

Particles with bosonic statistics can macroscopically occupy a single mode at low enough temperature, even in the absence of correlation. This phenomenon is known as Bose–Einstein condensation (BEC) and leads to a variety of phases in strongly correlated bosonic systems. A typical example is $^4$He, which exhibits normal, superfluid, solid and possibly supersolid phases. Another example is dilute ultracold atomic gases, which are well described by a Bogoliubov Hamiltonian. Strong interaction effects can be induced by adding lasers producing an optical lattice. The resulting system is an essentially clean realization of the Bose–Hubbard model, which describes the competition between hopping and on-site repulsion. Commensurability effects in the lattice lead to a phase transition from a superfluid to a Mott...
insulator at integer fillings and strong enough interaction [1]. Both cold gases and $^4$He can be controlled experimentally with great accuracy and are virtually free from impurities and disorder. Cold atomic gases have the additional flexibility of tunable interaction strengths, and provide the freedom of changing the mass by choosing different alkali atoms.

For both $^4$He and ultracold bosonic gases in an optical lattice, powerful numerical methods exist for the strongly interacting regime. Path integral simulations based on the worm algorithm can sample up to 10,000 bosonic atoms at $T = 1$ K for supersolid $^4$He, enabling the study (for a review see [2]) of individual defects, such as vacancies [3], dislocations [4] and grain boundaries [5]. For cold gases, up to $1.5 \times 10^6$ atoms were studied [6] and compared directly with experiment, with excellent agreement in time-of-flight images [7]. Such simulations involve a stochastic evaluation of all connected and disconnected diagrams occurring in a high-temperature series expansion on a finite lattice, which is an expansion in the hopping or kinetic energy (over temperature) around the atomic limit [8–10].

The Monte Carlo simulation of fermionic lattice models suffers from the notorious sign problem, which prevents the study of large systems in the most interesting parameter regime. A computationally tractable approximate method for simulating these models is dynamical mean-field theory (DMFT) [11–15]. In these calculations, the many-body self-energy is approximated by all local skeleton diagrams involving local propagators only, which implies a self-consistent determination of the self-energy and the local propagators. Non-local contributions are neglected. This simplification is convenient because the approximated self-energy can be evaluated efficiently from an appropriately defined impurity action [12]. By using sign-free (for single-site DMFT) efficient continuous-time Monte Carlo solvers [16], one obtains the full Green’s function as a solution to the effective impurity action in polynomial time [17–19]. The simplification of the diagrammatic structure [11] allows one to define DMFT for arbitrary dimensions and lattice structures. A major success of DMFT lies in the understanding it has provided of the Mott metal–insulator transition [13, 15]. DMFT has been extensively used to study model systems and—in conjunction with band structure techniques—to compute material properties for a wide range of compounds [15, 20]. Several extensions make the approximation systematic and controlled: cluster methods [14], such as the dynamical cluster approximation [21] or the cellular DMFT [22, 23], reintroduce momentum dependence by considering multi-site impurity clusters. Methods such as dynamical vertex approximation (DVA) [24] or dual fermions [25, 26] systematically consider non-local diagrams beyond DMFT. In principle, a diagrammatic Monte Carlo evaluation of all neglected contributions to the self-energy allows one to estimate its accuracy, as, e.g., recently done for the Anderson localization problem [27].

The formulation of an analogous dynamical mean-field theory for bosonic lattice models has proved difficult. On the one hand, from the perturbative diagrammatic point of view, the idea of retaining an infinite subclass of bare diagrams may seem dubious since standard Feynman diagrammatic expansions in $U$ fail notoriously for the Bose–Hubbard model due to Dyson’s collapse argument: in the complex plane, the convergence radius is zero as all bosons would collapse to a single point for negative interactions, with an infinite negative energy in the thermodynamic limit. Hence, it seems impossible to think of meaningful diagrammatic expansions in $U$ for bosons, and only a few techniques are known for dealing with this problem: for example, Kleinert’s variational perturbation theory [28], the cutting off of large field contributions [29] or the use of a sequence with appropriately chosen counter-terms rendering an infinite convergence radius in the absence of phase transitions [30]. In the Baym–Kadanoff
approach to DMFT, a subset of diagrams consisting of all the contributions from local dressed propagators is retained. These skeleton diagrams may have convergence properties radically different from those of the bare series, but those properties are essentially unknown. In the case of absolutely convergent series, the bare and skeleton series are equivalent and physically meaningful, but owing to Dyson’s collapse argument for the bare series, there is no guarantee that the skeleton approach will converge.

On the other hand, keeping knowledge of the series provenance and using the effective action for a single site (i.e. restoring the action on the basis of the series) may still be worthwhile. In the normal phase, the usual DMFT formalism can be applied in the same way as it is usually done for fermions. By using an effective action on a single site (which can be solved with the method of choice), most of the aforementioned convergence issues can be sidestepped. It is in fact only the occurrence of a condensate (which happens in the single-particle channel) in the broken symmetry phase that poses a challenge in the development of a B-DMFT formalism (cf [31]). We will define our B-DMFT theory at the one-loop level beyond this self-consistently defined mean field (condensate). As shown in appendix B, our effective action for the impurity problem is the most general action for an impurity with a broken $U(1)$ symmetry and a one-loop correction [32]. The hybridizations are then determined self-consistently with the underlying lattice problem. The approximations involved can still be understood in the language of diagrams, but a full interpretation in terms of Baym–Kadanoff functionals remains subjective in light of the asymptotic series expansions. In this work we therefore prefer to use alternative derivation schemes that do not rely on an expansion in the bosonic repulsion $U$.

In the limit of infinite coordination number, the decoupling approximation for the Bose–Hubbard model becomes exact (see the appendix of [1]). This decoupling approximation is recovered in our action at the mean-field level, since the one-loop correction vanishes. The original B-DMFT paper by Byczuk and Vollhardt [33] (as well as subsequent work presented by Hu and Tong [34]) is based on the assumption that in this limit the kinetic and potential energy contributions in the broken symmetry phase can still be comparable to each other, in apparent contrast to [1]. Their work postulates a scaling ansatz with different scalings for condensed and non-condensed bosons, leading to an effective action that is different from the one we shall describe. The authors of [35] performed an expansion in the inverse of the coordination number around the limit of infinite coordination number (i.e. the static mean-field result of [1]), but treated the condensate in a perturbative way only valid on the Bethe lattice. After the publication of our results [36], they corrected for this and also derived a fully self-consistent (and general) version of the B-DMFT formalism [37].

The virtue of extending the DMFT framework to interacting Bose systems lies in the fact that certain model systems otherwise not amenable to bosonic simulations, e.g. models with frustrated interactions, or Bose–Fermi mixtures, can now be studied numerically. The quality of the approximation $\Sigma(k, \omega) \rightarrow \Sigma^{\text{ske}}(\omega)[G_{\text{loc}}]$ is system dependent and needs to be established on a case-by-case basis. We will see that the B-DMFT approximation is very good for the single-component Bose–Hubbard model in 3D and thus may serve as a good starting point for more complicated systems.

In both the fermionic and the bosonic versions of dynamical mean-field theory, the computationally challenging part is the solution of the impurity problem. For fermionic systems, exact diagonalization (ED) [38], semi-analytical resummation of diagrams [39, 40], quantum Monte Carlo (QMC) [41] and numerical renormalization group [42] methods are in wide use for single-orbital models. In recent years, significant progress has been made.
with the development of diagrammatic Monte Carlo impurity solver techniques, based on an expansion of the partition function in powers of the interaction [17, 18] or the impurity–bath hybridization [19, 43], allowing access to much larger impurity clusters, lower temperatures and more general interactions [16].

In this paper, we present a detailed derivation of the B-DMFT equations and show how the impurity–condensate coupling must be chosen to obtain a consistent theory. We quantify the errors introduced by the dynamical mean-field approximation for a system with finite coordination number by comparing with lattice Monte Carlo methods, and we describe the impurity solver proposed in [36] in such detail that the implementation of the method becomes straightforward.

This paper is organized as follows. Section 2 introduces the Bose–Hubbard model, and in section 3, we derive the B-DMFT formalism, which is summarized in section 4. In section 5, we describe the diagrammatic Monte Carlo impurity solver. Section 6 discusses solvable limits, while B-DMFT results for interacting bosons on a Bethe and a 3D simple cubic lattice are presented in section 7. Section 8 provides the summary and outlook.

2. The Bose–Hubbard model

We consider a model of spinless bosons on a lattice, described by the Bose–Hubbard Hamiltonian in standard lattice notation,

$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i,$$

where $t$ denotes the hopping amplitude, $U$ the on-site interaction and $\mu$ the chemical potential. Unless otherwise mentioned, our unit will be the hopping amplitude, $t = 1$. This model has three phases: (i) a normal phase at high temperature, (ii) a Mott insulating phase at zero temperature and commensurate filling for $U \gg zt$ and (iii) a superfluid phase occurring at low temperature.

In the following, we will develop an effective theory that goes beyond static mean-field theory by including temporal (in imaginary time) fluctuations, but which is restricted to a single site and therefore contains no momentum fluctuations.

The local terms of the action on a single site are

$$S_{\text{int}} = \int_0^\beta d\tau b_{\text{int}}^\dagger(\tau)(\partial_\tau - \mu) b_{\text{int}}(\tau) + \frac{U}{2} n_{\text{int}}(n_{\text{int}} - 1).$$

The subscript ‘int’ denotes the internal degrees of freedom. This local action correctly describes the physics of the system in the case of zero hopping ($t = 0$), when a factorization over each lattice site is exact. Hence, it already contains the low-energy physics occurring deep in the Mott phase. At very high temperature, the action is also accurate because, in terms of Feynman’s path integrals, the world lines describing the evolution of particles in imaginary time remain almost straight lines, i.e. a few hopping processes are present. Our task then is to replace this action with an effective action that also describes the physics deep in the superfluid phase (when the interaction is weak, compared with the hopping amplitude), i.e. in the regime where the Bogoliubov theory of the weakly interacting Bose gas (WIBG) applies. In terms of the treatment of the WIBG of [44], there is reason to believe that such an accurate DMFT-like effective action exists: to leading and subleading order (in the interaction), the normal and anomalous self-energies are momentum independent at zero frequency, which is precisely the DMFT approximation.
Note that in [44] an explicit small symmetry-breaking field was added, which introduced a gap in the spectrum (and removed IR divergences in leading orders). Although this violates the requirement that the spectrum of a superfluid should be gapless [45, 46], it was argued in [44] that the leading orders of thermodynamic observables are found on short-range distances and provided by Beliaev’s diagrammatic technique, whereas for long-range physics (i.e. the long-range wavelength fluctuations of the order parameter) one has to resort to Popov’s hydrodynamic theory. Similar considerations hold for our effective action where the gap is not fixed but depends on the condensate $\phi$. The short-range physics can be computed, but the long-range fluctuations are not part of the theory. In particular, the explicit symmetry breaking still leads to a finite condensate density in two dimensions at finite temperature (see section 7.2), which greatly simplifies the theory. However, while the explicit but fixed symmetry breaking field of [44] made the superfluid–normal transition first order, we expect in our case a second-order transition (see section 7.1.2) with non-universal critical exponents different from static mean-field theory because of the dynamical corrections in the hybridization terms that form a one-loop correction to mean-field theory [32].

3. Derivation of the bosonic dynamical mean-field theory (B-DMFT) equations

In this section, we present the derivation of the B-DMFT equations (the action and the self-consistency relations). For completeness, we present alternative (but equivalent) derivations of the DMFT formalism, such as a quantum cavity reasoning (appendix A) and an effective medium approach (appendix B), in the appendix. Here we implement an expansion around the atomic limit, following almost literally the lecture notes of Georges [47] and consider B-DMFT as an approximation to the kinetic energy functional. This derivation can to a large extent also be found in the supplementary material accompanying our previous paper [36]. The atomic reference system is interpreted as the impurity problem. We use the coupling constant integration method and introduce source fields (Lagrange multipliers) to constrain the condensate field and the connected Green’s function for the normal bosons to their physical values. By doing so, we avoid the collapse arguments associated with an expansion in $U$ mentioned in the introduction.

3.1. Expansion parameter

We introduce a parameter $\alpha \in [0, 1]$ such that

$$H_\alpha = \frac{U}{2} \sum_i n_i (n_i - 1) - \alpha t \sum_{\langle i, j \rangle} b_i^\dagger b_j.$$  \hfill (3)

When $\alpha = 0$, the atomic limit is recovered and the partition function factorizes over all sites. When $\alpha = 1$, the full hopping is recovered, and this is the model we are ultimately interested in.

3.2. Source fields and constraining fields

Constraining the normal/anomalous Green’s functions and the condensate to specified values can be done by introducing conjugate source fields (Lagrange multipliers) in the action. In order to constrain the condensate to $\Phi$, we introduce the source field $J$, and analogous for the connected Green’s function $G_c$ with source field $\Delta$. Throughout this paper, we use the Nambu
notation in which $\Phi^\dagger = (\phi^*, \phi)$, $J^\dagger = (J^*, J)$ and the individual components of $G_c$ and $\Delta$ are given by

$$G_c(\tau) = \begin{pmatrix} G_c(\tau) & \tilde{G}_c(\tau) \\ \tilde{G}_c^*(\tau) & G_c(-\tau) \end{pmatrix}$$

and

$$\Delta(\tau) = \begin{pmatrix} F(-\tau) & 2K(\tau) \\ 2K^*(\tau) & F(\tau) \end{pmatrix}.$$  \hfill (4)

We can then explicitly write down the grand potential per site (there are $N_s$ sites), which is a functional of the source fields and also depends on the constraining fields,

$$\Omega_{\alpha}[J, \Phi, \Delta, G_c] = -\frac{1}{N_s \beta} \ln \int \mathcal{D}[b^*, b] \exp \left\{ \int_0^\beta d\tau \left( \sum_i (\sum_i b_i(\tau) - \phi_i(\tau)) + \sum_i J(\tau) [b_i^*(\tau) - \phi_i^*(\tau)] \right) \right. \left. + \int_0^\beta d\tau \sum_i (J_i^*(\tau) [b_i(\tau) - \phi_i(\tau)] + J(\tau) [b_i^*(\tau) - \phi_i^*(\tau)]) \right. \left. + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i F(\tau - \tau') [\delta b_i(\tau) \delta b_i^*(\tau') + G_c(\tau - \tau')] \right. \left. + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i K(\tau - \tau') [\delta b_i^*(\tau) \delta b_i(\tau') + \tilde{G}_c(\tau - \tau')] \right. \left. + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i K^*(\tau - \tau') [\delta b_i(\tau) \delta b_i(\tau') + \tilde{G}_c(\tau - \tau')] \right\}.$$  \hfill (6)

Here, $\delta b$ is the non-condensed part of the operator $b$ given by $b = \langle b \rangle + \delta b$.

\subsection*{3.3. Atomic limit: impurity model}

Let us consider the atomic limit $\alpha = 0$. There the problem is local on every site with grand potential

$$\Omega_0[J_0, \Phi, \Delta_0, G_c] = -\frac{1}{N_s \beta} \ln \int \mathcal{D}[b^*, b] \exp \left\{ \int_0^\beta d\tau \left( \sum_i b_i^*(\tau) (-\partial_t + \mu) b_i - \frac{U}{2n_i(n_i - 1)} \right) \right. \left. + \int_0^\beta d\tau \sum_i (J_0^*(\tau) [b_i(\tau) - \phi_i(\tau)] + J_0(\tau) [b_i^*(\tau) - \phi_i^*(\tau)]) \right. \left. + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i F_0(\tau - \tau') [\delta b_i(\tau) \delta b_i^*(\tau') + G_c(\tau - \tau')] \right. \left. + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i K_0(\tau - \tau') [\delta b_i^*(\tau) \delta b_i(\tau') + \tilde{G}_c(\tau - \tau')] \right. \left. + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i K_0^*(\tau - \tau') [\delta b_i(\tau) \delta b_i(\tau') + \tilde{G}_c(\tau - \tau')] \right\}.$$  \hfill (7)
From $\delta \Omega_0/\delta J_0 = 0$ and $\delta \Omega_0/\delta J_0^* = 0$, we obtain

$$\Phi = \langle b \rangle_{\text{imp}},$$

and from $\delta \Omega_0/\delta F = 0$, $\delta \Omega_0/\delta K = 0$ and $\delta \Omega_0/\delta K^* = 0$, the relation

$$G_c(\tau) = G(\tau) + \Phi \Phi^\dagger,$$

with $G(\tau) = -\langle T b(\tau) b^\dagger(0) \rangle_{\text{imp}}$. The expectation values $\langle \ldots \rangle_{\text{imp}} = \text{Tr} [ T e^{-S_{\text{imp}}} \ldots ] / \text{Tr} [ T e^{-S_{\text{imp}}} ]$ are defined with respect to an impurity action,

$$S_{\text{imp}} = -\frac{1}{2} \int_0^\beta \int_0^\beta d\tau d\tau' \delta b^\dagger(\tau) \Delta_0(\tau - \tau') \delta b(\tau')$$

$$- \mu \int_0^\beta d\tau n(\tau) + U \int_0^\beta d\tau n(\tau) [n(\tau) - 1]$$

$$- \int_0^\beta d\tau J_0^\dagger(\tau) b(\tau).$$

Inverting expressions (8) and (9) yields $J[\Phi, G_c]$ and $\Delta_0[\Phi, G_c]$ and thus a functional $\Gamma_0$ of the condensate and connected impurity Green’s function,

$$\Gamma_0[\Phi, G_c] = \Gamma_{\text{imp}}[\Phi, G_c] + \int_0^\beta d\tau [F_0(\tau) G_c(\tau) + K_0(\tau) \tilde{G}_c^* (\tau) + K_0^* (\tau) \tilde{G}_c(\tau)]$$

$$+ \frac{1}{N_s \beta} \int_0^\beta d\tau \sum_i [J_i^\dagger(\tau) \phi_i(\tau) + J_o(\tau) \phi_i^*(\tau)],$$

where $F_{\text{imp}}$ is the free energy of the local quantum impurity model.

### 3.4. Full model

The exact functional of the (local) Green’s function and condensate is constructed by using the coupling constant integration method, starting from the atomic limit,

$$\Gamma = \Gamma_{\alpha=1} = \Gamma_0 + \int_0^1 d\alpha \frac{d\Gamma_\alpha}{d\alpha}.$$ 

By using the stationarity of $\Omega$ ($\alpha$-derivatives of the Lagrange multipliers do not contribute), we obtain

$$\frac{d\Gamma_\alpha}{d\alpha} = -\frac{1}{N_s \beta} \int_0^\beta d\tau t \sum_{\langle i,j \rangle} \langle b_i^\dagger(\tau) b_j(\tau) \rangle$$

$$= -\frac{1}{N_s \beta} \int_0^\beta d\tau t \sum_{\langle i,j \rangle} \langle \phi_i^*(\tau) \phi_j(\tau) \rangle$$

$$= -\frac{1}{2N_s \beta} \text{Tr} \sum_{n,k} \epsilon_k G_c^\alpha(k, i\omega_n) |_{\Phi, G_c} - \frac{1}{N_s \beta} \int_0^\beta d\tau t \sum_{\langle i,j \rangle} \langle \phi_i^*(\tau) \phi_j(\tau) \rangle,$$

where $\omega_n = 2\pi n / \beta$ are even Matsubara frequencies and $\epsilon_k$ is the dispersion relation of the non-interacting bosons.

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We now arrive at the formal expression for the exact functional $\Gamma = \Gamma_{\alpha=1}$,
\[
\Gamma[\Phi, G_c] = \Gamma_0[\Phi, G_c] + \mathcal{K}[\Phi, G_c],
\]
with the kinetic energy functional given by
\[
\mathcal{K}[\Phi, G_c] = \int_0^1 d\alpha \frac{\delta \Gamma_0}{\delta \alpha}[\Phi, G_c].
\]
Requiring stationarity ($\delta \Gamma / \delta \phi^*_\alpha(\tau) = 0$, $\delta \Gamma / \delta \phi_\alpha(\tau) = 0$) determines the value of the source field conjugate to the condensate (assume a homogeneous condensate over the lattice),
\[
J_0 = z t \Phi.
\]
Since the condensate is time independent (and taken real), we drop the $\tau$ dependence of $J_0$ as well. The other stationarity requirement ($\delta \Gamma / \delta G_c = 0$, $\delta \Gamma / \delta G_\alpha = 0$) determines the hybridization function appearing in the impurity action,
\[
F_0(\tau) = \frac{\delta \mathcal{K}}{\delta G_\alpha(\tau)}, \quad K^*_0(\tau) = \frac{\delta \mathcal{K}}{\delta G_\alpha(\tau)}.
\]
Note that for the case $z = \infty$, we have identically $\delta b = 0$ following appendix A in [1] and only static mean-field theory exists, which is physically clear: for a thermodynamic condensate to be gapless, the $k = 0$ component of the Green’s function should not decay in time. The infinite connectivity of the lattice removes any $k$ dependence, and in combination with bosonic statistics one then sees that the decoupling approximation is exact.

3.5. Approximation to the kinetic energy functional

B-DMFT can now be considered as an approximation to the kinetic energy functional. With the single-particle Green’s function of the Bose–Hubbard model in the presence of source fields and for arbitrary coupling constants, we can define a self-energy,
\[
G_c^{\alpha}(k, i\omega_n) = [i\omega_n \sigma_3 + (\mu - \alpha \epsilon_k) I + \Delta_\alpha - \Sigma_\alpha[k, i\omega_n]]^{-1},
\]
where $\sigma_3$ is the Pauli matrix with $\pm 1$ on the diagonal.

The DMFT approximation consists in replacing the self-energy $\Sigma_\alpha$ for arbitrary $\alpha$ by the impurity model self-energy $\Sigma_0$. Hence,
\[
G_c^{\alpha}(k, i\omega_n) = [i\omega_n \sigma_3 + (\mu - \alpha \epsilon_k) I + \Delta_\alpha - \Sigma_\alpha=0[i\omega_n]]^{-1} - \Delta_\alpha - \Sigma_\alpha=0[1\omega_n],
\]
\[
= [\Delta_\alpha - \Delta_0 + G_c^{-1} - \alpha \epsilon_k I]^{-1},
\]
where we have used that the impurity self-energy satisfies the Dyson equation
\[
\Sigma_\alpha=0[i\omega_n] = G_0^{-1} - G_c^{-1} = i\omega_n \sigma_3 + \mu I + \Delta_0 - G_c^{-1}
\]
and $G_0^{-1}$ is the bare Green’s function. Summing over $k$ and using the constraint on the local lattice Green’s function, we obtain the following relation between $G_c$ and the hybridization function,
\[
G_c(i\omega_n) = \int d\epsilon D(\epsilon)(\zeta - \alpha \epsilon I)^{-1} = \frac{1}{\alpha} \tilde{D}(\frac{\zeta}{\alpha}),
\]
with $\zeta = \Delta_\alpha - \Delta_0 + G_c^{-1}$. We used the non-interacting density of states $D(\epsilon) = \frac{1}{N} \sum_k \delta(\epsilon - \epsilon_k)$ and its Hilbert transform $\tilde{D}(z) = \int d\epsilon D(\epsilon)(z - \epsilon I)^{-1}$. By introducing its inverse,
\[ \tilde{D}(R(g)) = g, \text{ the relation above can be inverted } (\alpha R(\alpha G_c) = \zeta = \Delta_a - \Delta_0 + G_c^{-1}) \] and yields the hybridization function as a functional of the local Green’s function,

\[ \Delta_0[\omega_n; \Phi, G_c] = -G_c^{-1} + \Delta_0[\Phi, G_c] + \alpha R(\alpha G_c). \quad (22) \]

Inserting the above relation into (19), the lattice Green’s function expressed as a functional of \( G_c \) becomes

\[ G_c^\beta(k, \omega_n)|_{B-DMFT} = \left( \alpha R(\alpha G_c) - \alpha \epsilon_k I \right)^{-1}. \quad (23) \]

Equation (13) can now be evaluated with \( G_c^\beta(k)|_{B-DMFT} \),

\[ -\frac{1}{2N_s \beta} \text{Tr} \sum_{n,k} \epsilon_k G_c^n(k, \omega_n)|_{B-DMFT} - \frac{1}{N_s \beta} \int_0^\beta d\tau \sum_{i,j} [\phi_i^*(\tau)\phi_j(\tau)] \\
= -\frac{1}{2\alpha \beta} \text{Tr} \sum_n \int d\epsilon D(\epsilon)(R(\alpha G_c) - \epsilon I)^{-1} - \frac{1}{N_s \beta} \int_0^\beta d\tau \sum_{i,j} [\phi_i^*(\tau)\phi_j(\tau)]. \]

An explicit expression for the B-DMFT approximation to \( \mathcal{K}[\Phi, G_c] \) therefore reads as

\[ \mathcal{K}_{B-DMFT}[\Phi, G_c] = -\frac{1}{2 \beta} \text{Tr} \sum_n \int_0^1 d\alpha \left[ G_c R(\alpha G_c) - \frac{1}{\alpha} I \right] - \frac{1}{N_s \beta} \int_0^\beta d\tau \sum_{i,j} [\phi_i^*(\tau)\phi_j(\tau)], \quad (25) \]

where the last term reduces to \(-zt\phi^*\phi\) for a constant, homogeneous condensate.

3.6. Stationarity conditions

It immediately follows from equation (25) that the stationarity condition for the condensate is unaltered in the B-DMFT approximation \( (J_0 = zt \Phi) \), while the stationarity condition for the connected Green’s function \( (\delta \Gamma/\delta G_c = 0, \delta \Gamma/\delta \tilde{G}_c = 0) \) reads in the B-DMFT approximation \( (use R(\alpha G) + \alpha G R'(\alpha G) = \partial_\alpha [\alpha R(\alpha G)] \) and the cyclical properties of the trace,

\[ \Delta_0[\omega_n; \Phi, G_c]|_{B-DMFT} = -R[G_c(\omega_n)] + G_c(\omega_n)^{-1} \]

\[ = -\omega_n \sigma_3 - \mu I + \Sigma_{imp} + G_c^{-1}. \quad (26) \]

Here we have used again the Dyson equation for the second equality. Applying \( \tilde{D}(\cdot) \) to both sides of equation (26) gives

\[ G_c(\omega_n) = \int d\epsilon D(\epsilon)(\omega_n \sigma_3 + (\mu - \epsilon) I - \Sigma_{imp})^{-1}. \quad (27) \]

This equation defines the B-DMFT self-consistency condition.

B-DMFT maps the bosonic lattice problem to a self-consistent solution of an impurity model, whose action (expressed in terms of the full operators \( b \), therefore dropping the term \( \partial_\tau \)) now takes the form

\[ S_{imp} = -\frac{1}{2} \int_0^\beta d\tau d\tau' b^\dagger(\tau)\Delta_0(\tau - \tau')b(\tau') - \mu \int_0^\beta d\tau n(\tau) + \frac{U}{2} \int_0^\beta d\tau n(\tau)[n(\tau) - 1] \]

\[ -\Phi^\dagger \left( zt - \int_0^\beta d\tau' \Delta_0(\tau') \right) \int_0^\beta d\tau b(\tau). \quad (28) \]
Assuming $K = K^*$, $\phi = \phi^*$ and dropping all subscripts, we can write the action in our final version as

$$S_{\text{imp}} = -\frac{1}{2} \int_0^\beta \int_0^\beta d\tau d\tau' b^\dagger(\tau) \Delta(\tau - \tau') b(\tau') - \mu \int_0^\beta d\tau n(\tau) + \frac{U}{2} \int_0^\beta d\tau n(\tau)[n(\tau) - 1]$$

$$-\kappa \Phi^\dagger \int_0^\beta d\tau \Phi(\tau), \quad (29)$$

where the coefficient $\kappa$ is given by

$$\kappa = z t - \Delta_{11}(i\omega_n = 0) - \Delta_{12}(i\omega_n = 0). \quad (30)$$

The solution of the impurity problem yields the condensate $\Phi$ (equation (8)), the connected Green’s function $G_c$ (equation (9)) and the self-energy $\Sigma_{\text{imp}}$ of the impurity model. The right-hand side of equation (27) then defines the local lattice Green’s function, which is identified with the impurity Green’s function and thus allows one to obtain the new hybridization function for the next iteration by using equation (26).

4. DMFT procedure

Solving the single-site impurity model means computing the local Green’s function,

$$G(\tau) = -\langle T b(\tau) b^\dagger(0) \rangle_{\text{imp}}, \quad (31)$$

and the condensate $\Phi$ for the impurity action given by equation (29). The hybridization function $\Delta(\tau)$ and the condensate order parameter $\Phi$, which is constant in time, are calculated by a self-consistent procedure starting from some arbitrary initial values (usually obtained from the non-interacting or static mean-field limit). We then solve the impurity problem and calculate the new updated parameters $\Delta(\tau)$ and $\Phi$ for the action via the Dyson equation. This procedure is repeated until convergence is reached. The self-consistency equation for the condensate takes the simple form

$$\Phi = \langle b(\tau) \rangle_{\text{imp}}. \quad (32)$$

The new hybridization function $\Delta(\tau)$ is obtained as follows. From equations (31) and (8), we obtain the connected Green’s function via

$$G_c(\tau) = G(\tau) + \Phi \Phi^\dagger. \quad (33)$$

We then Fourier transform $G_c(\tau)$ to obtain $G_c(i\omega_n)$. In appendix C, we show how to obtain accurate Fourier transforms in spite of a finite number of measurement time steps. With this we calculate the matrix self-energy via the Dyson equation,

$$\Sigma(i\omega_n) = G_0^{-1}(i\omega_n) - G_c^{-1}(i\omega_n). \quad (34)$$

Here, $G_0^{-1}(i\omega_n)$ is the bare Green’s function, which is related to the hybridization function $\Delta(i\omega_n)$ via

$$\Delta(i\omega_n) = -i\omega_n \sigma_3 - \tilde{\mu} I + G_0^{-1}(i\omega_n). \quad (35)$$

The parameter $\tilde{\mu} = \mu - \langle \epsilon \rangle$ is chosen such that $\Delta(i\omega_n) \to 0$ in the limit $\omega_n \to \infty$. As we only consider symmetric density of states ($\langle \epsilon \rangle = 0$) here, we write $\mu$ from now on. Equation (35) allows us to rewrite the Dyson equation as

$$\Sigma(i\omega_n) = i\omega_n \sigma_3 + \mu I + \Delta(i\omega_n) - G_c^{-1}(i\omega_n). \quad (36)$$
Employing the DMFT approximation that the lattice self-energy coincides with the impurity self-energy, i.e. the self-energy loses its momentum dependence: \( \Sigma(k, i\omega_n) = \Sigma(i\omega_n) \), we can calculate the \( k \)-summed (or local) lattice Green’s function with

\[
G_{\text{latt}}(i\omega_n) = \sum_k \left[ i\omega_n \sigma_3 + (\mu - \epsilon_k) \mathbf{1} - \Sigma(i\omega_n) \right]^{-1},
\]

where \( \epsilon_k \) is the dispersion of the lattice. For some dispersions \( \epsilon_k \), it may be more convenient to transform the summation over wave vectors \( k \) into an integration over the density of states \( D(\epsilon) \). With \( D(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k) \), equation (37) transforms to

\[
G_{\text{latt}}(i\omega_n) = \int \frac{d\epsilon}{D(\epsilon)} \left[ \left( i\omega_n \sigma_3 + (\mu - \epsilon) \mathbf{1} - \Sigma(i\omega_n) \right)^{-1} \right].
\]

We now use the Dyson equation again to calculate the new updated hybridization function,

\[
\Delta(i\omega_n) = -i\omega_n \sigma_3 - \mu \mathbf{1} + \Sigma(i\omega_n) + G_{\text{latt}}^{-1}(i\omega_n),
\]

and the new value for \( \kappa \),

\[
\kappa = \zeta t - \Delta_{11}(i\omega_n = 0) - \Delta_{12}(i\omega_n = 0).
\]

After an inverse Fourier transform, we obtain \( \Delta(\tau) \) and the self-consistency loop is closed. We then solve the impurity problem again with the updated action, until convergence is reached.

4.1. Convergence

In this section, we discuss two problems that may occur in the iteration process but that can easily be overcome. The first problem is that in the first few iterations, when the solution is still far from the converged result, the Hilbert transformation may diverge for some Matsubara frequencies. The origin of the problem can be understood by writing equation (38) for the individual components

\[
G_{\text{latt}}(i\omega_n) = \int d\epsilon D(\epsilon) \left[ \frac{\zeta^* - \epsilon}{|\zeta - \epsilon|^2 - \Sigma^2} \right],
\]

\[
\tilde{G}_{\text{latt}}(i\omega_n) = \tilde{\Sigma} \int d\epsilon D(\epsilon) \left[ \frac{1}{|\zeta - \epsilon|^2 - \tilde{\Sigma}^2} \right],
\]

where \( \zeta = i\omega_n + \mu - \Sigma(i\omega_n) \), \( \Sigma (\tilde{\Sigma}) \) are the diagonal (off-diagonal) components of the matrix self-energy and we have used that \( \tilde{\Sigma} = \Sigma^* \). Obviously, the denominator of equation (41) can vanish for certain values of \( \Sigma \) and \( \tilde{\Sigma} \). If the divergence is due to the statistical errors on \( \Sigma \) and \( \tilde{\Sigma} \), the problem can be cured by running more accurate simulations. However, another reason for a divergent integral can be that the initial approximations for \( \Delta(\tau) \) and \( \Phi \) are unphysical (‘too far away’ from the converged solution). In almost all cases, this problem can be avoided by choosing suitable initial hybridization functions \( \Delta(\tau) \) and condensates \( \Phi \). We found that a good choice for the initial \( \Phi \) was the static mean-field value, corresponding to \( \Delta(\tau) = 0 \). For this value of \( \Phi \), we then calculated \( G_c(\tau) \) and obtained our initial hybridization function \( \Delta(\tau) \) using the lattice Hilbert transform. Should the integral still be divergent, which happens only in the first few iterations, one can shift (increase) the value of \( \Sigma \) such that the integral becomes well
defined. Another strategy to fix this problem is to apply a damping procedure to the self-energy in the first few iterations.

The second problem is related to the convergence properties of the condensate \( \Phi \). Sufficiently far away from the SF–Mott transition, we typically need about 10–20 iterations to reach convergence. Close to the SF–Mott transition, however, the convergence of \( \Phi \) is very slow, and sometimes up to 500 iterations are needed in order to reach a converged solution. With a runtime of a few minutes per iteration, this translates into a large numerical effort. Such slowing down of the convergence close to the phase transition can be overcome by using overrelaxation of the condensate \( \Phi \). The updating for \( \Phi \) is changed from equation (8) to

\[
\Phi = \alpha \left( \langle b(\tau) \rangle_{\text{imp}} - \Phi_{\text{old}} \right) + \Phi_{\text{old}},
\]

where \( \Phi_{\text{old}} \) is the condensate from the previous iteration and \( \alpha > 1 \).

5. Monte Carlo method

To formulate our Monte Carlo method, we start by writing the impurity action equation (29) in the non-matrix form

\[
S_{\text{imp}} = -\int_0^\beta d\tau \, d\tau' [b(\tau) F(\tau - \tau') b^\dagger(\tau') + b^\dagger(\tau) K(\tau - \tau') b(\tau')] - \mu \int_0^\beta d\tau n(\tau) + \frac{U}{2} \int_0^\beta d\tau n(\tau) [n(\tau) - 1] - \kappa \int_0^\beta d\tau [\phi^* b(\tau) + \phi b^\dagger(\tau)].
\]

With this action, we expand the partition function \( Z = \text{Tr} [T e^{-S_{\text{imp}}}] \) in powers of the hybridization functions \( F, K \) and \( K^* \) and the source fields \( \phi \) and \( \phi^* \). This leads to the series

\[
Z = \sum_n \sum_m \int_0^\beta d\tau_1^F \ldots \int_0^\beta d\tau_{m_F}^F \int_0^\beta d\tau_1^K \ldots \int_0^\beta d\tau_{m_K}^K \int_0^\beta d\tau_1^* \ldots \int_0^\beta d\tau_{m_\phi}^* \times \left[ \int_0^\beta d\tau_1^\phi \ldots \int_0^\beta d\tau_{m_\phi}^\phi \right] \langle n | T e^{\mu \int_0^\beta d\tau \ln n(\tau)} | n(\beta) \rangle \]

\[
\times b(\tau_1^F) \ldots b(\tau_{m_F}^F) b^\dagger(\tau_{m_F}^F) b(\tau_1^K) \ldots b(\tau_{m_K}^K) b(\tau_1^*) \ldots b(\tau_{m_\phi}^*) \phi(\tau_1^F) \ldots \phi(\tau_{m_\phi}^F) | n \rangle \]

\[
\times F(\tau_1^F - \tau_{m_F}^F) \ldots F(\tau_{m_F}^F - \tau_1^F) K(\tau_1^K - \tau_{m_K}^K) \ldots K(\tau_{m_K}^K - \tau_1^K) \times K^*(\tau_1^* - \tau_{m_\phi}^*) \ldots K^*(\tau_{m_\phi}^* - \tau_1^*) \phi(\tau_1^F) \ldots \phi(\tau_{m_\phi}^F) \phi(\tau_1^K) \ldots \phi(\tau_{m_\phi}^K) \phi(\tau_1^*) \ldots \phi(\tau_{m_\phi}^*) \phi(\tau_1^*). \tag{44}
\]
Figure 1. Diagram corresponding to perturbation orders $m_F = 1$, $m_K = 1$, $m_{K^*} = 1$, $m_\phi = 2$, $m_{\phi^*} = 2$ and $n(\tau = 0) = 2$. The hybridization function $F$ determines the amplitude for transitions of bosons from the impurity into the normal reservoir, while operators coupling to source fields $\phi$ and $\phi^*$ represent transitions between the impurity and the BEC reservoir. The off-diagonal hybridization functions $K$ and $K^*$, present only in the BEC phase, represent the amplitudes for creating or annihilating two bosons at different times.

where $|n\rangle$ denotes the eigenstate with $n$ bosons and $m = (m_F, m_K, m_{K^*}, m_\phi, m_{\phi^*})$. We can now sample individual diagrams with weight,

$$w(n; \tau_1^F, \ldots, \tau_{m_F}^F, \tau_1^K, \ldots, \tau_{m_K}^K, \tau_1^{K^*}, \ldots, \tau_{m_{K^*}}^{K^*}, \tau_1^{\phi}, \ldots, \tau_{m_\phi}^{\phi}) = \langle n| T \, e^{\mu \int_0^\beta d\tau \, U(n)} |n(\tau)\rangle$$

These contributions, illustrated in figure 1, can be represented by a collection of $m_F + 2m_{K^*} + m_\phi = m_F + 2m_{K^*} + m_\phi$ creation and annihilation operators on the imaginary time interval $[0, \beta]$. Hybridization functions $F$ connect $m_F$ pairs of creation and annihilation operators, off-diagonal hybridization functions $K (K^*)$ connect $m_K (m_{K^*})$ pairs of creation (annihilation) operators, and $m_\phi (m_{\phi^*})$ creation (annihilation) operators are linked to source fields $\phi (\phi^*)$. The configuration is fully specified by additionally giving the occupation $n$ of the impurity at times $\tau = 0$, which in combination with the collection of operators determines $n(\tau)$.

5.1. Updates and detailed balance

An ergodic sampling of all possible diagrams requires the following updates:

1. insertion/removal of a pair $b(\tau) F(\tau - \tau') b^\dagger(\tau')$,
2. exchange of the bath type:
   (a) $b(\tau) F(\tau - \tau') b^\dagger(\tau') \leftrightarrow \kappa \phi^* b(\tau) \kappa \phi^* b^\dagger(\tau')$,
   (b) $b(\tau) K^*(\tau - \tau') b(\tau') \leftrightarrow \kappa \phi^* b(\tau) \kappa \phi^* b(\tau')$,
   (c) $b^\dagger(\tau) K(\tau - \tau') b^\dagger(\tau') \leftrightarrow \kappa \phi^* b^\dagger(\tau) \kappa \phi^* b^\dagger(\tau')$. 

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In order to improve the efficiency, additional moves can/should be used. Updates that may improve the efficiency are shifts in operator positions, moves that reconnect the hybridization lines and moves that increase/decrease $n$ by one. For example, in the normal or Mott phase, where $\phi = K = 0$, or close to the SF transition, where $\phi$ is small, it is useful to have an additional move that reconnects two $F$-lines. The reason for this is that update 1 is the most time consuming and no $F$-lines can be reconnected via source fields $\phi$. Deep in the Mott phase, the insertion of $F$-lines is strongly suppressed. In order to have an efficient sampling, we now need an update that increases/decreases the occupation in the whole imaginary time interval without inserting new operators. A graphical representation of the updates is shown in figure 2.

In order to satisfy a detailed balance, we decompose the transition probability to go from state $i$ to state $j$ as

$$p(i \rightarrow j) = p^{\text{prob}}(i \rightarrow j) p^{\text{acc}}(i \rightarrow j),$$

where $p^{\text{prob}}$ ($p^{\text{acc}}$) is the probability to propose (accept) this move.

The only move that changes the number of operators in the imaginary time interval, and therefore the total perturbation order $m$, is the move to insert or remove an $F$-line. If we choose to insert an operator pair ($F$-line) at random times $\tau$ and $\tau'$ drawn from a uniform distribution $[0, \beta)$ and propose to remove this pair with probability $1/(m_F + 1)$, the proposal probability becomes

$$p^{\text{prob}}(m_F \rightarrow m_F + 1) = \frac{2d\tau d\tau'}{\beta^2},$$

Figure 2. Illustration of the different updates described in section 5.1.
The Green’s function matrix $G$ can be written as $C^2 \sum_{\tau} \langle n, \tau | \phi^* b(\tau) \rangle = \sum_{\tau} \langle n, \tau | \phi^* b(\tau) \rangle$.

For moves that increase/decrease the occupation of the impurity by one, we have $p_{\text{prop}} = 1$, so the acceptance probabilities satisfy

$$\frac{p_{\text{acc}}(n \rightarrow n+1)}{p_{\text{acc}}(n+1 \rightarrow n)} = \frac{w_{\text{Tr}}(n+1; \tau_1^F, \ldots, \tau_{m_F}^F, \tau_1^F, \ldots, \tau_{m_F}^F, \ldots)}{w_{\text{Tr}}(n; \tau_1^F, \ldots, \tau_{m_F}^F, \tau_1^F, \ldots, \tau_{m_F}^F, \ldots)}.
$$

Moves that interchange hybridization lines are easiest, since the operator trace term $\text{Tr} \frac{\partial}{\partial \phi} \langle \phi^* b(\tau) \rangle$ does not change. The probability of proposing such a move is given by the inverse of the number of possibilities to choose the line (or lines) to exchange. For moves that exchange $\phi^* b(\tau)\phi b(\tau')$, the detailed balance condition reads

$$\frac{p_{\text{acc}}([m_F, m_\phi, m_{\phi^*}] \rightarrow [m_F - 1, m_\phi + 1, m_{\phi^*} + 1])}{p_{\text{acc}}([m_F - 1, m_\phi + 1, m_{\phi^*} + 1] \rightarrow [m_F, m_\phi, m_{\phi^*}])} = \frac{m_F}{(m_\phi + 1)(m_{\phi^*} + 1)} \frac{\kappa \phi^* \kappa \phi}{F(\tau - \tau')}.
$$

For moves that change an off-diagonal hybridization line into two condensate lines, we have to consider that the $K$-lines do not have a defined direction like the $F$-lines. Therefore, the probability of choosing one $K$-line in a state with $m_K$ $K$-lines is given by $p_{\text{prop}} = 2/m_K$. Similarly, the probability of choosing two $\phi$-lines in a state with $m_\phi$ $\phi$-lines is given by $p_{\text{prop}} = 2/(m_\phi(m_\phi - 1))$. The detailed balance condition for moves that exchange $\phi^* b(\tau)\phi b(\tau')$ is therefore given by

$$\frac{p_{\text{acc}}([m_K, m_\phi] \rightarrow [m_K - 1, m_\phi + 2])}{p_{\text{acc}}([m_K - 1, m_\phi + 2] \rightarrow [m_K, m_\phi])} = \frac{m_K}{(m_\phi + 2)(m_\phi + 1)} \frac{\kappa \phi \phi}{K(\tau - \tau')}.
$$

and similarly for the complex conjugate.

### 5.2. Measurement of observables

By taking functional derivatives of the partition function with respect to $F(\tau - \tau'$), $K(\tau - \tau'$), $K^*(\tau - \tau')$, or both $\phi^* (\tau)$ and $\phi (\tau')$, one can calculate the diagonal and off-diagonal parts of the Green’s function matrix $G(\tau)$ and the condensate order parameter $\phi$.

For the condensate, the functional derivative yields

$$\phi(\tau) = \langle b(\tau) \rangle_{\text{imp}} = \left( \sum_{i=1}^{m_\phi^*} \frac{\delta(\tau, \tau_i^{\phi^*})}{\kappa \phi^* (\tau_i^{\phi^*})} \right)_{\text{MC}}.$$
where \( \langle A \rangle_{MC} \) means that the quantity \( A \) should be averaged over all configurations obtained in the Monte Carlo sampling. Due to the time independence of \( \phi \), this reduces to

\[
\phi = \langle b(\tau) \rangle_{\text{Simp}} = \frac{\langle m_{\phi^*} \rangle_{\text{MC}}}{\beta \kappa \phi^*}.
\]

One can see from equation (54) that one needs a condensate in order to measure a condensate. Therefore, one always chooses \( \phi \neq 0 \) as the initial value in the simulation.

The diagonal and off-diagonal Green’s functions can be measured in two different ways: either by taking the functional derivative with respect to \( F(\tau - \tau') \), \( K(\tau - \tau') \) and \( K^*(\tau - \tau') \) or by differentiating with respect to both \( \phi^*(\tau) \) and \( \phi(\tau') \). This yields

\[
G(\tau) = -\langle Tb(\tau)b^\dagger(0)\rangle_{\text{Simp}} = -\left\langle \frac{m_{\phi^*}}{\beta \kappa \phi^*} \sum_{i=1}^{m_F} \delta(\tau, \tau_i^F - \tau_i^F) \right\rangle_{\text{MC}},
\]

\[
\tilde{G}(\tau) = -\langle Tb(\tau)b(0)\rangle_{\text{Simp}} = -\left\langle \frac{m_{\phi^*}}{\beta \kappa \phi^*} \sum_{i=1}^{m_K} \delta(\tau, \tau_i^K - \tau_i^K) \right\rangle_{\text{MC}},
\]

in terms of the hybridization and

\[
G(\tau) = -\langle Tb(\tau)b^\dagger(0)\rangle_{\text{Simp}} = -\left\langle \frac{m_{\phi^*}}{\beta \kappa \phi^*} \sum_{i=1}^{m_F} \sum_{j=1}^{m_F} \delta(\tau, \tau_i^\phi - \tau_j^\phi) \right\rangle_{\text{MC}},
\]

\[
\tilde{G}(\tau) = -\langle Tb(\tau)b(0)\rangle_{\text{Simp}} = -\left\langle \frac{m_{\phi^*}}{\beta \kappa \phi^*} \sum_{i=1}^{m_K} \sum_{j=1}^{m_K} \delta(\tau, \tau_i^{K^*} - \tau_j^{K^*}) \right\rangle_{\text{MC}},
\]

in terms of the condensate with

\[
\delta(\tau, \bar{\tau}) = \begin{cases} 
\delta(\tau - \bar{\tau}) & \text{for } \bar{\tau} \geq 0, \\
\delta(\tau - \bar{\tau} - \beta) & \text{for } \bar{\tau} < 0,
\end{cases}
\]

and similarly for the adjoint. The end point \( G(\beta_-) \) can be accurately measured through the density,

\[
G(\beta_-) = -\langle n \rangle_{\text{MC}} = -\left\langle \frac{1}{\beta} \int_{0}^{\beta} d\tau \, n(\tau) \right\rangle_{\text{MC}}
\]

and \( G(0_+) = G(\beta_-) - 1 \). In the condensate phase, the expansion order of \( \phi \) and \( \phi^* \) is much higher than the expansion order of the hybridization (see section 5.4). Therefore, the Green’s functions are measured by using the condensate. Close to the SF transition, where \( \phi \) is very small, it is more efficient to measure the diagonal Green’s function according to equation (55).

In the normal or Mott phase, where \( \phi = 0 \), the diagonal Green’s function can only be calculated.
in this way. In practice, the off-diagonal Green’s function is always measured with $\phi$, even close to the SF transition. This is because the expansion order of $K$ and $K^*$ is always lower than $m_\phi$.

The kinetic and potential energy can also be evaluated easily and very accurately. The potential energy is given by

$$E_{\text{pot}} = \frac{U}{2} \langle n(n-1) \rangle - \mu \langle n \rangle$$  \hspace{1cm} (58)

and can be computed directly in the Monte Carlo simulation. As shown in section 3.4, the kinetic energy in the DMFT approximation is given by $E_{\text{kin}} = \frac{dE}{d\tau} |_{\tau=1}$. Equation (24) in the presence of a constant, homogeneous condensate then yields

$$E_{\text{kin}} = -\frac{1}{2\beta} \text{Tr} \sum_n \left[ G_c(\omega_n) R(G_c(\omega_n)) - I \right] - zt \phi^2.$$  \hspace{1cm} (59)

By using equation (22) and $\Delta_{\alpha=1} = 0$, we obtain

$$E_{\text{kin}} = \frac{1}{2\beta} \text{Tr} \sum_n \left[ G_c(\omega_n) \Delta_0(\omega_n) \right] - zt \phi^2.$$  \hspace{1cm} (60)

Going back to imaginary time, we can write this in the individual components as

$$E_{\text{kin}} = \int_0^\beta d\tau \left[ F(\tau) G_c(\tau) + K(\tau) \tilde{G}_c(\tau) + K^*(\tau) \tilde{G}_c(\tau) \right] - zt \phi^2,$$  \hspace{1cm} (61)

or in terms of the full Green’s function,

$$E_{\text{kin}} = \int_0^\beta d\tau \left[ F(\tau) G(\tau) + K(\tau) \tilde{G}^*(\tau) + K^*(\tau) \tilde{G}(\tau) \right] - \kappa \phi^2.$$  \hspace{1cm} (62)

By plugging equations (54) and (55) into the above expression, we see that the kinetic energy is directly related to the expansion order via

$$E_{\text{kin}} = -\frac{1}{\beta} \langle m_{\text{tot}} \rangle,$$  \hspace{1cm} (63)

where $m_{\text{tot}} = m_F + m_K + m_{K^*} + (m_\phi + m_{\phi^*})/2$ is the total number of operator pairs in the interval $[0, \beta)$.

This algorithm is a bosonic version of the hybridization expansion method of [19]. Aside from the condensate term and the anomalous hybridization, the main difference lies in the fact that for bosons we do not use any summation of diagrams. In the fermionic case, the analytical summation of all diagrams corresponding to a given sequence of creation and annihilation operators (i.e. all diagrams obtained by linking these operators in different ways by hybridization functions) results in a determinant, and was the essential step that allowed us to suppress the sign problem and to formulate an efficient algorithm. In a bosonic model, a similar summation of diagrams would lead to a matrix permanent whose evaluation is #P-complete. The only efficient way of evaluating permanents is by their stochastic sampling, which is exactly our algorithm of individually sampling the different diagrams (as illustrated in figure 1) instead of summing them up explicitly.

Since the off-diagonal hybridization function $K$ is negative, some diagrams have negative weights, which leads to a sign problem. However, as we will show later, this becomes an issue only at very low temperatures in the presence of a condensate and does not prevent an accurate computation of phase diagrams and dynamical quantities.
5.3. Solver test

To check if the diagrammatic sampling and measurement procedure have been implemented correctly, we compare the QMC result with ED. In a Hamiltonian formulation, the impurity model can be written as

$$H_{\text{imp}} = \sum_i \left[ V_i (a_i^\dagger b + a_i b^\dagger) + W_i (a_i b + a_i^\dagger b^\dagger) \right] + \sum_i \epsilon_i a_i^\dagger a_i - \mu n + \frac{U}{2} n(n-1) - \kappa (\phi^* b + \phi b^\dagger).$$

(64)

The hybridization functions $F$ and $K$ in equation (29) are related to the hybridization parameters $V_i$ and $W_i$ through

$$F(i\omega_n) = \sum_i \left( \frac{V_i V_i}{\epsilon_i + i\omega_n} + \frac{W_i W_i}{\epsilon_i - i\omega_n} \right),$$

(65)

$$K(i\omega_n) = \frac{1}{2} \sum_i \left( \frac{V_i W_i}{\epsilon_i + i\omega_n} + \frac{V_i W_i}{\epsilon_i - i\omega_n} \right).$$

(66)

For the test, we represent the bosonic bath by a finite number $n_{\text{bath}}$ of levels with creation (destruction) operators $a_i^\dagger$ ($a_i$) and energies $\epsilon_i$. By Fourier transforming equation (66), we obtain

$$F(\tau) = \sum_{i=1}^{n_{\text{bath}}} \left( \frac{V_i^2}{e^{\epsilon_i \beta} - 1} e^{\epsilon_i \tau} + \frac{W_i^2}{1 - e^{-\epsilon_i \beta}} e^{-\epsilon_i \tau} \right),$$

(67)

$$K(\tau) = \frac{1}{2} \sum_{i=1}^{n_{\text{bath}}} \left( \frac{V_i W_i}{e^{\epsilon_i \beta} - 1} e^{\epsilon_i \tau} + \frac{V_i W_i}{1 - e^{-\epsilon_i \beta}} e^{-\epsilon_i \tau} \right).$$

For the comparison, we choose one orbital ($n_{\text{bath}} = 1$) and the following parameters: $t = 1$, $\beta = 1$, $\mu = 20$, $U = 20$, $\kappa = 6$, $\phi = 1$, $\epsilon = 1$, $V = 1$ and $W = -0.2$. In figure 3, we show the diagonal and off-diagonal Green’s functions calculated with ED and Monte Carlo simulations.

The density and the condensate order parameter are $n_{\text{ED}} = 1.6762$ and $\phi_{\text{ED}} = 1.07976$ for ED, and $(n_{\text{MC}}) = 1.67619(3)$ and $(\phi_{\text{MC}}) = 1.07974(9)$ for the Monte Carlo simulations. Note that for this set of parameters the average sign $\langle s \rangle$ in the Monte Carlo simulation is $\langle s \rangle = 0.40695(7)$. The perfect agreement with the ED result shows that the diagrammatic sampling and measurement procedure have been implemented correctly. Since the model we considered here contains both diagonal and off-diagonal hybridization terms and since a bath with a finite number of levels is as difficult to treat as any other bath, this serves as a non-trivial test for the Monte Carlo solver.

5.4. Perturbation order and average sign

In this section, we show how the expansion order of the hybridization function scales with interaction and how the sign problem, caused by the off-diagonal hybridization $K$, scales at the transition from the Mott insulator (or normal phase) to the SF. Since we sample the operator configuration in the imaginary time interval $[0, \beta)$, the perturbation order grows roughly in proportion to $\beta$ in all phases.

In figure 4, we show how the mean perturbation order grows as one goes from the normal phase to the SF phase at filling $n = 1$. In the normal phase, we have only contributions from the
Figure 3. Comparison of the diagonal and off-diagonal Green’s functions calculated by Monte Carlo (black circles) and ED (red curve) for a hybridization function that can be described by a bath with one orbital. For the parameters, see text.

Figure 4. Mean perturbation order versus $t/U$ at filling $n = 1$ and inverse temperature $\beta t = 2$ for the 3D cubic lattice. The superfluid phase sets in where $m_\phi$ and $m_K$ become nonzero.

diagonal hybridization $F$, and the perturbation order $m_F$ decreases with increasing $U$. In the SF phase, the perturbation order grows rapidly with decreasing interaction $U/t$, mainly because of the condensate contribution $m_\phi$ and the off-diagonal hybridization contribution $m_K$.

Figure 5 illustrates the sign problem we encounter when going from the Mott phase to the SF phase. At the phase boundary where the condensate vanishes (and therefore $K$ vanishes), the
Figure 5. Average sign versus $t/U$ at filling $n = 1$ for the 3D cubic lattice at different temperatures. The sign is negative (positive) for odd (even) expansion orders in $m_K$. Hence, the point where the average sign starts to deviate from 1 is indicative of the phase transition into the superfluid phase.

sign problem disappears. Therefore, the sign problem does not prevent an accurate computation of phase diagrams. The sign problem is only severe deep in the condensate phase.

6. Simple limits

6.1. Non-interacting bosons

For an ideal Bose gas ($U = 0$), the total number of particles is given by

$$n = |\phi|^2 + \int \frac{D(\epsilon)}{e^{\beta(\epsilon - \mu)} - 1}, \quad |\epsilon| \leq zt,$$

(68)

where $zt$ is the half-bandwidth of the lattice. Just as in the case of an ideal Bose gas in continuous space, the chemical potential $\mu$ has to be lower than the bottom of the band, $\mu \leq -zt$, in order to keep the number of particles finite.

For temperatures $T > T_c$, the condensate vanishes, $|\phi|^2 = 0$, and the above equation determines the density $n$ as a function of the chemical potential $\mu$. For $T < T_c$, the chemical potential must be pinned at the lower edge of the band, $\mu = -zt$, in order to have condensation. The total number of particles is then a function of the condensate density $|\phi|^2$. In the non-interacting limit, the off-diagonal hybridization functions $K$ and $K^*$ vanish and the B-DMFT equations become exact. The impurity action now takes the simple form

$$S_{imp} = -\int_0^\beta d\tau' d\tau F(\tau - \tau')b(\tau')b^\dagger(\tau) - \int_0^\beta d\tau n(\tau) - \kappa \int_0^\beta d\tau [\phi^\star(\tau)b(\tau) + \phi(\tau)b^\dagger(\tau)].$$

(69)
This is a quadratic action that can be solved analytically. The solutions for the non-interacting Green’s function and hybridization function are given by

\[ G(i\omega_n) = G_0(i\omega_n) = \int \frac{d\epsilon}{i\omega_n + \mu - \epsilon} \left( |\epsilon| \leq zt \right), \]
\[ F(i\omega_n) = i\omega_n - \mu + G^{-1}_0(-i\omega_n). \]  

(70)

6.2. Static mean field

One obtains a self-consistent mean-field theory (the decoupling approximation) by substituting

\[ b^+_i b_j = \langle b^+_i \rangle b_j + b^+_i \langle b_j \rangle - \langle b^+_i \rangle \langle b_j \rangle = \phi (b^+_i + b_j) - \phi^2 \]  

(71)

into our Hamiltonian defined by equation (1). If one drops the term \(-\phi^2\), which is just a constant shift in energy, one obtains the following Hamiltonian,

\[ H_{MF} = -\kappa \phi \sum_i (b^+_i + b_i) + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu \sum_i n_i, \]  

(72)

where \( \kappa = \sum_{\langle i,j \rangle} t = zt \) is the hopping term summed over the nearest neighbors. For the 3D cubic lattice \((z = 6)\), this just gives the half-bandwidth \( \kappa = 6t \). This Hamiltonian can be expressed as a matrix in the occupation number basis (truncated at some maximum occupation) and solved by ED. One chooses an initial value for the condensate \( \phi \) and determines \( \phi \) iteratively by solving \( \phi = \langle b \rangle \) until convergence is reached.

By using B-DMFT, we can reproduce the static mean-field results by setting the hybridization function to zero, i.e. \( \Delta(\tau) = 0. \) Since there is no hybridization, equation (30) reduces to \( \kappa = zt. \)

7. Numerical results

In this section, we present results for the Bose–Hubbard model on a 3D cubic and a 2D square lattice obtained with B-DMFT. All our results are compared with other methods, such as static mean-field theory and worm-type QMC simulation on a lattice of up to \( 40^3 \) sites [8, 10] and with a recently developed numerically exact method on the Bethe lattice [49]. Since the Bethe lattice can also be directly simulated with B-DMFT, we will show a direct comparison between B-DMFT and the numerically exact solution.

7.1. Three-dimensional (3D) cubic lattice

7.1.1. Kinetic and total energy. In this section, we present the results for the 3D cubic lattice. Since DMFT can be considered as an approximation to the kinetic energy functional, equation (25), it is interesting to see how the kinetic energy per site obtained from B-DMFT compares to results from lattice Monte Carlo simulations [48] and static mean-field theory. In figure 6, we show the kinetic energy as a function of temperature as one goes from the SF to the normal phase. In the case of static mean-field theory, the kinetic energy is just given by \( E_{kin} = -zt \phi^2, \) where \( \phi = \langle b \rangle \) is the condensate order parameter. In the ground-state regime, this gives a good approximation of the kinetic energy. For \( T > T_c, \) where \( \phi = 0, \) the kinetic energy vanishes since
hopping of the normal bosons is completely neglected. There is excellent agreement between the B-DMFT results and the exact QMC results over the entire temperature range. Only close to $T_c$ there is some small deviation. For the QMC simulation, we used $10^3$ lattice sites, except for temperatures in the range $4 \leq T/t \leq 6$, where $40^3$ sites were used. In figure 7, we show the total energy as a function of temperature. The remarkable accuracy of the B-DMFT result for the total energy at all temperatures implies that entropies may also be computed reliably using B-DMFT.

In figure 8, we show the finite-temperature phase diagram (top panel) and the ground-state phase diagram (bottom panel) for the first and second Mott lobes of the Bose–Hubbard model on a 3D cubic lattice and compare the B-DMFT results to exact results from lattice QMC simulations, to the exact solution for the Bethe lattice with coordination number $z=6$ [49] and to static mean-field results [36]. The SF phase is characterized by a finite value of $\phi = \langle b \rangle$, while we have $\phi = \langle b \rangle = 0$ in the Mott insulating and normal phases. For the calculation of the ground-state phase diagram, we used $\beta t = 2$, which is shown in figure 8 to be a sufficiently low temperature. Based on simulations done at $\beta t = 4$ and $\beta t = 8$, we found that any systematic error is smaller than the statistical error.

The excellent agreement between our B-DMFT results and the full solution of the Bose–Hubbard model shows that the Mott transition is a local phenomenon well described by a momentum-independent self-energy and that the condensed bosons are accurately described by a uniform condensate.
7.1.2. Critical exponents. We now examine the critical exponent of the order parameter $\phi$. In [50], fermionic DMFT was employed to study the superfluid state. The temperature dependence of the condensate order parameter $\Delta$ goes as $\Delta \sim |(T_c - T)/T_c|^{\beta}$ in the vicinity of the critical temperature $T_c$, with $\beta = 1/2$ being the mean-field exponent. The symmetry breaking happens on the mean-field level in the two-particle channel given by a spin-up and a spin-down fermion. For any fermionic operator, we find that $\langle c \rangle \equiv 0$ such that condensation can occur the earliest in the two-particle channel, e.g. $\langle c^+_1 c_1 \rangle$ may be nonzero. For a bosonic operator, a single operator $b$ may already have a nonzero expectation value, $\langle b \rangle \neq 0$, leading to condensation at the one-body level. The B-DMFT action allows for this, while at the two-body level (i.e. the self-consistently determined hybridization terms) the one-loop correction to the condensate will change the critical exponents from their mean-field values. The exponents we obtain are therefore not universal but depend on the parameters $t$, $\mu$, $U$, $\beta$ and the lattice dispersion $\epsilon_k$. Whenever $\kappa = \text{const}$, we recover the mean-field exponents. This happens of course in the static mean-field limit ($\kappa = zt$) and for non-interacting bosons ($\kappa = -G_0^{-1}(i\omega_n = 0)$), where the mean-field exponent $\beta = 1/2$ is exact. In [49], mean-field exponents were also found for the exact solution on the Bethe lattice.

In figure 9 (main panel), we show the condensate order parameter $\phi$ as a function of temperature obtained by B-DMFT and compare the results with lattice QMC and static mean-field theory. Close to the critical point, the condensate goes as $\phi \sim |(T_c - T)/T_c|^{\beta}$ for $T < T_c$. The QMC results are obtained on a lattice with $40^3$ sites, which still leads to a rounding of
Figure 8. Top panel: phase diagram (superfluid to normal liquid transition) of the cubic lattice Bose–Hubbard model in the space of interaction and temperature for $n = 1$. The dashed line shows the static mean-field result, the red curve the exact solution for a Bethe lattice with coordination number $z = 6$ [49] and the blue curve with open diamonds the QMC result from lattice simulations [48]. The black line with open circles corresponds to the B-DMFT solution, which yields a second-order transition. Bottom panel: ground-state phase diagram in the space of $t/U$ and $\mu/U$, showing the first two Mott lobes surrounded by superfluid. The B-DMFT phase boundary was computed at $\beta t = 2$. The error bars are much smaller than the symbol size.

the data compared with the thermodynamic limit. They are based on the $k = 0$ component of the Fourier transform of the equal-time density matrix. By plotting $\phi$ as a function of $T_c - T$ in a log–log plot, we can extract the critical exponent $\beta$ from the slope of the line as $T \to T_c$, which is shown in the inset of figure 9. Static mean-field theory of course gives the mean-field
Figure 9. Main panel: condensate order parameter $\phi$ as a function of temperature of the Bose–Hubbard model on the 3D cubic lattice for $\mu/t = 8$ and $U/t = 20$ ($n \approx 1$). Results obtained from B-DMFT (black circles) are compared with lattice QMC (blue diamonds) and with static mean-field theory (black dashed line). Inset: zoom-in of the region close to the SF–normal transition, showing the critical exponent $\beta$. Here, $\phi$ is plotted as a function of $T_c - T$ for $T < T_c$. The full lines are fits to $\phi = A|T_c - T|^\beta$ (B-DMFT: $\beta = 0.194(2)$, $T_c/t = 4.365(3)$, $At = 0.6463$, QMC: $\beta = 0.35$, $T_c/t = 4.43(3)$, $At = 0.6517$, mean-field: $\beta = 0.5$, $T_c/t = 6.5661$, $At = 0.535$). The QMC results are obtained on a lattice with $40^3$. The error bars are smaller than the symbol size.

The weakly interacting Bose gas (WIBG) regime. When bosonic field theories are expanded in $U$ (cf the WIBG of [44]), the effect of the chemical potential is non-perturbative. The chemical potential is negative for the ideal Bose gas and has to change sign in the presence of repulsive interactions. There is an implicit relation between the condensate density $n_0 = |\phi|^2$ and the chemical potential, which follows from the condition of thermodynamic equilibrium [52],

$$\left[ \frac{\partial \Omega(T = 0, V, \mu, n_0)}{\partial n_0} \right]_{V, \mu} = 0,$$

(73)

leading to $\mu = \langle 0 | \frac{\partial \hat{H}_{\text{int}}}{\partial n_0} | 0 \rangle$, with $\hat{H}_{\text{int}}$ being the interacting two-body terms and $| 0 \rangle$ the ground state (finite-temperature extensions also exist [44]). In any expansion order, this remains valid and can be worked out to yield

$$\mu = \Sigma(k = 0, \omega = 0) - \tilde{\Sigma}(k = 0, \omega = 0),$$

(74)

which is the famous relation for a gapless spectrum first derived by Hugenholtz and Pines [53].
The Hugenholtz–Pines relation does not hold in our B-DMFT formalism. To start the discussion, let us consider a mean-field approach in which the condensate is determined self-consistently but the hybridization functions are not. Then it is easy to see that the Hugenholtz–Pines relation is shifted to \( \mu = \Sigma(\omega_n = 0) - \tilde{\Sigma}(\omega_n = 0) - zt \). If, however, the hybridization functions are also determined self-consistently (as in the full B-DMFT scheme), they will also depend on and influence the condensate density (and contain \( \mu \) in them), leading to the breakdown of the Hugenholtz–Pines relation. Indeed, although the authors of \cite{44} use a skeleton approach for the description of the WIBG, the discussion of the Hugenholtz–Pines relation is provided in terms of bare Green’s functions in order not to mix the expansion orders.

However, it turns out that the deviations from the (shifted) Hugenholtz–Pines theorem are minimal. This is shown in figure 10, where we plot the relative deviation from the Hugenholtz–Pines relation at a value of \( U/t = 10 \) across the SF-to-normal transition. One clearly sees that the deviation grows with inverse temperature when one goes deeper into the SF phase. When lowering \( U \) or the density \( n \) at low temperature, the deviations become smaller. In the Mott and normal phases, where \( \phi = 0 \), the Hugenholtz–Pines relation is not valid.

As already mentioned in the introduction, it was shown in \cite{45, 46} that gapless field theories have self-energies that should be momentum dependent and, in particular, that the anomalous self-energy has to go to zero for small momenta at zero frequency. In Beliaev’s diagrammatic approach of the WIBG, the first-order self-energies are momentum and frequency independent, and this condition is not satisfied, questioning Beliaev’s approach. Similarly, in the B-DMFT scheme, the self-energies are momentum independent. In figure 11, one sees that the anomalous self-energy is nonzero for zero frequency, as could be expected from the explicit symmetry-breaking terms in the B-DMFT action. On the other hand, the arguments of \cite{44}
Figure 11. Self-energy of the Bose–Hubbard model on the 3D cubic lattice as a function of Matsubara frequencies in the SF phase, $\beta t = 1$, $\mu / t = 8$ and $U / t = 20$ ($\langle n \rangle \approx 1$). The curve with blue circles (diamonds) shows the real (imaginary) part of the self-energy $\Sigma (i\omega_n)$ and the curve with red triangles shows the off-diagonal self-energy $\Sigma_{off}(i\omega_n)$. The dashed lines show the analytically known high-frequency tail where $\Sigma (i\omega_n) = \Sigma_0 + \frac{\Sigma_1}{i\omega_n} + O(1/(i\omega_n)^2)$ and $\Sigma_{off}(i\omega_n) = \tilde{\Sigma}_0 + O(1/(i\omega_n)^2)$ with $\Sigma_0 = 2U\langle n \rangle$, $\Sigma_1 = U^2(3\langle n^2 \rangle - \langle n \rangle - 4\langle n \rangle^2 + \langle bb \rangle)$ and $\tilde{\Sigma}_0 = U\langle bb \rangle$.

for the WIBG also hold for B-DMFT. In particular, the authors of [44] argued that the system reaches its thermodynamic limit for properties such as the energy and the entropy for small system sizes. In figures 6 and 7, we have already seen that the (kinetic) energy is reproduced remarkably well over the entire temperature range in 3D, except in the fluctuation region near the normal–superfluid phase transition point.

From the viewpoint that DMFT and B-DMFT sum up all skeleton diagrams built with local propagators only (which is an (asymptotic) expansion in $U$), we expect that our B-DMFT theory should recover the physics of the WIBG (Bogoliubov Hamiltonian), which is known to be an excellent approximation at low values of $nU$. It is the only limit for which it is not obvious that the B-DMFT formalism will be successful, while the other regimes of strong $U$ or high temperature are well captured by a single-site action. In the skeleton approach to the WIBG theory [44], the self-energies are to leading and subleading order given by $\Sigma = 2\langle n \rangle U$ and $\tilde{\Sigma} = \langle bb \rangle U$ (see figure 15). To this order of accuracy, the chemical potential is given by $\mu^{(1)} = 2\langle n \rangle U - \langle bb \rangle U \approx \langle n_0 \rangle U$. The latter approximation is made to keep the equations simple (it is not fundamental) since we do not want to go into the technical details of the WIBG theory here [44], but it allows us to simply relate the condensate $\langle n_0 \rangle$ to the chemical potential $\mu^{(1)} \approx \mu$ in this limit, after also taking the shift $-6t$ from the band edge into account. Because the chemical potential in B-DMFT is an input parameter and fully renormalized from the start, this is another way of understanding the deviations from the Hugenholtz–Pines relation.
Figure 12. Self-energy of the Bose–Hubbard model on the 3D cubic lattice as a function of Matsubara frequencies in the SF phase, $\beta t = 4$, $\mu/t = -5.75$ and $U/t = 0.5$ ($\langle n \rangle \approx 0.5$). The parameters are in the regime where the WIBG theory applies, which predicts $\Sigma^{(1)} = 2\langle n \rangle U$ and $\tilde{\Sigma}^{(1)} = \langle bb \rangle U$. The self-energies are almost frequency independent and are in very good agreement with the WIBG predictions.

We now discuss the numerical results for the WIBG limit. In order to see some depletion effects, we choose parameters such that $\langle n \rangle = 0.5$ and $\beta t = 4$. The main result is shown in figure 12, where one sees that the self-energy and the anomalous self-energy become frequency independent and approach their WIBG values, which are precisely the leading terms in the high-frequency expansions used in B-DMFT.

For the normal self-energy it is $\Sigma = 2\langle n \rangle U$, while for the anomalous self-energy it is $U \langle bb \rangle$.

In figure 13, the chemical potential is calculated such that the density is $\langle n \rangle = 0.5$. The chemical potentials found by B-DMFT are in excellent agreement with those found by QMC worm-type simulations. This shows again that the deviation from the Hugenholtz–Pines relation in B-DMFT is minimal, and goes to zero as $U/t \to 0$. We also compare the condensate densities for these theories in figure 14, a more challenging quantity than the total density. The agreement with QMC simulations and with the WIBG theory for $U/t < 0.5$ is remarkable, and the difference from static mean-field theory is significant. Technically, calculations in this limit are hampered by the low values of the self-energies and the proximity of the band edge because of which very precise calculations are needed. For the density $\langle n \rangle = 0.5$, the sign problem is not the limiting factor (the average sign is approximately $\langle s \rangle = 0.7$), but the situation deteriorates quickly for higher densities at these temperatures.

To conclude this section, we briefly comment on the difference between the anomalous self-energy found here ($\tilde{\Sigma}^{(1)} = \langle bb \rangle U$) and that found in [44] ($\tilde{\Sigma}^{(1)} = \langle n_0 \rangle U_{ps}$, with $U_{ps}$ being the pseudo-potential). The difference between the two comes exclusively from the use of the bare potential here and the pseudo-potential in [44], justified by equation (3.44) in [44], but which cannot be applied for B-DMFT. The diagram given by the convolution of the anomalous
Figure 13. The chemical potential as a function of $U/t$ such that the density is approximately $\langle n \rangle = 0.5$ for the cases of the WIBG (WIBG), B-DMFT, QMC worm-type simulations on a lattice of size $L = 10^3$ and static mean-field theory. The temperature is $T/t = 0.25$. For low $U$, both static mean-field theory and B-DMFT approach the WIBG theory well, while in the intermediate regime, B-DMFT is doing a superior job for the chemical potential despite the local approximation for the self-energy.

Green's function with the interaction line, at finite momenta (that is the second diagram for $\tilde{\Sigma}^{(1)}$ in figure 15), appears in B-DMFT in first order, while in [44] this diagram was not present in first order for the anomalous self-energy for the following reason: the leading piece of the second diagram is absorbed into the first one when the pseudo-potential is used, after which the second diagram can be neglected to leading order. In subleading order, the corrections (expressed in terms of bare potentials to avoid double counting) can then be read from equation (4.9) and figures 9 and 10 in [44], and these are precisely the missing terms compared with the B-DMFT first-order diagrams.

7.2. 2D square lattice

In this section, we present the results for the 2D square lattice. As in the previous section, data from B-DMFT are compared with those from lattice QMC [54], static mean-field theory and an exact solution of this model on a Bethe lattice with connectivity $z = 4$ [49]. In figure 16, we show the finite-temperature phase diagram (top panel) and the ground-state phase diagram (bottom panel) for the first and second lobes on the 2D square lattice. The ground-state phase diagram was calculated at $\beta t = 8$, which is sufficiently low, as can be seen from the top panel of figure 16. As one might expect, the agreement of B-DMFT with exact Monte Carlo lattice simulations is not as good in 2D as in 3D. We note here that figure 16 compares the condensate transition obtained by B-DMFT to the SF transition obtained by Monte Carlo lattice simulations. Since B-DMFT is just a dynamical extension to static mean-field theory, we obtain (as in the
Figure 14. The condensate fraction as a function of $U/t$ such that the density is approximately $\langle n \rangle = 0.5$ for the case of the WIBG, B-DMFT and static mean-field theory. The temperature is $T/t = 0.25$. For low and intermediate $U$, B-DMFT is in better agreement with the WIBG than with static mean-field theory.

Figure 15. First-order skeleton diagrams of the self-energy valid in the WIBG regime, with the results $\Sigma^{(1)} = 2\langle n_0 \rangle U + 2G_c(\tau = 0^-)U = 2\langle n \rangle U$ and $\tilde{\Sigma}^{(1)} = \langle n_0 \rangle U + \tilde{G}_c(\tau = 0^-)U = \langle bb \rangle U$. Note that in single-site B-DMFT all momenta are equal, and our interactions are instantaneous.
and low temperatures the agreement with QMC worm-type simulations is excellent, in contrast with static mean-field theory. Only in the vicinity of the transition point relatively are small deviations found. As in 3D, B-DMFT predicts a kink in the kinetic energy curve at the transition point and is hence not well equipped to describe Kosterlitz–Thouless phase transitions. Still, it
Figure 17. Kinetic energy of the Bose–Hubbard model on the 2D square lattice as a function of temperature for $\mu/t = 3.52$ and $U/t = 10$ ($n \approx 1$). The results obtained from B-DMFT (black circles) are compared with lattice QMC (blue diamonds) and with static mean-field theory (black dashed line). Inset: energy difference from the QMC data for the same parameters. The QMC results are obtained on a lattice with $100^2$ sites. The error bars are smaller than the symbol size.

gives a substantially improved finite-temperature phase diagram compared with static mean-field theory (top panel of figure 16) and a ground-state phase diagram (bottom panel) in good agreement with the QMC result.

7.3. Bethe lattice

7.3.1. Finite connectivity. In this section, the solution of the B-DMFT equation on the Bethe lattice is compared with the exact solution of Semerjian et al [49]. Since both methods are formulated in the thermodynamic limit, this allows us to directly compare results and to check the accuracy of the B-DMFT formalism. For the Bethe lattice with connectivity $z$, the density of states is given by

$$D(\epsilon) = \frac{1}{V} \delta(\epsilon + zt) + D_c(\epsilon),$$

with $V$ being the volume of the system. The continuum part $D_c$ reads

$$D_c(\epsilon) = \frac{\sqrt{4(z-1)t^2 - \epsilon^2}}{2\pi(zt^2 - \epsilon^2/z)}, \quad |\epsilon| \leq 2t\sqrt{z-1},$$

where $t$ is the hopping between the sites. The isolated state at $\epsilon = -zt$ matters for condensation and prevents the existence of Goldstone modes in the symmetry-broken phase [55]. Figure 18 shows a comparison of the density $n$ and the condensate order parameter $\phi$ between B-DMFT and the exact solution for a Bethe lattice with connectivity $z = 4$. As one can see in figure 19, the agreement is excellent except for the condensate $\phi$ very close to the SF–Mott transition. This comes from the fact that B-DMFT does not reproduce the mean-field exponents like the
Figure 18. The density $n$ and the condensate order parameter $\phi = \langle b \rangle$ as a function of $\mu/U$ for $t/U = 0.02$ and $\beta t = 1$ on the Bethe lattice with connectivity $z = 4$. The open black circles are the result obtained with B-DMFT and the solid red line the numerically exact solution [49].

exact solution [49] but has a smaller exponent in this case, i.e. the transition is much sharper. This excellent agreement of the B-DMFT condensate $\phi$ with the exact solution also shows that the definition of the condensate used both in this work and in our previous paper [36] is correct, unlike the condensate defined in the comment [56] on our previous work [36], which corresponds to the blue diamonds in figure 19.

7.3.2. Limit of infinite connectivity. For systems without symmetry breaking, the isolated state in the non-interacting density of states, is negligible. It is customary in (fermionic) DMFT to rescale the hopping in the limit $z \to \infty$ as $t = \tilde{t}/\sqrt{z}$ for the density of states to remain finite. Equation (76) reduces then to the semi-circular density of states given by

$$D(\epsilon) = \frac{1}{2\pi \tilde{t}^2} \sqrt{4\tilde{t}^2 - \epsilon^2}, \quad |\epsilon| \leq 2\tilde{t}. \quad (77)$$

For this density of states, the self-consistency equations simplify since the Hilbert transformation can be performed analytically. This allows us to formulate the whole self-consistency loop in $\tau$-space, i.e. we do not have to go to Matsubara frequencies. We obtain a simple relationship between the hybridization and the Green’s function given by

$$\Delta(\tau) = -\tilde{t}^2 G_c(\tau). \quad (78)$$

For bosons, however, the isolated state in the non-interacting density of states is not negligible. As soon as $z > 2$, the condensation temperature is nonzero, and one has then to keep track of the uniform mode [55]. Integer scaling $t = \tilde{t}/z$ is then the only possibility, and the static mean-field theory [1] becomes exact for $z \to \infty$ (for all temperatures). This integer scaling is also compatible with equation (30) such that the hybridization terms become identically zero for $z \to \infty$, again in line with [1, 55] but in contrast with the different scalings postulated in [33].
Figure 19. Condensate order parameter $\phi = \langle b \rangle$ as a function of $\mu/U$ for $t/U = 0.02$ and $\beta t = 1$ on the Bethe lattice with connectivity $z = 4$ (blow-up of $\phi$ in figure 18 around $\mu/U = 2$). The open black circles are the result obtained by B-DMFT, the solid red line is the numerically exact solution [49] and the blue diamonds are the results for the condensate $\phi$ as defined in [56].

8. Conclusions

In summary, we have derived the B-DMFT formalism in three different ways: (i) by approximating the kinetic energy functional, (ii) by considering a cavity method or $1/z$ expansion and (iii) by using an effective medium approach. We highlighted similarities and differences with previous approaches [33–35], [37, 49]. The action we derived differs from the action in the original paper by Byczuk and Vollhardt [33] and subsequent work by Hu and Tong [34]. In [33], different scaling Ansätze for normal and condensed bosons were suggested, so that the hybridization term survives in the limit $z \to \infty$. This scaling behavior is unlike what one expects on the basis of [1, 55]. In our formulation, the local action is the same as that in theories with a broken continuous symmetry [32], where the hybridization terms express the two-point corrections to the condensate. In the case of a uniform and constant condensate, the differences between the approaches amount to a different equation for the parameter $\kappa$, which describes the coupling of the condensate with the bosonic fields. This modification (with respect to [33]) is crucial for obtaining a consistent theory and good agreement with numerically exact lattice simulations. In the work by Hubener et al [35], an approximate form of our self-consistency equation [36] was used, but the full derivation of the correct self-consistency condition was eventually presented in [37].

We discussed the Monte Carlo impurity solver in great detail, including detailed balance of the updates, technical difficulties one may encounter and the measurement procedure. We have shown results for the 3D Bose–Hubbard model, where the zero-temperature phase diagram and the finite-temperature phase diagram are in excellent agreement with QMC worm algorithm results. We compared the results with those of the WIBG theory in the regime of weak repulsion.
The kinetic energy is reproduced at the 1–2% level over the full range of temperatures, except in very close proximity to the superfluid-to-normal transition where deviations are larger. We studied the critical exponents of this transition on the superfluid side, and found non-universal values depending on the parameters of the Bose-Hubbard model that are different from the mean-field values and from the universal ones found in the 3D $XY$ universality class. The reason is that the contribution of the hybridization terms can be understood as a one-loop correction to the condensate. In 2D, the ground state phase diagram is still in good agreement with quantum Monte Carlo worm simulations, but at finite temperature the superfluid-to-normal transition is less accurately reproduced, because of the Kosterlitz-Thouless nature of the phase transition: in B-DMFT there is still a genuine condensate at finite temperature in 2D, and we miss the long-range fluctuations of the phase. However, quantities that are local, such as the energy, are still remarkably accurately reproduced over the entire parameter regime, just as in 3D. We also compared B-DMFT with the exact solution of [49] on the Bethe lattice, and found again good agreement except in very close proximity to the phase transition points. The agreement over the whole parameter regime (except in the vicinity of the phase transitions) was argued to be the result of fast diagrammatic convergence of thermodynamic quantities with system size, just as in the case of the WIBG system [44]. Our approach thus constitutes a natural extension of the Bogoliubov mean-field theory of the weakly interacting system (which is unable to find a Mott insulator) to a dynamical mean-field theory successful over the entire parameter regime of the Bose–Hubbard model. It shows that when technical difficulties such as the asymptotic behavior of the series are properly taken care of or sidestepped, elusive diagrammatic expansions for bosonic systems are in fact promising, in line with the spirit of (bold) diagrammatic Monte Carlo [57] studies, whether or not in combination with DMFT [27].

The virtue of developing a DMFT formalism for the Bose–Hubbard model lies in the possible extension of the formalism to models where known numerical methods fail. Prime examples are the Bose–Fermi mixtures in 2D or 3D [58–61], where previous calculations treated the spinless fermions within DMFT and the bosons at the mean-field level [62]. The formalism can also be generalized to mixtures with spinful fermions. Cluster expansions are possible along the lines of [43], but it remains to be seen whether the sign problem remains tolerable in the condensed phase. Developing the formalism for real-time applications can be considered along the same lines as for fermionic DMFT [63], but here too it remains to be seen how the sign (as well as a complex condensate) behaves.

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Appendix A. Quantum cavity method (1/z expansion)

In a recent paper [49], Semerjia et al derived an exact solution for the Bose–Hubbard model on the Bethe lattice (lattices with tree structure). Their final result is a self-consistency equation that can easily be solved numerically. The paper mentions that B-DMFT can be considered as the first-order approximation to this equation. This is indeed the case, and leads to an equivalent derivation of the B-DMFT equations. The expressions in [49] are, however, for the cavity condensate and Green’s function and not for the true (observable) condensate and Green’s function. In this appendix, we provide their equations for the observable quantities and compare them with our B-DMFT action.

Computations on a tree can benefit from the recursive structure of the tree. Following [49], the quantity \[ Z_{i\rightarrow j}(\{n\}) \] for the two adjacent sites \( i \) and \( j \) is defined as the partial partition function for the subtree rooted at \( i \) and excluding the branch to \( j \) for given quantum numbers \( \{n\} \).

We note that a Suzuki–Trotter decomposition for the quantum action preserves the structure of the lattice for every time slice. Normalized quantities that can be interpreted as probabilities can then be defined as \[ \eta_{i\rightarrow j}(\{n\}) = Z_{i\rightarrow j}(\{n\})/ \sum_{\{n'\}} Z_{i\rightarrow j}(\{n'\}) \]. See [49] for more details.

When taking an infinite number of Suzuki–Trotter slices, the cavity field on a Bethe lattice of connectivity \( z \) can self-consistently be expressed as [49]

\[
\eta_{\text{cav}}(b^*, b) = \frac{1}{Z_{\text{cav}}} w(b^*, b) \int \prod_{i=1}^{z-1} D[b_i, b_i] \eta_{\text{cav}}(b_i^*, b_i) \times \exp \left[ t \int_0^\beta d\tau \left( b^*(\tau) \sum_{i=1}^{z-1} b_i(\tau) + b(\tau) \sum_{i=1}^{z-1} b_i^*(\tau) \right) \right], \tag{A.1}
\]

with the on-site weight of the path given by

\[
w(b^*, b) = \exp \left[ - \int_0^\beta d\tau \left( b^*(\tau)(\partial_\tau - \mu) b(\tau) + \frac{U}{2} n(\tau)(n(\tau) - 1) \right) \right]. \tag{A.2}
\]

In the Nambu notation, this reads

\[
\eta_{\text{cav}}(b) = \frac{1}{Z_{\text{cav}}} w(b) e^{(z-1)\Gamma_0 b}, \tag{A.3}
\]

\[
\Gamma(\Phi) = \ln \left[ \int D b \eta_{\text{cav}}(b) \exp \int_0^\beta d\tau b^\dagger(\tau) \Phi(\tau) \right].
\]

This self-consistency equation can only be solved exactly for \( U = 0 \). For the interacting case, \( U > 0 \), a solution can be sought in the large connectivity limit, where in the leading order 1/z B-DMFT is recovered. This follows from an expansion of the generating functional of connected correlation functions \( \Gamma \),

\[
\Gamma(\Phi) = \int_0^\beta d\tau \langle b^\dagger(\tau) \rangle_{\text{cav}} \Phi(\tau) + \frac{1}{2} \int_0^\beta d\tau d\tau' \Phi^\dagger(\tau) G_{\text{cav}}(\tau - \tau') \Phi(\tau') + \cdots. \tag{A.4}
\]

4 The presentation in this section is based on private discussions with the authors of [49], as well as on private notes of F Zamponi, which they allowed us to use in order to clarify this minor issue.
The connected part of the two-point correlator satisfies
\[ G_{\text{cav}}^c(\tau - \tau') = \langle b^\dagger(\tau)b(\tau') \rangle_{\text{cav}} - \langle b^\dagger(\tau) \rangle_{\text{cav}} \langle b(\tau') \rangle_{\text{cav}}. \] (A.5)

We now plug equation (A.4) into (A.3) and obtain
\[
\eta_{\text{cav}}(b) = \frac{1}{Z_{\text{cav}}} \exp[-S_{\text{cav}}],
\]
\[ S_{\text{cav}} = \frac{1}{2} \int_0^\beta d\tau d\tau' b^\dagger(\tau) G_{-1,\text{cav}}(\tau - \tau') b(\tau') + \int_0^\beta d\tau \left[ \frac{U}{2} n(\tau)(n(\tau) - 1) - t(z - 1) \Phi_{\text{cav}}^\dagger b(\tau) \right],
\]
\[ G_{-1,\text{cav}}(\tau - \tau') = (\partial_\tau \sigma_3 - \mu I) \delta(\tau - \tau') - t^2(z - 1) G_{\text{cav}}^c(\tau - \tau'). \] (A.6)

In the limit of large connectivity, one has to scale the hopping as \( t \sim 1/z \); hence \( z t \sim 1 \) and \( t^2 z \sim 1/z \).

We now proceed to the equations for the true fields, which cannot be found in [49] (see footnote 4). To this end, the true marginal \( \eta(b) = \frac{1}{2} \ln \langle \exp[G(b)] \rangle \) is needed. It is still expressed in terms of the cavity field (and not the true field) and is obtained by replacing \( z - 1 \) by \( z \) in equation (A.6). We try to find now suitable expressions for the true connected Green’s function and condensate, valid for the impurity problem ‘imp’ instead of for the cavity problem ‘cav’.

The action for the impurity problem is valid up to order \( 1/z \). Since the prefactor of the cavity Green’s function is already of \( O(1/z) \), we can identify the impurity Green’s function with the cavity Green’s function without loss of accuracy,
\[ G_{\text{imp}}^c(\tau - \tau') = G_{\text{cav}}^c(\tau - \tau') = \langle b^\dagger(\tau)b(\tau') \rangle_{\text{imp}} - \langle b^\dagger(\tau) \rangle_{\text{imp}} \langle b(\tau') \rangle_{\text{imp}}, \] (A.7)
where the average can now be taken with respect to the impurity action.

The prefactor of the condensate in equation (A.6) is of the order of unity; hence we need the impurity condensate to \( O(1/z) \). We have
\[ S_{\text{imp}} = S_{\text{cav}} - t \int_0^\beta d\tau \Phi_{\text{imp}}^\dagger b(\tau). \] (A.8)

The condensate is now found for the total impurity action \( S_{\text{imp}} \),
\[ \Phi_{\text{imp}} = \langle b \rangle_{\text{imp}} \sim \Phi_{\text{cav}} + t \int_0^\beta d\tau G_{\text{imp}}^c(\tau) \Phi_{\text{cav}}, \] (A.9)
which can be inverted (accurate up to this order),
\[ \Phi_{\text{cav}} \sim (I - t G_{\text{imp}}^c(\omega_n = 0)) \Phi_{\text{imp}}. \] (A.10)

By plugging this equation into equation (A.8), a closed set of equations for the true condensate is found, which is tantamount to B-DMFT. The iteration scheme proceeds in the usual way. Note that the last step does not rely on the scaling in equations (78) and (77), but does use the recurrence relation of a tree. We note that the derivation presented in [37] is conceptually equivalent to that presented in [49], on which this appendix is based.
Appendix B. Effective medium approach

In this section, we will expand the full Bose–Hubbard action around a single site, identify the low-energy modes and re-exponentiate them. The derivation in this section is similar to the derivation found in [33], but differs in the treatment of the condensate. We provide a microscopic RG-like picture for the condensate field and hybridization fields in the effective action. The total action of the full Bose–Hubbard model is split into three parts, with the first one being the local part defined in equation (2),

\[ S_{\text{int}} = \int_0^\beta d\tau b_{\text{int}}^*(\tau)(\partial_\tau - \mu)b_{\text{int}}(\tau) + \frac{U}{2}n_{\text{int}}(n_{\text{int}} - 1). \] (B.1)

The second part \( \Delta S \) describes the coupling with the rest of the lattice,

\[ \Delta S = \int_0^\beta \Delta S(\tau) = \int_0^\beta \sum_{\text{(int, ext)}} -t(b_{\text{int}}^\dagger b_{\text{ext}} + b_{\text{ext}}^\dagger b_{\text{int}}), \] (B.2)

and the third part is the remaining, external part ‘ext’ with the action

\[ S_{\text{ext}} = \int_0^\beta d\tau b_{\text{ext}}^*(\tau)(\partial_\tau - \mu)b_{\text{ext}} + \frac{U}{2}n_{\text{ext}}(n_{\text{ext}} - 1). \] (B.3)

We had that \( S = S_{\text{int}} + S_{\text{ext}} + \Delta S \), but would like to derive an action \( S \approx S_{\text{imp}} + S_{\text{ext}} \) by expanding the exponential function with respect to the action \( \Delta S \), and perform the functional integral over the external degrees of freedom, and incorporate this into a new effective internal action \( S_{\text{imp}} \) and a decoupled, external action \( S_{\text{ext}} \).

We assume that ‘ext’ is a thermodynamic system that can spontaneously break the symmetry, if needed, and develop a condensate. If so, we decompose

\[ b_{\text{ext}} = \phi_{\text{ext}} + \delta b_{\text{ext}}, \] (B.4)

where \( \langle b_{\text{ext}} \rangle = \phi_{\text{ext}} \) represents the condensate wave function. It is a classical field (c-number, taken to be real) that breaks the symmetry, and its presence forces us to consider anomalous averages, such as \( \langle b_{\text{ext}}b_{\text{ext}} \rangle \), which are nonzero. The commutation relations are now \([\delta b_{\text{ext}}^j, \delta b_{\text{ext}}^k] = \delta_{j,k}\) and zero otherwise. The impurity part ‘int’ is by itself small and cannot spontaneously break the symmetry and develop a nonzero expectation value for its local operators.

In our perturbative expansion in \( \Delta S \), an atom from the ‘int’ part will hop to the ‘ext’ part and acquire an expectation value through the full correlators in ‘ext’. A nonzero expectation value corresponds to the condensate mode and is not possible for the bosons outside the condensate. We do not attempt here to build in all low-energy modes via ‘ext’; only the classical field contributions from the condensate will suffice. Let us anticipate such a possibility and allow

\[ b_{\text{int}} = \phi_{\text{int}} + \delta b_{\text{int}}, \quad \langle b_{\text{int}} \rangle = \phi_{\text{int}}. \] (B.5)

We also have the commutation relations \([\delta b_{\text{int}}^j, \delta b_{\text{int}}^k] = \delta_{j,k}\) and \([\delta b_{\text{int}}^j, \delta b_{\text{ext}}^k] = 0\). In second order, we then also have to allow for \( \langle b_{\text{int}}^j b_{\text{int}}^k \rangle \) to become large. The validity of equation (B.5) can then be checked \textit{a posteriori}. 

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The coupling between the internal and external degrees of freedom, expressed in equation (B.2), can then be written as

\[ \Delta S = \int_0^\beta \sum_{\text{int,ext}} -t \left( b_{\text{int}}^\dagger b_{\text{ext}} + b_{\text{ext}}^\dagger b_{\text{int}} \right) \]

\[ = -t \int_0^\beta d\tau z \phi_{\text{int}} (\delta b_{\text{ext}} + \delta b_{\text{ext}}^\dagger) + z \phi_{\text{ext}} (\delta b_{\text{int}} + \delta b_{\text{int}}^\dagger) + \sum_{\text{int,ext}} \delta b_{\text{int}}^\dagger \delta b_{\text{ext}} + \delta b_{\text{ext}}^\dagger \delta b_{\text{int}}, \]  

(B.6)

where we have omitted terms in \( \phi_{\text{int}} \phi_{\text{ext}} \) since the condensate is treated as a \( c \)-number and such terms involve an arbitrary shift in the condensate energy. There are four terms in \( \Delta S \), of which two have the condensate directly in them and two do not. Since we are interested in adding the physics of the WIBG to the action, we have to treat the condensate as a large contribution compared with the small contributions coming from the depleted atoms, while the third term will be contributing to one- (and higher-) loop corrections. We can now immediately write down the contribution of the parts with the condensate lines to the action,

\[ S_1 = z t \phi_{\text{ext}} \int \delta b(\tau) + \delta b^\dagger(\tau) = z t \phi_{\text{ext}} \int b(\tau) + b^\dagger(\tau), \]  

(B.7)

and we keep only the following terms in \( \Delta S \) (the other one factorizes), which we treat as a small term,

\[ \Delta S = -t \int_0^\beta \sum_{\text{int,ext}} \delta b_{\text{int}}^\dagger \delta b_{\text{ext}} + \delta b_{\text{ext}}^\dagger \delta b_{\text{int}}. \]  

(B.8)

The advantage of our approach is that we have first added the condensate to the impurity action, before looking at depletion (fluctuation) terms. In this picture, the stationarity and time independence of the condensate are immediately built in. We are now in a position to expand in \( \Delta S \). This results in an infinite series,

\[ Z \sim Z^{\text{ext}} \int D[b_{\text{int}}^\ast, b_{\text{int}}] e^{-S_{\text{int}}(b_{\text{int}}^*, b_{\text{int}}) - S_{\text{ext}}(b_{\text{int}}^*, b_{\text{int}})} \xi, \]

\[ \xi = 1 - \int_0^\beta d\tau \langle \Delta S(\tau) \rangle_{\text{ext}} + \frac{1}{2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle \Delta S(\tau_1) \Delta S(\tau_2) \rangle_{\text{ext}} + \cdots. \]  

(B.9)

We start with the evaluation of the first-order term,

\[ \int_0^\beta \langle \Delta S \rangle_{\text{ext}} = -t \int_0^\beta d\tau \sum_{\text{int,ext}} \langle \delta b_{\text{int}}^\dagger \delta b_{\text{ext}} \rangle_{\text{ext}} + \text{h.c.}, \]  

(B.10)

which is zero, as could have been expected from symmetry.

The second-order term is the lowest order term that survives,

\[ \frac{1}{2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle \Delta S(\tau_1) \Delta S(\tau_2) \rangle_{\text{ext}} = t^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{j, k \in \text{ext}} \left[ S^j + S^2 + S^3 + S^4 \right], \]  

(B.11)
with \( S^j, j = 1, \ldots, 4, \)
\[
S^1 = \langle \delta b_{\text{int}}(\tau_1) \delta b_{\text{int}}(\tau_2) \delta \phi^{*}_\text{ext}(\tau_1) \delta \phi_{\text{ext}}(\tau_2) \rangle_{\text{ext}}, \\
S^2 = \langle \delta b_{\text{int}}(\tau_1) \delta \phi^{*}_\text{int}(\tau_2) \delta \phi^{*}_\text{ext}(\tau_1) \delta \phi_{\text{ext}}(\tau_2) \rangle_{\text{ext}}, \\
S^3 = \langle \delta \phi^{*}_\text{int}(\tau_1) \delta b_{\text{int}}(\tau_2) \delta \phi^{*}_\text{ext}(\tau_1) \delta \phi_{\text{ext}}(\tau_2) \rangle_{\text{ext}}, \\
S^4 = \langle \delta \phi_{\text{int}}(\tau_1) \delta b_{\text{int}}(\tau_2) \delta \phi^{*}_\text{ext}(\tau_1) \delta \phi_{\text{ext}}(\tau_2) \rangle_{\text{ext}}.
\]

(B.12)

The notation \((j)\) and \((k)\) denotes different sites that are coupled to the impurity through the hopping term in the Bose–Hubbard Hamiltonian. The anomalous terms survive in the presence of a condensate, which tells us that there are four terms in second order. Let us analyze \( S^1 \) in more detail,
\[
S^1 = \langle \delta b_{\text{int}}(\tau_1) \delta b_{\text{int}}(\tau_2) \delta \phi^{*}_\text{ext}(\tau_1) \delta \phi_{\text{ext}}(\tau_2) \rangle_{\text{ext}}.
\]

(B.13)

This describes the anomalous process of a depleted boson hopping from the impurity site to the environment, propagating there according to the full (but unknown to us) anomalous two-particle Green’s function, and finally being annihilated on the impurity site. We will now perform a cumulant re-exponentiation of this term in the presence of a condensate, for which only the connected diagrams can be kept,
\[
e^{-S^1} = e^{-\int_0^\beta d\tau \int_0^\beta d\tau' \delta b_{\text{int}}(\tau) K_{\text{ext}}(\tau - \tau') \delta b_{\text{int}}(\tau')},
\]

(B.14)

where \( K \) will be a function that we treat as unknown and that originates from the connected diagrams only. The DMFT self-consistency iteration scheme will determine \( K \) self-consistently.

In a numerical algorithm, it is practical to work with full operators \( b \) instead of \( \delta b \), so we will write \( b_{\text{int}}(\tau) - \phi_{\text{int}} \) instead of \( \delta b_{\text{int}} \). The other terms \( S^j, j = 2, 3, 4, \) are treated in the same way as \( S^1 \), but we will not write this out explicitly.

After convergence, we wish that our site is in equilibrium with the surroundings. We thus impose a first self-consistency relation,
\[
\phi = \phi_{\text{ext}} = \phi_{\text{int}} = \langle b \rangle_{\text{int}}.
\]

(B.15)

The meaning of this relation is that in every iteration we have to compute \( \langle b \rangle \) and equate the condensate with this value. It can always be taken as real and time independent. We collect now all terms needed for our effective impurity action,
\[
S_{\text{imp}} = \int_0^\beta d\tau b_{\text{int}}^\dagger(\tau) (\partial_\tau - \mu) b_{\text{int}}(\tau) + \frac{U}{2} n_{\text{int}}(n_{\text{int}} - 1) - z f_{\text{ext}} \int_0^\beta d\tau b_{\text{int}}(\tau) \\
+ \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' (b_{\text{int}}^\dagger(\tau) - \Phi_{\text{int}}(\tau)) (\Phi_{\text{int}}(\tau') - \Phi_{\text{int}}(\tau'))
\]

(B.16)

where the elements of the hybridization matrix are (dropping the subscript ‘c’ for connected).

The remaining hybridization term can now be treated similarly to the hybridization term in fermionic DMFT and hence has a similar self-consistency relation [13] (see section 4).

**Appendix C. High-frequency expansions**

Within our self-consistency loop, we need to perform Fourier transforms between the imaginary time \( \tau \) domain and Matsubara frequencies \( \omega_n \). Even though we use a continuous time method,
we measure the Green’s function $G(\tau)$ on a grid with a fixed number of time slices. We can therefore only obtain accurate data for a finite number of Matsubara frequencies. In order to perform accurate Fourier transforms, we supplement the Green’s function with the analytically known high-frequency behavior, given by

$$G(i\omega_n) = \frac{g_1}{i\omega_n} - \frac{g_2}{(i\omega_n)^2} + \frac{g_3}{(i\omega_n)^3} + \Delta G(i\omega_n), \quad (C.1)$$

where $\Delta G(i\omega_n)$ goes to zero as $1/(i\omega_n)^4$ for $i\omega_n \to \infty$. For the static component ($n = 0$), we let $\Delta G(i\omega_n) = G(i\omega_n)$. Computing these coefficients analytically improves the accuracy of our Fourier transformation significantly [65]. By using

$$\frac{1}{\beta} \sum_{n \neq 0} e^{-i\omega_n \tau} \frac{1}{i\omega_n} = \frac{1}{2\beta} (2\tau - \beta),$$

$$\frac{1}{\beta} \sum_{n \neq 0} e^{-i\omega_n \tau} \frac{1}{(i\omega_n)^2} = \frac{1}{12\beta} (-6\tau^2 + 6\tau\beta - \beta^2), \quad (C.2)$$

$$\frac{1}{\beta} \sum_{n \neq 0} e^{-i\omega_n \tau} \frac{1}{(i\omega_n)^3} = \frac{1}{12\beta} (2\tau^3 - 3\beta\tau^2 + \beta^2 \tau),$$

we can write the inverse Fourier transformation as

$$G(\tau) = \frac{1}{\beta} \sum_n G(i\omega_n) e^{-i\omega_n \tau}$$

$$= g(\tau) + \frac{1}{\beta} \sum_n \Delta G(i\omega_n) e^{-i\omega_n \tau}, \quad (C.3)$$

where

$$g(\tau) = \frac{g_1}{2\beta} (2\tau - \beta) - \frac{g_2}{12\beta} (-6\tau^2 + 6\tau\beta - \beta^2) + \frac{g_3}{12\beta} (2\tau^3 - 3\beta\tau^2 + \beta^2 \tau), \quad (C.4)$$

and the Fourier transformation as

$$G(i\omega_n) = \frac{g_1}{i\omega_n} - \frac{g_2}{(i\omega_n)^2} + \frac{g_3}{(i\omega_n)^3} + \int_0^\beta \Delta G(\tau) e^{i\omega_n \tau}, \quad (C.5)$$

with $\Delta G(\tau) = G(\tau) - g(\tau)$.

The coefficients for the Green’s function are obtained by evaluating commutators,

$$g_1 = \langle [b, b^\dagger]\rangle = 1,$$

$$g_2 = \langle [[[H, b], b^\dagger]\rangle = \mu - 2U \langle n \rangle,$$

$$g_3 = \langle [[[H, [H, b]], b^\dagger]\rangle = \langle \epsilon^2 \rangle + \mu^2 + 3U^2 \langle n^2 \rangle - \langle n \rangle (4\mu U + U^2),$$

$$\tilde{g}_1 = \langle [b, b] \rangle = 0,$$

$$\tilde{g}_2 = \langle [[[H, b], b]\rangle = U \langle bb \rangle,$$

$$\tilde{g}_3 = \langle [[[H, [H, b]], b]\rangle = 0.$$
where \( g_i \) are the coefficients for the diagonal and \( \tilde{g}_i \) for the off-diagonal Green’s function. All odd coefficients of the anomalous functions are zero, as these functions are purely real since all anomalous functions are symmetric in imaginary time.

Similar coefficients can be obtained for the hybridization function \( \Delta(i\omega_n) \). Here we find

\[
\begin{align*}
  f_1 &= \langle \epsilon^2 \rangle, \\
  f_2 &= -\langle \epsilon^2 \rangle g_2, \\
  f_3 &= \langle \epsilon^4 \rangle + \langle \epsilon^2 \rangle (g_3 - 2\langle \epsilon^2 \rangle)
\end{align*}
\] (C.7)

for the diagonal component \( F(i\omega_n) \) and

\[
\begin{align*}
  k_1 &= 0, \\
  k_2 &= -0.5\langle \epsilon^2 \rangle \tilde{g}_2, \\
  k_3 &= 0
\end{align*}
\] (C.8)

for the off-diagonal component \( K(i\omega_n) \).

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