PAPER

Self-energy functional theory with symmetry breaking for disordered lattice bosons

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Abstract

We extend the self-energy functional theory to the case of interacting lattice bosons in the presence of symmetry breaking and quenched disorder. The self-energy functional we derive depends only on the self-energies of the disorder-averaged propagators, allowing for the construction of general non-perturbative approximations. Using a simple single-site reference system with only three variational parameters, we are able to reproduce numerically exact quantum Monte Carlo (QMC) results on local observables of the Bose–Hubbard model with box disorder with high accuracy. At strong interactions, the phase boundaries are reproduced qualitatively but shifted with respect to the ones observed with QMC due to the extremely low condensate fraction in the superfluid phase. Deep in the strongly-disordered weakly-interacting regime, the simple reference system employed is insufficient and no stationary solutions can be found within its restricted variational subspace. By systematically analyzing thermodynamical observables and the spectral function, we find that the strongly interacting Bose glass is characterized by different regimes, depending on which local occupations are activated as a function of the disorder strength. We find that the particles delocalize into isolated superfluid lakes over a strongly localized background around maximally-occupied sites whenever these sites are particularly rare. Our results indicate that the transition from the Bose glass to the superfluid phase around unit filling at strong interactions is driven by the percolation of superfluid lakes which form around doubly occupied sites.

1. Introduction

Ever since the seminal work by Giamarchi and Schulz [1, 2] in one dimension and the extension to any dimension by Fisher et al [3], the intricate interplay of disorder and interactions in bosonic lattice systems has been an active field of research. The advent of cold atom experiments in optical lattices [4, 5], where disorder can be realized e.g. through the overlap of optical potentials with incommensurate wavelengths [6, 7] or speckle-laser patterns [8–10], has further invigorated the interest in this class of systems. More recently, the field has moved to research frontiers such as many-body-localization [11] thanks to advances in monitoring real-time dynamics and state preparation.

The theoretical understanding of disordered and interacting lattice bosons has been primarily driven by numerical simulations. Exact diagonalization [12] can only be applied to relatively small finite system sizes, while the extension of the density matrix renormalization group [13–16] to disorder [17] is restricted to low-dimensional systems. In higher dimensions the state of the art method is path integral quantum Monte Carlo (QMC) with worm updates [18–21]. This algorithm provides numerically exact results for large but finite-sized bosonic lattice systems, while the disorder can be accounted for by averaging over many disorder realizations [21]. However, dynamical quantities such as the single-particle spectral function can only be determined by
performing analytic continuation of imaginary-time propagators with stochastic noise \[22, 23\]. The continuation is an inherently ill-posed problem, and cannot resolve sharp resonances. While the methods mentioned above excel with a high numerical accuracy, they rely on finite system sizes, which can represent a problem when rare disorder-driven fluctuations play an important role, which can only be captured once one approaches the thermodynamical limit. The available methods in the thermodynamical limit rely on approximations. The mean-field decoupling approximation \[3\] can be applied to disordered systems using an arithmetically averaged condensate. However, this overestimates the phase coherence and the extent of the superfluid phases, as locally condensed bosons are mistaken for a global condensate \[24\]. In fact, in mean-field methods with position-space resolution the geometric percolation of condensed regions appears to be a more accurate quantity to evaluate the global superfluid response \[25\]. A more accurate mean-field approach is the stochastic mean-field theory \[26, 27\], where the condensate order parameter is treated as a disorder-dependent quantity. However, mean-field methods are self-consistent only in terms of the condensate (i.e. the one-point propagator). This severely hampers the ability to describe uncondensed phases, which are simply approximated by the zero hopping limit (i.e. the atomic limit).

A non-perturbative method which includes also a self-consistency in terms of the two-point propagator is the dynamical mean-field theory (DMFT), originally formulated for fermions \[28, 29\] and later generalized to bosons \[30–35\]. For fermions the formalism has been extended to disordered systems \[36–39\] by averaging the systems propagators over all disorder configurations. While an arithmetic averaging in this framework works well for weak disorder, it misses the essential physics in non-self-averaging phases. In such phases, like the Anderson-localized regime \[37, 40\], observables show broad tails in their disorder distribution. An interesting idea for incorporating non-self-averaging effects is the typical medium theory \[36–39\], where the arithmetic average is replaced by a geometrical mean. However, it is not clear what the range of validity is for this approach. We would like to point out that the works above employing disorder and DMFT all study fermionic systems. As of today we are not aware of any works applying DMFT to disordered bosonic systems.

A more general theoretical framework for constructing non-perturbative approximations for interacting many-body systems is the self-energy functional theory (SFT) \[41–48\], from which DMFT can be derived as a certain restriction of the variational space. The formalism was first developed for fermions \[41–44\] and later extended to bosonic systems \[45–48\]. Our recent derivation \[48\] based on the bosonic Baym–Kadanoff functional \[49, 50\] correctly includes $U(1)$-symmetry breaking, and simplifies to bosonic DMFT \[30–35\] in a particular limit. Within SFT, non-perturbative approximations are readily constructed by restricting the self-energy domain of the original lattice system to the self-energies of a simpler exactly solvable reference system. This reduces the full complexity of the original problem to a search for stationary solutions in terms of the variational free propagators of the reference system. The generalization of SFT to systems with disorder has been developed for fermions in \[51\] and applied in a variational cluster approximation (VCA) to bosons in the absence of $U(1)$-symmetry breaking in \[52\].

The aim of this paper is to extend the bosonic SFT formalism of \[48\] to disordered lattice bosons including the possibility of $U(1)$-symmetry breaking. As argued for fermions in \[51\], the geometrical mean used in the context of DMFT \[36–39\] is hard to reconcile with the variational SFT framework. We therefore derive an arithmetically averaged formalism, where, through the introduction of an appropriate $\hat{T}_{PV}$ functional, the functional depends only on the self-energies of the arithmetically averaged propagators. Just as the version for clean systems \[48\], we find that SFT incorporates a disorder-averaged generalization of bosonic DMFT \[30–35\] in a certain limit. The resulting functional is, however, more general than DMFT by being amenable to a more general variational space.

The prototypical model for interacting disordered bosonic lattice systems is the Bose–Hubbard model (BHm) in the presence of local disorder (for a review, see \[53\]). In addition to the Mott insulating and superfluid phases of the clean system, the groundstate phase diagram exhibits a new phase: the Bose glass \[1–3\]. This is an insulating but gapless and compressible phase, which always intervenes between the Mott insulator and the superfluid phase at finite disorder \[21, 54, 55\]. While certain single-particle states can show a high (but not macroscopic) occupation, the disorder does not allow for global phase coherence as observed in the superfluid. The statistical fluctuations of the local potential, on the other hand, locally exceed the gaps of adding/removing a particle \[21\], creating gapless regions which induce a non-vanishing density of states at zero energy \[3\]. In the groundstate phase diagram of the disordered BHm on a cubic lattice the superfluid phase extends to surprisingly large values of the interaction $U$ and the disorder strength $D$. For low/intermediate interactions and high disorder it can be argued that this is related to the percolation between localized states \[21\]. At stronger interaction and lower disorder, the phase diagram is characterized by the so-called ‘superfluid finger’ which extends to much larger interactions than the critical value of the clean system and is characterized by an extremely low condensate fraction. The critical temperature at which the condensate vanishes is thus extremely low, making it very hard to access this regime in experiments \[21\].
We apply SFT to the BHm with local box disorder on the cubic lattice using the simplest imaginable reference system, comprising a single bosonic mode. This restriction to the minimal reference system produces a self-energy approximation with three variational degrees of freedom, which we will denote by SFA3. In the clean BHm the SFA3 approach has been shown to be in quantitative agreement with numerically exact QMC results [48]. In this work we investigate the disordered BHm in the vicinity of the superfluid finger, where the condensate density is extremely fragile, leading to a substantial shift in the phase boundaries even if the numerical error is very low. Nonetheless, we observe excellent agreement of the thermodynamic quantities computed with SFT and the QMC reference results.

Since the SFA3 reference system can be solved exactly, we can also evaluate the lattice spectral function and thereby obtain spectroscopic information not readily available from QMC. By systematically analyzing the local excitations of the SFA3 spectral functions, we find that the strongly interacting Bose glass is characterized by different regimes, depending on which local occupations $n$ are activated as a function of the disorder strength $D$. While local observables are described well by the atomic limit, we find that the particles delocalize into isolated superfluid lakes over the strongly localized background around highly occupied sites whenever these sites are particularly rare. In particular, our results indicate that the transition from the strongly interacting Bose glass to the superfluid phase close to unit filling is driven by the percolation of superfluid lakes which form around doubly occupied sites. As $D$ is further increased and the number of highly occupied sites increases accordingly, the particles are localized by the increasing particle number fluctuations and interaction energy, explaining the reentrant behavior of the superfluid finger at larger $D$.

We also present results deeper in the superfluid phase (i.e. at weaker interactions), showing excellent agreement with QMC for thermodynamical quantities at low disorder. When the disorder dominates both over the bandwidth and the interaction, the restricted variational subspace of our SFA3 reference system is however insufficient, as we no longer can stabilize a stationary solution. Whether this can be remedied by a more general reference system construction is an open question.

This paper is organized as follows. In section 2 we derive the SFT for disordered lattice bosons: starting from the free-energy functional (section 2.1), we generalize the bosonic Baym–Kadanoff functional to the case of disorder (section 2.2), perform a Legendre transform to the self-energy effective action (section 2.3), average the effective action over all disorder configurations (section 2.4), and finally arrive at the disorder-averaged self-energy functional (section 2.5). In section 3 we introduce the disordered BHm, discuss the SFA3 reference system used in the SFT calculations (section 3.1) and derive analytic results in the atomic limit (section 3.2). The numerical results are presented in section 4, where we investigate the strongly-interacting Bose glass (section 4.1), the strongly-interacting superfluid phase transition (section 4.2), and the superfluid phase (section 4.3). Finally, section 5 is devoted to the conclusion.

2. Self-energy functional theory for disordered lattice bosons

In this section we derive the SFT for disordered lattice bosons. In analogy to the formalism for clean systems derived in [48], we do so by a series of Legendre transformations starting from the free-energy functional and introduce a simpler exactly solvable reference system sharing the same local interaction and disorder distribution. As was done in a previous work on fermions [51], we average over all possible disorder configurations, arriving at a functional which only depends on the self-energies of the arithmetically averaged propagators of the system.

Note that, in order to keep track of the various additional dependencies arising through the disorder, we introduce a slightly more complex notation than in our work on disorder-free bosons in [48], by denoting the explicit dependencies on system parameters as subscripts. Further, we will denote Nambu objects (i.e. matrices or vectors) as bold letters (e.g. $\mathbf{O}$), scalars as simple letters (e.g. $O$), and functionals with a hat (e.g. $\hat{O}$). Finally, for notational simplicity, we denote the one-point self-energy (formerly $\Sigma_{1/\omega}$ in [48]) as $S$.

2.1. Free-energy functional

Consider a lattice system of bosons in the presence of quadratic disorder, with creation (annihilation) operator $b_i^\dagger$ ($b_i$) on site $i$. Using the Nambu operators $\mathbf{b}_i^\dagger \equiv \mathbf{b}_{i\nu}^\dagger \equiv (b_i^\dagger, b_i)$, with commutator $[\mathbf{b}_i^\dagger, \mathbf{b}_j] = (1 \otimes \sigma_3)^\alpha_{ij}$, where $\alpha$ is a superindex spanning both the site index $i$ and the Nambu index $\nu$, the Hamiltonian $\hat{H}$ of the system can be written as

$$\hat{H} = \mathbf{F}_i \mathbf{b}_{i\nu}^\dagger + \frac{1}{2} \mathbf{t}_i \mathbf{b}_{i\nu}^\dagger \mathbf{b}_{i\nu} + \frac{1}{2} \mathbf{t}_i \mathbf{\eta}_{i\nu}^\dagger \mathbf{b}_{i\nu} + \mathbf{\eta}_i^\dagger \mathbf{\eta}_i + \mathbf{\nu},$$

(1)

where repeated indices are summed over, $\mathbf{F}$ is an explicit symmetry breaking field, $\mathbf{t}_i \equiv \mathbf{t}_{i\nu} = t_{ij} \otimes 1_{\nu}$ is the hopping, the quadratic disorder $\mathbf{\eta}_{i\nu}^\dagger \equiv \mathbf{\eta}_{i\nu}^\dagger = \eta_{ij} \otimes 1_{\nu}$ has the probability distribution $P(\eta)$, and the general
three and four-body interaction \( \hat{V} \) can be expressed as \( \hat{V} \equiv V_{a}^{(4)} b^{a}\bar{b}^{a} b^{b}\bar{b}^{b} + V_{\alpha\beta}^{(4)} b^{a}\bar{b}^{a} b^{b}\bar{b}^{b} \). To keep the notation compact we will henceforth suppress the lattice-Nambu superindices.

At finite temperature \( T \equiv \beta^{-1} \) the free-energy functional of the interacting system is given by

\[
\tilde{\Omega}_{V}[\mathbf{F}, \mathbf{G}^{-1}] = -\ln(\text{Tr}[e^{-S_V[\mathbf{F}, \mathbf{G}^{-1}]}]) / \beta,
\]

where the subscript ‘\( V \)’ means that in addition to \( \mathbf{F} \) and \( \mathbf{G}^{-1} \) the functional also depends on the interaction vertex \( \hat{V} \), and \( S_V \) is the imaginary time action

\[
S_V[\mathbf{F}, \mathbf{G}^{-1}] \equiv \int_0^\beta d\tau \mathbf{F} b(\tau) + \int_0^\beta d\tau \hat{V}[b(\tau)] - \frac{1}{2} \int_0^\beta \int_0^\beta d\tau d\tau' \mathbf{G}^{-1}(\tau, \tau') b(\tau') b(\tau').
\]

The free-energy functional \( \tilde{\Omega}_{V}[\mathbf{F}, \mathbf{G}^{-1}] \) is equal to the free-energy \( \Omega_{\text{lat}}^{(V)} \) of the lattice system in equation (1) with fix-disorder configuration \( \eta \), when evaluated at the symmetry breaking field \( \mathbf{F} \) and the free single-particle propagator \( \mathbf{G}_{\text{lat}}^{-1} \), i.e.

\[
\tilde{\Omega}_{V}[\mathbf{F}, \mathbf{G}^{-1}] = \Omega_{\text{lat}}^{(V)},
\]

where the non-interacting (\( \hat{V} = 0 \)) single-particle propagator of equation (1) is given by

\[
\mathbf{G}_{\text{lat}}^{-1}(\tau, \tau') = \delta(\tau - \tau') (-[1 \otimes \sigma_Date subscripts mean that in addition to hopping \( t \) and the disorder configuration \( \eta \) only. By taking functional derivatives of the free-energy functional \( \tilde{\Omega}_{V} \) with respect to \( \mathbf{F} \) and \( \mathbf{G}^{-1} \) we obtain the two functionals

\[
\tilde{\phi}_{\nu}[\mathbf{F}, \mathbf{G}] \equiv \beta \frac{\delta \tilde{\Omega}_{V}[\mathbf{F}, \mathbf{G}^{-1}]}{\delta \mathbf{F}},
\]

\[
\tilde{\gamma}_{\nu}[\mathbf{F}, \mathbf{G}^{-1}] \equiv 2\beta \frac{\delta \tilde{\Omega}_{V}[\mathbf{F}, \mathbf{G}^{-1}]}{\delta \mathbf{G}^{-1}} + (\tilde{\phi}_{\nu} \tilde{\gamma}_{\nu})[\mathbf{F}, \mathbf{G}^{-1}],
\]

that reproduce the physical one- and two-point propagators (i.e. the condensate \( \Phi_{\text{lat}}^{(V)} \) and the connected Green’s function \( \mathbf{G}_{\text{lat}}^{(V)} \)) of the disordered interacting system in equation (1) when evaluated at \( \mathbf{F} \) and \( \mathbf{G}_{\text{lat}}^{-1} \), i.e.,

\[
\tilde{\phi}_{\nu}[\mathbf{F}, \mathbf{G}_{\text{lat}}^{-1}] = \Phi_{\text{lat}}^{(V)} = \langle b \rangle,
\]

\[
\tilde{\gamma}_{\nu}[\mathbf{F}, \mathbf{G}_{\text{lat}}^{-1}] = \mathbf{G}_{\text{lat}}^{(V)} = -\langle b(\tau)\bar{b}^{\dagger}(0) \rangle + \langle b \rangle \langle \bar{b}^{\dagger} \rangle.
\]

2.2. Baym–Kadanoff functional

When exchanging the functional dependence of the free-energy functional \( \tilde{\Omega}_{V} \) in equation (2), from \( \mathbf{F} \) and \( \mathbf{G}_{\text{lat}}^{-1} \) to \( \Phi \) and \( \mathbf{G} \) by means of a Legendre transformation, one obtains the bosonic Baym–Kadanoff functional \([48–50]\)

\[
\Gamma_{\text{BK}}^{(V)}[\Phi, \mathbf{G}] = \mathbf{F}^\dagger \Phi - \frac{1}{2} \Phi \mathbf{G}^{-1} \Phi + \frac{1}{2} \text{Tr}[\mathbf{G}^{-1} \mathbf{G}] + \frac{1}{2} \text{Tr}[-\mathbf{G}^{-1}] + \Phi^{(\text{LW})}[\Phi, \mathbf{G}].
\]

Here, the entire complexity of the many-body system is contained in the Luttinger–Ward functional \( \Phi^{(\text{LW})}[\Phi, \mathbf{G}] \) which contains all two-particle irreducible diagrams \([56, 57]\). For a more detailed discussion of the Luttinger–Ward functional in the context of SFT, see \([48]\).

At the physical interacting one and two-point propagators, the Baym–Kadanoff functional \( \Gamma_{\text{BK}}^{(V)} \) is stationary

\[
\partial_{\Phi} \Gamma_{\text{BK}}^{(V)}[\Phi, \mathbf{G}, \Phi_{\text{lat}}^{(V)}, \mathbf{G}_{\text{lat}}^{-1}] = 0, \quad \partial_{\Phi} \Gamma_{\text{BK}}^{(V)}[\Phi_{\text{lat}}^{(V)}, \mathbf{G}_{\text{lat}}^{-1}, \mathbf{G}_{\text{lat}}^{-1}] = 0,
\]

and equal to the free energy

\[
\Gamma_{\text{BK}}^{(V)}[\Phi_{\text{lat}}^{(V)}, \mathbf{G}_{\text{lat}}^{-1}] = \Omega_{\text{lat}}^{(V)}.
\]

The explicit functional derivatives take the form

\[
\frac{\delta \Gamma_{\text{BK}}^{(V)}}{\delta \Phi} = \mathbf{F} - \mathbf{G}_{\text{lat}}^{-1} \Phi + \frac{\delta \Phi^{(\text{LW})}}{\delta \Phi}, \quad \frac{\delta \Gamma_{\text{BK}}^{(V)}}{\delta \mathbf{G}} = \mathbf{G}_{\text{lat}}^{-1} - \mathbf{G}^{-1} + 2 \frac{\delta \Phi^{(\text{LW})}}{\delta \mathbf{G}}.
\]

By identifying the variations of the Luttinger–Ward functional \( \Phi^{(\text{LW})} \) as the one and two-point self-energies \([48–50]\)
and applying the stationarity conditions (equation (10)) we find that the interacting propagators fulfill the two Dyson equations

\[
G^{-1}_0 \Phi = F - S, \quad G^{-1} = G_0^{-1} - \Sigma.
\]

Consider now the result of substituting \( F \) and \( G_0^{-1} \) using equation (14) in the functionals \( \hat{\Phi}_V \) and \( \hat{\Sigma}_V \) (equations (6) and (7)). This gives the highly nonlinear coupled equations

\[
\hat{\Phi}_V[(G^{-1} + \Sigma) \Phi + S, G^{-1} + \Sigma] = \Phi, \tag{15}
\]

\[
\hat{\Sigma}_V[(G^{-1} + \Sigma) \Phi + S, G^{-1} + \Sigma] = \Sigma. \tag{16}
\]

For given self-energies \( S \) and \( \Sigma \) the concomitant solution of equations (15) and (16) implicitly defines the functionals

\[
\hat{\Phi}_V[S, \Sigma] = \Phi, \quad \hat{\Sigma}_V[S, \Sigma] = \Sigma, \tag{17}
\]

depending solely on the self-energies \( S \) and \( \Sigma \) and the interaction \( V \), producing the physical interacting propagators when evaluated at the physical self-energies, i.e.

\[
\hat{\Phi}_V[S_{\text{Fin}}, \Sigma_{\text{Fin}}] = \Phi_{\text{Fin}}, \quad \hat{\Sigma}_V[S_{\text{Fin}}, \Sigma_{\text{Fin}}] = \Sigma_{\text{Fin}}. \tag{18}
\]

### 2.3. Bosonic self-energy effective action

By means of a further Legendre transform the Baym–Kadanoff functional \( \hat{I}^{(BK)}_{\text{FinV}} \) with functional dependence on \( \Phi \) and \( G \) can be transformed into the self-energy effective action

\[
\hat{I}^{(SE)}_{\text{FinV}}[S, \Sigma] = \frac{1}{2}(F - S)/G_{\text{mp}}(F - S) + \frac{1}{2} \text{Trln}[-(G_{\text{mp}}^{-1} - \Sigma)] + \hat{\Phi}_V[S, \Sigma], \tag{19}
\]

depending on the self-energies \( S \) and \( \Sigma \), where the universal functional \( \hat{\Phi}_V[S, \Sigma] \) is the Legendre transform of the universal Luttinger–Ward functional \( \hat{\Phi}^{(LW)}_V[\Phi, G] \), with variations (see [48] for details)

\[
\delta_S \hat{\Phi}_V = \Phi, \quad \delta_{\Sigma} \hat{\Phi}_V = \Sigma. \tag{20}
\]

The variations of the self-energy effective action give

\[
\frac{\delta \hat{I}^{(SE)}_{\text{FinV}}}{\delta S^i} = -G_{\text{mp}}(F - S)^i + \Phi^i, \quad \frac{\delta \hat{I}^{(SE)}_{\text{FinV}}}{\delta \Sigma} = -[G_{\text{mp}} - \Sigma]^{-1} + G, \tag{21}
\]

whence \( \hat{I}^{(SE)}_{\text{FinV}} \) is stationary at the physical self-energies

\[
\delta_S \hat{I}^{(SE)}_{\text{FinV}}[S_{\text{FinV}}, \Sigma_{\text{FinV}}] = 0, \quad \delta_{\Sigma} \hat{I}^{(SE)}_{\text{FinV}}[S_{\text{FinV}}, \Sigma_{\text{FinV}}] = 0. \tag{22}
\]

and equal to the free energy

\[
\hat{I}^{(SE)}_{\text{FinV}}[S_{\text{FinV}}, \Sigma_{\text{FinV}}] = \Omega_{\text{FinV}}. \tag{23}
\]

### 2.4. Disorder-averaged self-energy effective action

While we up till now have treated a system with a single disorder realization \( \eta \), we are interested in describing the averaged ensemble of systems with disorder probability distribution \( P(\eta) \) and its ensemble averaged free energy

\[
\Omega_{\text{FinPV}} \equiv \langle \Omega_{\text{FinV}} \rangle_p \equiv \int d\eta P(\eta) \Omega_{\text{FinV}}. \tag{24}
\]

In terms of the self-energy functional equation (19) the averaged free energy can be expressed as

\[
\Omega_{\text{FinPV}} = \langle \hat{I}^{(SE)}_{\text{FinV}}[S_{\text{FinV}}, \Sigma_{\text{FinV}}] \rangle_p \tag{25}
\]

using equation (23). However, a direct application of the averaged self-energy functional does not lend itself to the construction of approximations using disorder-averaged propagators and self-energies.

To describe the combined effect of disorder and interaction we seek to construct an extended disorder-averaged functional parameterized by the disorder-averaged propagators

\[
\hat{\Phi} \equiv \langle \hat{\Phi}_{\eta} \rangle_p, \quad \hat{G} \equiv \langle \hat{G}_{\eta} - \hat{\Phi}_{\eta} \hat{\Phi}_{\eta}^\dagger \rangle_p + \hat{\Phi} \hat{\Phi}^\dagger, \tag{26}
\]

using the short-hand notation \( \hat{G}_{\eta} \equiv \hat{G}_V[S_{\eta}, \Sigma_{\eta}] \) and \( \hat{\Phi}_{\eta} \equiv \hat{\Phi}_V[S_{\eta}, \Sigma_{\eta}] \), where \( S_{\eta} \) and \( \Sigma_{\eta} \) denote the self-energies for the disorder configuration \( \eta \), see equation (18). The corresponding average self-energies \( S \) and \( \Sigma \) are defined through the Dyson equations
\[ S = F - G_{00}^{-1} \Phi, \quad \Sigma = G_{00}^{-1} - G^{-1}, \]

where \( G_{00} \) is the free propagator for the disorder-free system \( G_{00} \equiv G_{00}|_{\eta=0} \). By insertion of the averaged Dyson equations (equation (27)) in the definitions of the averaged propagators \( \Phi \) and \( G \) (equation (26)) we obtain the relations

\[ \Phi = \langle A_\eta^{-1} B_\eta \rangle, \]
\[ G = \Phi \Phi^\dagger = \langle [A_\eta^{-1} - \Sigma)_\eta^{-1} - [A_\eta^{-1} B_\eta]\rangle \langle [A_\eta^{-1} B_\eta]\rangle, \]

where

\[ A_\eta = G^{-1} + \Sigma - \eta, \quad B_\eta = S - S_\eta + [G^{-1} + \Sigma] \Phi. \]

The concomitant solution of equations (28) and (29) implicitly defines the two universal functionals

\[ \hat{\Phi}(S, \Sigma; [S_\eta, \Sigma_\eta]) \equiv \Phi, \quad \hat{G}(S, \Sigma; [S_\eta, \Sigma_\eta]) \equiv G. \]

Using the universal averaged propagator functionals we define the extended averaged self-energy effective action

\[ \hat{\Gamma}_{PV}^{(SE)}[S, \Sigma; [S_\eta, \Sigma_\eta]] = \frac{1}{2} (F - \hat{S})^\dagger G_{00}(F - \hat{S}) + \frac{1}{2} \text{Trln}[-(G_{00}^{-1} - \Sigma)] + \hat{T}_{PV}[S, \Sigma; [S_\eta, \Sigma_\eta]] + \langle \hat{\Phi}_V[S_\eta, \Sigma_\eta]\rangle, \]

where \( \hat{T}_{PV} \) is a universal functional of the averaged self-energies

\[ \hat{T}_{PV}[S, \Sigma; [S_\eta, \Sigma_\eta]] \equiv -\frac{1}{2} \langle \Phi \rangle (G + \Sigma) \Phi - \frac{1}{2} \langle \Phi \langle \Phi \rangle G^{-1} + \Sigma - \eta \rangle \Phi \rangle + \langle [\hat{S}^\dagger - S_\eta] + \Phi \rangle \langle \hat{G}^{-1} + \Sigma \rangle \hat{\Phi} \rangle + \frac{1}{2} \langle \text{Trln}[-(\hat{G}^{-1} + \Sigma - \eta - \Sigma_\eta)]\rangle \]

\[ -\frac{1}{2} \text{Trln}[-\hat{G}^{-1}]. \]

Here, we have extended the variational space from the fixed-disorder self-energies \([S_\eta, \Sigma_\eta]\) to both the fixed-disorder and average self-energies \([S, \Sigma; [S_\eta, \Sigma_\eta]]\). However, when evaluated at the physical self-energies, \( \hat{\Gamma}_{PV}^{(SE)} \) takes the value of the disorder average of the self-energy functional \( \hat{\Gamma}_{PV}^{(SE)} \) by equation (25).

The variations of \( \hat{T}_{PV} \) are derived in appendix A and give, \( \delta S \hat{T}_{PV} = \hat{\Phi} \) and \( 2\delta \Sigma \hat{T}_{PV} = \hat{G} \), showing that \( \hat{T}_{PV} \) is the analog of the \( \hat{\Phi}_V \) functional for the averaged self-energies, as by equation (20), \( \delta S \hat{\Phi}_V = \hat{\Phi}_V \) and \( 2\delta \Sigma \hat{\Phi}_V = \hat{G} \). The functional derivatives with respect to the self-energies at fixed-disorder configuration \( \eta \) yield

\[ \delta S \hat{T}_{PV} = -P(\eta) \hat{\Phi}_\eta + \delta S \hat{\Phi}_V^{\dagger} P(\eta) \hat{Q}_\eta, \]
\[ 2\delta \Sigma \hat{T}_{PV} = -P(\eta) \hat{G}_\eta + 2\delta \Sigma \hat{\Phi}_V^{\dagger} P(\eta) \hat{Q}_\eta, \]

where \( \hat{Q}_\eta \) is defined in appendix A and vanishes at the physical self-energies.

The variations of the averaged self-energy effective action \( \hat{\Gamma}_{PV}^{(SE)} \) (equation (32)) therefore give

\[ \delta S \hat{\Gamma}_{PV}^{(SE)} = -G_{00}(\hat{F} - \hat{S}) + \hat{\Phi}, \]
\[ 2\delta \Sigma \hat{\Gamma}_{PV}^{(SE)} = -[G_{00}^{-1} - \Sigma]^{-1} + \hat{G}, \]

\[ \delta S \hat{\Gamma}_{PV}^{(SE)} = -P(\eta) \hat{\Phi}_\eta + \delta S \hat{\Phi}_V^{\dagger} P(\eta) \hat{Q}_\eta + \delta S \hat{\Phi}_V^{\dagger} P(\eta) \hat{Q}_\eta, \]
\[ 2\delta \Sigma \hat{\Gamma}_{PV}^{(SE)} = -P(\eta) \hat{G}_\eta + 2\delta \Sigma \hat{\Phi}_V^{\dagger} P(\eta) \hat{Q}_\eta. \]

Hence, at the physical self-energies

\[ S, \Sigma; [S_\eta, \Sigma_\eta] = S_{PV}, \Sigma_{PV}, [S_{PV}, \Sigma_{PV}], \]

the averaged self-energy effective action \( \hat{\Gamma}_{PV}^{(SE)} \) is stationary

\[ \delta S \hat{\Gamma}_{PV}^{(SE)} = \delta S \hat{\Gamma}_{PV}^{(SE)} = \delta \Sigma \hat{\Gamma}_{PV}^{(SE)} = \delta \Sigma \hat{\Gamma}_{PV}^{(SE)} = 0, \]

and equal to the average free energy

\[ \hat{\Gamma}_{PV}^{(SE)}[S_{PV}, \Sigma_{PV}, [S_{PV}, \Sigma_{PV}]] = \Omega_{PV}. \]

The crucial part of the disorder-averaged self-energy effective action is that the functionals \( \hat{T}_{PV} \) and \( \hat{\Phi}_V \) are universal, in the sense that they do not depend on the non-interacting propagator \( G_{00} \) or the symmetry breaking
field $F$ (see appendix B for the explicit derivatives of $\hat{T}_{PV}$ and [48] for the universality of $\hat{F}_V$), but only on the interaction $V$, the disorder probability distribution $P(\eta)$, the disorder-dependent self-energies $\{S_\eta, \Sigma_\eta\}$, and the average self-energies $\overline{S}$ and $\overline{\Sigma}$. In the following we will make use of this property in order to derive consistent approximations of $I_{\text{PV}}^{(SE)}$.

2.5. Disorder-averaged SFT

A versatile approach to non-perturbative approximations of the self-energy effective action $I_{\text{PV}}^{(SE)}$ is the SFT pioneered by Potthoff [41–44] for fermionic systems and later extended to bosonic systems [45, 47, 48]. The formalism for systems with disorder has been developed for fermions in [51] and applied in a VCA to bosons without symmetry breaking in [52]. Here, we generalize the bosonic case to also include $U(1)$-symmetry breaking and general reference systems.

We consider the general interacting bosonic system with quadratic disorder of equation (1), and introduce a second reference system with the same interaction $\hat{V}$ and disorder $P(\eta)$ but with some arbitrary linear symmetry breaking field $F'$, arbitrary free propagator

$$G_{\Delta}\bigg(\tau, \tau'\bigg) = \delta(\tau - \tau')(\mathbb{1} \otimes \sigma_3)\partial_{\tau'} - \eta) - \Delta(\tau, \tau'),$$

and self-energy effective action $I_{\text{PV}}^{(SE)}$. Here, the free propagator $G_{\Delta\eta\eta}$ is parametrized by replacing the hopping $t$ by a completely general matrix $\Delta(\tau, \tau')$.

Now, since the self-energy effective actions of both systems contain the same universal functionals $\hat{T}_{PV}$ and $\hat{T}_{PV}$ we can evaluate $I_{\text{PV}}^{(SE)}$ in terms of $I_{\text{PV}}^{(SE)}$ as

$$I_{\text{PV}}^{(SE)}[\mathcal{S}, \mathcal{\Sigma}, \{S_\eta, \Sigma_\eta\}] = I_{\text{PV}}^{(SE)}[\mathcal{S}, \mathcal{\Sigma}, \{S_\eta, \Sigma_\eta\}] + \frac{1}{2} \text{Tr} \ln \left[G_{\Delta\eta\eta}^{-1} - \mathcal{\Sigma}\right]
- \frac{1}{2} \text{Tr} \ln \left[G_{\Delta\eta\eta}^{-1} - \mathcal{\Sigma}\right] + \left(F - \mathcal{S}\right)G_{\Delta\eta\eta}(F - \mathcal{S})
- \frac{1}{2} \left(F' - \mathcal{S}\right)G_{\Delta\eta\eta}(F' - \mathcal{S}).$$

The stationary condition in equation (41) now translates into

$$\frac{\delta I_{\text{PV}}^{(SE)}}{\delta \mathcal{S}} = G_{\Delta\eta\eta}(F' - \mathcal{S}) - G_{\Delta\eta\eta}(F - \mathcal{S}) = 0,$$

$$2\frac{\delta I_{\text{PV}}^{(SE)}}{\delta \mathcal{\Sigma}} = \left[G_{\Delta\eta\eta}^{-1} - \mathcal{\Sigma}\right]^{-1} - \left[G_{\Delta\eta\eta}^{-1} - \mathcal{\Sigma}\right]^{-1} = 0.$$

If by an appropriate choice of $\Delta$ and $F'$ the reference system can be made simple enough to be exactly solvable, one can go one step further and evaluate the original systems functional $I_{\text{PV}}^{(SE)}$ at the physical self-energies of the reference system, i.e. at $S_{F\Delta} \equiv S_{F\Delta PV}, \Sigma_{F\Delta} \equiv \Sigma_{F\Delta PV},$ and $\{S_{F\eta\eta}^\prime, \Sigma_{F\eta\eta}^\prime\}$. This produces the SFT approximation for the system and the SFT functional

$$I_{\text{PV}}^{(SFT)}[\mathcal{S}_{F\Delta}, \mathcal{\Sigma}_{F\Delta}] = \Omega_{F\Delta PV} + \frac{1}{2} \text{Tr} \ln \left[G_{\Delta \eta \eta}^{-1} - \mathcal{\Sigma}_{F\Delta}\right] - \frac{1}{2} \text{Tr} \ln \left[G_{\Delta \eta \eta}^{-1} - \mathcal{\Sigma}_{F\Delta}\right]
+ \frac{1}{2} \left(F - S_{F\Delta}\right)G_{\Delta \eta \eta}(F - S_{F\Delta})
- \frac{1}{2} \left(F' - S_{F\Delta}\right)G_{\Delta \eta \eta}(F' - S_{F\Delta}),$$

where we have used that $I_{\text{PV}}^{(SE)}[\mathcal{S}_{F\Delta}, \mathcal{\Sigma}_{F\Delta}, \{S_{F\eta\eta}^\prime, \Sigma_{F\eta\eta}^\prime\}] = \Omega_{F\Delta PV},$ and

$$I_{\text{PV}}^{(SFT)}[\mathcal{S}_{F\Delta}, \mathcal{\Sigma}_{F\Delta}] \equiv I_{\text{PV}}^{(SE)}[\mathcal{S}_{F\Delta}, \mathcal{\Sigma}_{F\Delta}, \{S_{F\eta\eta}^\prime, \Sigma_{F\eta\eta}^\prime\}].$$

is the self-energy effective action of the original system $I_{\text{PV}}^{(SE)}$ restricted to the domain of physical self-energies of the reference system. Note that by replacing $I_{\text{PV}}^{(SE)}[\mathcal{S}_{F\Delta}, \mathcal{\Sigma}_{F\Delta}, \{S_{F\eta\eta}^\prime, \Sigma_{F\eta\eta}^\prime\}]$ with the scalar $\Omega_{F\Delta PV}$, we eliminate all explicit dependencies on the fixed-disorder self-energies $\{S_{F\eta\eta}^\prime, \Sigma_{F\eta\eta}^\prime\}$, such that the disorder-averaged self-energy effective action now only depends on the average self-energies $S_{F\Delta}$ and $\Sigma_{F\Delta}$.

The domain of $I_{\text{PV}}^{(SFT)}$ is therefore defined by the average physical self-energies of the reference system ($S_{F\Delta}$ and $\Sigma_{F\Delta}$) and parametrized by $\Delta$ and $F'$. By generalizing the variational principle of equation (41) to the restricted domain we obtain a thermodynamically optimal approximation when the self-energy variations are zero on the domain, i.e. we seek $\Delta$ and $F'$ such that

5 In e.g. the context of DMFT $\Delta(\tau - \tau')$ would represent a retarded hybridization of an impurity with a non-interacting bath, while in the case of e.g. an instantaneous $\Delta(\tau - \tau') = t'\delta(\tau - \tau')$ where $t'$ is diagonal in Nambu space, it can be considered to be a hopping amplitude.
where \( D (\Delta) \) is the disorder strength. Thus, the free propagator creates (annihilates) a boson at site \( i \), \( \hat{n}_i = b_i^\dagger b_i \) is the occupation number operator, \((i, j)\) denotes summation over nearest neighbors, \( J \) is the hopping amplitude, \( U \) the on-site interaction, and \( \mu \) the chemical potential. The local disorder potentials \( \eta \) are uncorrelated and are assumed to have a flat probability distribution

\[
P(\eta) = \prod_i p(\eta_i, \eta) = \begin{cases} 1/(2D), & |\eta| \leq D \\ 0, & \text{else} \end{cases}
\]

where \( D \) is the disorder strength. Thus, the free propagator (equation (5)) is given by

\[
G_{\text{FPV}}^{-1}(\tau, \tau') = \delta(\tau - \tau')( - \mathbf{1} \otimes \mathbf{e}_Z ) \partial_\tau^2 + \{ J \delta_{(i,j)} + [\mu - \eta_i] \delta_{(i,j)} \otimes \mathbf{1} \},
\]

where \( \delta_{(i,j)} \) is non-zero only for nearest neighbors \((i, j)\).

In addition to the superfluid and Mott insulating phase of the clean (i.e. non-disordered) model, the groundstate phase diagram of the disordered BHm exhibits the Bose glass phase. It is an insulating compressible phase that always intervenes between the superfluid and the Mott insulator at finite disorder \((D > 0)\) [21]. The phase is composed of local regions, including both strongly localized atomic levels, and isolated superfluid lakes which locally close the many-body gap. Since these superfluid lakes are spatially separated, global phase coherence is not reached, yielding a zero superfluid response. Hence, while the compressibility of the Bose glass is finite, the global condensate order parameter is zero as is the many-body gap. In our SFT formalism we therefore distinguish the Bose glass and the superfluid phase by the disorder-averaged condensate \( \Phi \). In the mean-field approach of [25] a different criterion was used, analyzing the spatial percolation of superfluid regions (i.e. isolated regions with non-zero quasi-condensates), allowing for a zero global superfluid response even though \( \Phi = 0 \). As in this work we will treat only disorder-averaged translational invariant quantities, such a real-space percolation of the condensate is not analyzed directly.

### 3.1. Minimal reference system

In this first application of SFT with symmetry breaking to the disordered BHm, we will make use of the simplest possible reference system, comprising a single bosonic mode per site. In this case the reference system Hamiltonian in the thermodynamic limit reads

\[
H_{\text{ref}}(\mathbf{F}, \Delta) = \sum_i \hat{H}_{i,0} \langle \mathbf{F}, \Delta \rangle,
\]
where the sum runs over an infinite number of independent single-site Hamiltonians

\[ \hat{H}_{i,j} = \frac{U}{2} b_i^\dagger b_i^\dagger b_i b_i + (\eta_i - \mu) \hat{n}_i + b_i^\dagger F^\dagger + b_i^\dagger b_i \Delta \hat{b}_i. \]  

(57)

The reference system is parametrized by three real translationally invariant parameters \( F', \Delta_{\eta}, \) and \( \Delta_{\Delta}, \) where \( F' = (F', F') \) and \( \Delta (\tau - \tau'') = \delta (\tau - \tau') \Delta \) is instantaneous in imaginary time and site-local as

\[ \Delta (\tau - \tau'') = \delta (\tau - \tau') [\hat{b}_j \otimes (\Delta_{\eta} + \Delta_{\Delta} \sigma_2)]. \]  

(58)

This minimal reference system yields a non-perturbative self-energy functional approximation that we denote by SFA3. It has previously been shown to yield quantitatively correct results for the clean BHm, comparing with numerically exact QMC results [48].

In the case of uncorrelated disorder considered here, the disorder-averaging of observables (equation (24)) gives translationally invariant results, see appendix D. The disorder-averaged free energy of the SFA3 reference system is therefore given by

\[ \Omega_{F,\Delta,PU} = N \langle \Omega_{i,F,\Delta,\eta,U} \rangle_p, \]  

(59)

where \( N \) is the number of lattice sites, \( \Omega_{i,F,\Delta,\eta,U} \) is the free energy of a single-site in the reference system, and

\[ \langle f(\eta) \rangle_p \equiv \int d\eta \ p(\eta)f(\eta). \]  

Analogously, the propagators are obtained as

\[ G_{F,\Delta,PU}(\tau - \tau'') = \delta_{ij} \otimes \langle G_{i,F,\Delta,\eta,U}(\tau - \tau'' \rangle_p, \]  

\[ \Phi_{F,\Delta,PU} = \langle \Phi_{i,F,\Delta,\eta,U} \rangle_p. \]  

(60)

Hence, to evaluate the disorder-averaged quantities of the reference system it suffices to solve the single-site Hamiltonian of equation (57) for all possible values of \( \eta \) and then average the result over the probability distribution \( p(\eta). \) The corresponding average self-energies \( \Sigma_{F,\Delta,PU} \) and \( \Sigma_{F,\Delta,PU} \) of the reference system are then obtained from equation (27).

Physical solutions of the lattice system can be found by searching for stationary values of the SFT functional in equation (47) fulfilling equation (52) using a standard root solver to find the point with zero gradient. This procedure is identical to the algorithm detailed in [48]. Once a stationary solution is found, lattice quantities can be computed using the corresponding self-energies at stationarity as detailed in appendix E.

3.2. Atomic limit

As in this work we mainly analyze the behavior of the disordered BHm at large interactions \( U/J \gg 1, \) we want to compare to the analytic atomic limit of having decoupled sites, i.e. \( J = 0. \) In this section we analyze the properties of the infinite system in this limit.

3.2.1. Local occupations

We start by analyzing the local occupations as a function of disorder in the atomic limit. For \( J = 0, \) we can have a local occupation \( n_i = \langle \hat{n}_i \rangle \) at zero temperature if the local potential \( \eta_i \) takes values \( \eta_{\min}(n_i) < \eta_i < \eta_{\max}(n_i). \) In order to derive this, we turn to the local energy of the decoupled site \( i \) with occupation number \( n_i \) and local potential \( \eta_i, \) i.e.

\[ E_{SS}(n_i, \eta_i) = \frac{U}{2} n_i(n_i - 1) + (\eta_i - \mu) n_i. \]  

(61)

The groundstate will have local occupation larger than \( n_i - 1 \) if \( E_{SS}(n_i, \eta_i) < E_{SS}(n_i - 1, \eta_i), \) i.e. if

\[ \eta_i < \eta_{\max}(n_i) = \left\{ \begin{array}{ll} \mu - U(n_i - 1) & \text{if } n_i > 0, \\ \infty & \text{if } n_i = 0, \end{array} \right. \]  

(62)

where we used that the local occupation \( n_i \) is bounded from below by zero, and therefore \( \eta_{\min}(0) = \infty. \)

Additionally, in order to have a local occupation \( n_i \) we need to fulfill the condition \( E_{SS}(n_i, \eta_i) < E_{SS}(n_i + 1, \eta_i), \) resulting in

\[ \eta_i > \eta_{\min}(n_i) = \mu - Un_i. \]  

(63)

As the minimum possible value of \( \eta_i \) is \( -D \) (see equation (54)), this implies that the maximal possible local occupation \( n_{\max} \) is given by

\[ n_{\max} = \left\{ \left\lfloor \frac{D + \mu}{U} + 1 \right\rfloor \right. \]  

(64)

Furthermore, as the maximum value of \( \eta_i \) is \( D \) and the local occupation is bounded from below by \( n_i = 0, \) we have a minimal possible local occupation of
\[ n_{\text{min}} = \text{Max}\left\{ \mu - D \frac{\eta}{U}, 0 \right\}. \] (65)

We can use the information above to derive the probability of sites with occupation \( n \) in the infinite system. We denote this quantity by \( r_n \), defined as the number of sites with local occupation \( n \) divided by the total number of sites, which can be computed by

\[
r_n = \begin{cases} 
0 & \text{if } n < n_{\text{min}} \text{ or } n > n_{\text{max}}, \\
\frac{1}{2D} \left( \text{Min} \{ D, \eta_{\text{max}}(n) \} - \text{Max} \{ -D, \eta_{\text{min}}(n) \} \right) & \text{else}.
\end{cases}
\] (66)

We can use the probabilities \( r_n \) in order to derive expressions for the total density \( n \) and the interaction energy \( E_{\text{int}} \), given by

\[ n = \sum_{m=0}^{\infty} r_m, \quad E_{\text{int}} = U \frac{1}{2} \sum_{m=0}^{\infty} r_m (m^2 - m). \] (67)

Note that, while the values of \( r_n \) depend on the disorder distribution \( P(\eta) \), the values of \( D \) where they become non-zero (and therefore the maximal and minimal possible occupations for a given disorder strength in equations (64) and (65)) depend only on the maximal and minimal values of the local potential \( \pm D \) (and the global parameters \( \mu \) and \( U \)). These are therefore universal, in the sense that they do not depend on the disorder distribution \( P(\eta) \) as long as it is uncorrelated and bounded (i.e. with \( P(|\eta| > D) = 0 \)).

**3.2.2. Local excitations**

On a single-site level, the process \( (n_i \rightarrow n_i + 1) \) on site \( i \) leads to the energy difference

\[ \Delta E[n_i \rightarrow n_i + 1] = U n_i - \mu + \eta_i. \] (68)

As discussed in section **3.2.1**, in the groundstate we can have a local occupation of \( n_i \) only if \( \eta_{\text{min}}(n_i) \leq \eta_i \leq \eta_{\text{max}}(n_i) \), see equations (62) and (63). If we average over all sites \( i \), we therefore find, that the local processes \( (n_i \rightarrow n_i + 1) \), with local groundstate occupations \( n_i \), span over the energy range given by

\[ \text{Max} \{ 0, U n_i - \mu - D \} \leq \Delta E[n_i \rightarrow n_i + 1] \leq \begin{cases} D - \mu & \text{if } n_i = 0, \\
\text{Min} \{ U, U n_i - \mu + D \} & \text{else}.
\end{cases} \] (69)

We can further derive the energy difference for the opposite process in the same way, yielding

\[ \text{Max} \{ 0, -D - U n_i \} \leq \Delta E[n_i + 1 \rightarrow n_i] \leq \text{Min} \{ U, \mu + D - U n_i \}. \] (70)

The disorder-averaged local spectral function is defined as

\[ A_{\text{loc}}(\omega) = -\frac{1}{N \pi} \sum_i \text{Im} [\tilde{G}_i(\omega)]. \] (71)

At zero temperature we have

\[ G_{i,n}(\omega) = \sum_{n' = \text{GS}} E_{\text{GS}} - E_n + \omega \frac{[n|b_i^\dagger | \text{GS}]^2}{E_{\text{GS}} - E_n - \omega^\epsilon} + \frac{[n|b_i | \text{GS}]^2}{E_{\text{GS}} - E_n - \omega^\epsilon} \] (72)

where \( \text{GS} \) is the groundstate, the sum runs over all other eigenstates, \( E_n \) is the energy of eigenstate \( n \), and \( \omega^\epsilon = \omega + i \epsilon \) with a small broadening parameter \( \epsilon \). Disorder-averaging over an infinite number of configurations therefore yields a translational invariant local Green’s function

\[ \tilde{G}_i(\omega) = \int_{-D}^{D} d\eta P(\eta) \left( \frac{\tilde{\eta}(\eta) + 1}{\omega^\epsilon - \Delta E[\tilde{\eta}(\eta) \rightarrow \tilde{\eta}(\eta) + 1]} + \frac{\tilde{\eta}(\eta)}{\Delta E[\tilde{\eta}(\eta) - 1 \rightarrow \tilde{\eta}(\eta)] - \omega^\epsilon} \right), \] (73)

where

\[ \tilde{\eta}(\eta_{\text{min}}) < \eta < \eta_{\text{max}}(\eta) = n. \] (74)

Using equations (69) and (70) we therefore find that the resonances of the spectral function for the processes \( (n \rightarrow n + 1) \) are bounded by equation (69), while the processes \( (n + 1 \rightarrow n) \) are bounded by equation (70). Therefore, the effect of the disorder strength \( D \) on the spectral function in the atomic limit—which in the absence of disorder consists of sharp delta peaks—is to broaden the peaks to a width which is proportional to \( D \). A consequence of this is that, apart from the process \( (0 \rightarrow 1) \), all local resonances are bounded by \( -U \leq \omega \leq U \). Further, it can easily be shown that for \( D \geq mU/2 \), with integer \( m \), we have
\( \omega_{\text{max}}(n \rightarrow n + 1) > \omega_{\text{min}}(n + m \rightarrow n + m + 1), \) leading to an overlap of the processes \((n \rightarrow n + 1)\) and \((n + m \rightarrow n + m + 1)\) (and equivalently for the reversed particle-removal processes).

4. Results

We analyze the BHm with box disorder using SFT with an SFA3 reference system, see section 3.1. The calculations are compared to disorder-averaged path integral QMC [20, 21, 58] simulations on a finite cubic lattice of 83 sites. In the strongly-interacting case we further compare to analytic results in the atomic limit. As either empty or doubly occupied sites are activated by the disorder depending on the value of the condensate density.

For stronger disorder the situation changes, in particular in the so-called superfluid finger, i.e., the narrow region of the superfluid phase extending to large values of the relative interaction strength \(U/J\). In the finger, the condensate density \(\rho_{c} = \frac{1}{2} \langle \bar{\Phi} \rangle \bar{\Phi} \) is extremely low, and therefore very hard to resolve experimentally [21]. Small deviations from numerically exact results in the SFA3 calculations therefore lead to a notable shift in the phase boundaries and an overestimation of the extent of the superfluid finger, as seen in figure 1. At even larger disorder when leaving the superfluid finger, the discrepancy between SFA3 and QMC results is reduced. The Mott insulator to Bose glass transition at fixed density \(n = 1\) is very hard to resolve numerically (unlike the transition at fixed chemical potential discussed later), as the finite compressibility in the Bose glass close to the phase boundary is exponentially small [21]. Instead, in figure 1 we show analytic results on the phase boundary from [21].

Note that, while it is always possible to find a Bose glass stationary solution at strong disorder in mean-field approaches (by setting the condensate to zero), arithmetically averaged mean-field always finds a groundstate with a finite condensate order parameter and lower free energy [24, 25]. In the context of SFT, the mean-field approximation can be understood as neglecting the kinetic contributions of uncondensed bosons in the self-energy functional [48]. By including these contributions in our SFA3 calculations, we are able to change the energy balance with respect to the mean-field approach, yielding a phase transition to the uncondensed Bose glass.

4.1. Strongly-interacting Bose glass phase

Using the local occupation probabilities \(r_{n}\) of section 3.2.1, it is possible to distinguish different regimes of the Bose glass in the atomic limit: the qualitative behavior of the Bose glass will change every time the disorder strength is large enough to activate a given local occupation \(n\) (i.e. if the probability of finding a site with local occupation \(n_{1}, r_{n_{1}}\) becomes non-zero as a function of \(D\)). Coming from the Mott insulating groundstate at density \(n = 1\) (where \(r_{n=1} = 0\)) and increasing the disorder strength \(D\), as we enter the Bose glass one of the probabilities \(r_{1}\) and \(r_{2}\) becomes non-zero, as either empty or doubly occupied sites are activated by the disorder depending on the value of the chemical potential. When the disorder is increased further, also higher occupancies are activated and other probabilities \(r_{n}\) become non-zero every time we enter a new regime of the strongly-interacting Bose glass.
For weak disorder $D < W$ the qualitative behavior remains the same. However, the Hubbard bands are broadened by the finite hopping, so the kinetic energy is increased, while the gap of the kinetic energy fluctuations decreases (see figure 3(b)).

At $D \approx \mu$ ($D/f \approx 56$) the gap goes to zero, and we enter the Bose glass phase. The disorder activates empty sites (i.e., $n_i > 0$, see figure 2(d)), and as a consequence the density drops (figure 2(a)), while the kinetic energy

While the atomic limit shows sharp transitions between the different regimes (see the values of $r_w$ in figure 2(d)), for finite hopping $J$, the kinetic fluctuations turn the transitions into crossovers. However, as we will discuss in this section, in the case of strong interactions the qualitative behavior of local observables changes drastically also in our numerical results whenever a new regime is entered. For the sweep in disorder strength of figure 2 the results for local quantities such as the density (figure 2(a)) and the interaction energy (figure 2(c)) show perfect agreement between the analytic results in the atomic limit and both SFA3 and QMC results, except right at the transition/crossover between the different regimes. In fact, the kinetic energy (figure 2(b))—which is the dominating additional contribution of the finite hopping in SFA3 and QMC, as compared to the atomic limit—is orders of magnitude smaller than the interaction energy at large disorder. In the following we will discuss these different strongly-interacting regimes in more detail, analyzing the qualitative behavior of the observables in figure 2 and extracting additional information from the corresponding local spectral functions $A_{loc}(\omega)$ shown in figure 3.

We start at $D = 0$, i.e., in the non-disordered Mott insulator. As every site has the same local occupation $n_i = 1$, the local spectral function (figure 3(b)) is characterized by the two Hubbard bands corresponding to the transitions ($1 \rightarrow 0$) at negative frequencies and ($1 \rightarrow 2$) at positive frequencies. While in the atomic limit these resonances would correspond to delta peaks, at finite hopping the shape of the spectral function depends on the non-interacting dispersion and its bandwidth $W = 2zJ$, where $z = 6$ is the coordination number of the lattice. In particular, the unit filling Mott insulator lower and upper Hubbard bands have the bandwidths $W$ and $2W$ respectively, see [59] for a derivation. For weak disorder $D < W$ the qualitative behavior remains the same. However, the Hubbard bands are broadened by the finite disorder strength $D$ and the spectral weight at the center of the bands is reduced, see figure 3(b).

The situation changes when $D > W$ (see figure 3(c)), where the spectral function is more similar to the one predicted by the atomic limit: as discussed in section 3.2.2, the width of the Hubbard bands now is fully determined by the disorder strength $D$, and the dispersive features of the spectral function are lost. As we are still in the Mott phase, the spectral function shows a finite gap, defined as the minimal distance between the Hubbard bands and $\omega = 0$. As the disorder strength $D$ is increased, so does the kinetic energy (see figure 2(b)), due to increasing kinetic fluctuations, while the gap of the spectral function decreases (see figure 3(a)).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Observables of the disordered BHm as a function of disorder strength $D/f$ for $U/f = 140$, $\mu/U = 0.4$, and $T/f = 0.1$. (a) Density $n$ computed with SFA3 (red), QMC (black squares), and in the atomic limit ($f = 0$, blue dashed). (b) Kinetic energy per site $E_{kin}/f$ computed with SFA3 (red), QMC (black squares), and in the atomic limit ($f = 0$, blue dashed). (c) Interaction energy per site $E_{int}/f$ computed with SFA3 (red), QMC (black squares), and in the atomic limit ($f = 0$, blue dashed). (d) Probabilities of having sites with local occupation 0 ($r_0$, blue dashed), 1 ($r_1$, black), 2 ($r_2$, red dashed), and 3 ($r_3$, green), as computed in the atomic limit. The vertical dashed lines show the transitions between the different regimes in the atomic limit, while the gray area is where the non-local Green’s function of SFA3 develops a pole, indicating the presence of isolated quasi-condensates.}
\end{figure}
which increases abruptly at \( \omega = 0 \), and we find a finite spectral weight at small positive frequencies corresponding to the local excitation \( 0 \rightarrow 1 \) of the unoccupied sites (figure 3(d)). In order to study trends in the spectral weight at zero frequency \( \omega = 0 \), we introduce the spectral weight measure

\[
\rho_0 \equiv \frac{1}{2} (|A_{\text{loc}}(\omega = \delta)| + |A_{\text{loc}}(\omega = -\delta)|),
\]

where \( \delta = 0.002U \). As shown in figure 3(a), in this first regime of the Bose glass, the spectral weight \( \rho_0 \) for finite hopping is very close to the atomic limit result. In fact, the spectral function (figure 3(d)) only differs from the atomic limit result at the edges of the upper Hubbard band, corresponding to the excitation \( 1 \rightarrow 2 \), indicating a strong localization around empty sites with large values of \( \eta_l \).

The situation changes abruptly for \( D \gtrsim U - \mu \ (D/J \gtrsim 84) \). As doubly occupied sites are activated by the disorder (see figure 2(d)), the density increases (figure 2(a)), and so does the kinetic energy (figure 2(b)), indicating an increase of non-local kinetic processes. The additional doublons lead to a substantial increase in interaction energy (figure 2(c)), which dominates over the kinetic energy. One would therefore naively expect a better agreement between the spectral functions computed with SFA3 and in the atomic limit. This is however not the case for the spectral weight around zero frequency \( \rho_0 \) which increases abruptly at \( D/J \approx 84 \), see figure 3(a), deviating markedly from the atomic limit prediction. The appearance of doubly occupied sites in the atomic limit drives additional excitations \((2 \rightarrow 1)\) and \((2 \rightarrow 3)\) in the spectral function (figure 3(e)), which overlap with other excitations, leading to additional ‘bands’ composed of multiple resonating excitations, see e.g. \((1 \rightarrow 0, \ 2 \rightarrow 1)\) at low negative frequencies in figure 3(e).

It is at the edges of these new ‘bands’ that the spectral function is strongly peaked showing a considerable difference with respect to the atomic-limit spectral function, indicating delocalization of quasi-particles and quasi-holes in the vicinity of the rare sites with occupation \( n > 1 \) (i.e. occupation 2 in the atomic limit). However, in the Bose glass discussed here, there is no global superfluid response, as the sites contributing to these peaks are rare. Instead the physics is described by the notion of isolated superfluid lakes [21] around rare sites with particularly low local potential.

In this regime (denoted by the gray area in figure 2), the non-local Green’s function of SFA3 develops a simple pole at zero Matsubara frequency, which can be integrated out when computing local quantities such as the local Green’s function, see appendix F for details. Whence, the self-energy functional and local observables can still be evaluated in this regime. In a homogeneous system, such a pole would indicate an instability towards
spontaneous $U(1)$-symmetry breaking and the particles would condense. Here, however, it is only the rare sites with $n > 1$ that contribute to the pole, not allowing for a global condensate. The pole therefore implies the presence of isolated quasi-condensates on the lattice, which can have different condensate density $\rho$ (inset, rescaled by $10^8$) as a function of $U/J$ computed with SFA3 (red), QMC (black squares), and in the atomic limit (blue dashed). (b) Spectral weight around $\omega = 0$, $\rho_{\omega}$ (see equation (73)), as a function of $U/J$ computed with SFA3 (red) and in the atomic limit (blue dashed). The vertical dashed line indicates the phase transition between the superfluid and the Bose glass phase in SFA3.

Figure 4. Strongly-interacting superfluid to Bose glass phase transition at $D/J = 100$, $\mu/U = 0.25$, and $T/J = 0.1$. (a) Density $n$ and condensate density $\rho$ (inset, rescaled by $10^8$) as a function of $U/J$ computed with SFA3 (red), QMC (black squares), and in the atomic limit (blue dashed). (b) Spectral weight around $\omega = 0$, $\rho_{\omega}$ (see equation (73)), as a function of $U/J$ computed with SFA3 (red) and in the atomic limit (blue dashed). The vertical dashed line indicates the phase transition between the superfluid and the Bose glass phase in SFA3.
the correction of the density with respect to the atomic limit close to the phase transition are extremely low (with a condensate density on the order of $10^{-4}$, see inset of figure 4(a)).

At density $n \approx 1$ and larger disorder strength, the increase of highly occupied sites is compensated by a proliferation of empty sites (see e.g. figure 2(d)). Thus, the probability of having neighboring sites with resonating low-energy excitations decreases, making the spontaneous breaking of $U(1)$-symmetry less likely. The increased interaction energy and particle number fluctuations therefore suppress the superfluid phase, explaining the reentrant behavior of the superfluid finger at larger disorder (see figure 1).

4.3. Superfluid phase

We now turn to lower interactions, i.e., deeper into the superfluid phase away from the superfluid finger. If $U/J$ is lower than the critical value of the clean system, the condensate density is much larger than in the superfluid finger, and the uncondensed background is no longer well described by the atomic limit.

In figure 5 we show a sweep of the thermodynamical observables as a function of $D/J$ deep in the superfluid phase at $U/J = 20$ and $\mu/U = 0.35$. At low disorder SFA3 shows excellent agreement with QMC, as the condensate density increases and the density decreases as a function of disorder (figure 5(a)). As a consequence of the larger condensate fraction, the magnitude of the kinetic energy increases as well (figure 5(b)). The interaction energy increases throughout the entire parameter range $0 \leq D/J \leq 25$, indicating increasing spatial particle number fluctuations (figure 5(c)).

When the disorder becomes comparable to the single-particle bandwidth $W = 2J$, these fluctuations reverse the trend of the condensate density which starts to decrease as a function of $D/J$. It is at this point that also the kinetic energy starts to decrease and the non-local connected Green’s function develops a pole at zero Matsubara frequency (see appendix F). As in the Bose glass (see section 4.1), the pole indicates the appearance of additional isolated quasi-condensates in the system: this is most likely related to the disorder inducing rare regions, explaining the decrease in condensate density and kinetic energy, and leading to a glassy behavior in the superfluid.

Eventually, deeper in the glassy regime of the superfluid where the disorder dominates over both the interaction and the single-particle bandwidth, our SFA3 approach of having translationally invariant variational parameters on the reference system becomes too simple to fully capture the groundstate behavior. In fact, the SFA3 results start to deviate from the QMC results, see figure 5(a). As shown in figure 5(d), eventually at
$D/J \approx 2W$ the variational parameters of the stationary SFA3 solution join with a metastable solution with higher free energy through a saddle-node bifurcation [60], vanishing for larger disorder.

A possibility to get around this problem, may be the introduction of a spatially modulated symmetry breaking field on the reference system, as was also done in stochastic mean-field theory [26, 27]. In SFT, this would however involve the inversion of a non-translationally invariant connected Green’s function, limiting us to very small system sizes, while we here want to analyze the thermodynamic limit.

5. Conclusion

In this work, we generalized the bosonic SFT to include quenched disorder. The derived formalism is a general framework for constructing non-perturbative approximations of disordered interacting bosonic lattice systems incorporating spontaneous $U(1)$-symmetry breaking. We showed that the resulting SFT functional depends only on the self-energies of the disorder-averaged interacting one- and two-point propagator, the condensate, and connected Green’s function, respectively. The lattice self-energies can then be parametrized by the self-energies of a simpler exactly solvable reference system having the same interaction and disorder distribution as the original system. The resulting formalism is a general non-perturbative approach that contains disorder-averaged bosonic DMFT as a certain limit.

We applied SFT in combination with a simple SFA3 reference system, consisting of a single bosonic mode with only three variational parameters, to the BHm with local box disorder. The SFA3 results were compared to numerically exact path integral QMC results and analytic calculations in the atomic limit.

Our results in the strongly-interacting regime close to unit filling, showing excellent agreement with QMC, indicate that the Bose glass phase is characterized by different regimes as a function of the disorder strength $D$. With increasing $D$, sites with local occupations $n = 1$ appear as predicted by the atomic limit, leading to crossovers between different regimes whenever a new local occupation $n$ is activated by the disorder. While QMC has to resort to analytic continuation in order to compute dynamical quantities, through SFT we were able to compute spectral functions within SFA3 directly.

By systematically analyzing the local spectral function we observed that the bosons delocalize into superfluid lakes around highly occupied sites whenever these are particularly rare. In particular, we found that the transition from the strongly-interacting Bose glass to the strongly-interacting superfluid phase (which extends to values of the interaction which are much larger than in the clean system) is driven by the percolation of superfluid lakes which form around doubly occupied sites, leading to a small condensate fraction over a strongly localized background. As $D$ is further increased and the density of doublons increases accordingly, the particles are localized by the strongly interacting background, explaining the reentrant behavior of the superfluid phase.

Due to the extremely low condensate fraction in the strongly-interacting superfluid, even though the numerical error is small, the phase boundaries observed with SFA3 are shifted with respect to the QMC results. Deeper in the superfluid phase (i.e. at lower interactions), our SFT results show excellent agreement with the QMC data as long as the disorder is smaller or comparable to the non-interacting bandwidth. In the strongly-disordered weakly-interacting regime, however, the restricted variational subspace of the SFA3 reference system employed in this work is no longer capable to find a stationary solution.

As opposed to QMC, SFT does not suffer from a general sign problem in the presence of e.g. gauge fields [61–63], or other complex Hamiltonian terms such as spin-orbit coupling [64–66]. The formalism derived in this work therefore represents a promising tool for future studies of such complex systems in the presence of disorder. In particular, an extension to real-time dynamics, as has been done for disorder-free fermionic systems [67, 68], seems a promising route to study the elusive physics of many-body-localized systems and is left for future work.

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Appendix A. Derivation of the disorder-averaged self-energy functional

In order to construct approximations using the disorder-averaged propagators we now seek a functional that is equal to the disorder average of the self-energy functional $(\hat{1}_{\text{pert}} | \mathbf{S}_n, \Sigma_n | \hat{1}_{\text{pert}})$ but that is defined in the extended
space of both averaged and explicit self-energies $S$, $\Sigma$, $\{S_\eta, \Sigma_\eta\}$ and stationary at the physical solution in all self-energies.

An ansatz that fulfills equality at the physical self-energies is equation (32). Repeated application of the Dyson equations (equations (27) and (14)) in equation (33) at the physical self-energies gives

$$
\tilde{T}_P[\tilde{S}_{FPV}, \tilde{\Sigma}_{FPV}, \{S_{FPV}, \Sigma_{FPV}\}] = \frac{1}{2} \left( F - \tilde{S}_{FPV} \right) G_{00} \left( F - \tilde{S}_{FPV} \right)
$$

and therefore

$$
\tilde{F}^{(SE)}_{FPV}[\tilde{S}_{FPV}, \tilde{\Sigma}_{FPV}, \{S_{FPV}, \Sigma_{FPV}\}] = \langle \tilde{F}^{(SE)}_{FPV}[\tilde{S}_{FPV}, \tilde{\Sigma}_{FPV}, \{S_{FPV}, \Sigma_{FPV}\}] \rangle_P,
$$

whence the disorder-averaged self-energy functional gives the physical disorder-averaged free energy at stationarity. To show stationarity of $\tilde{F}^{(SE)}_{FPV}$ we consider the variations of the universal functional $\tilde{T}_P$

$$
\delta_S \tilde{T}_P = \langle \tilde{G}_{0p} \rangle_P + \langle \delta_S \tilde{h} \rangle_P + \langle \delta_S \tilde{h} \rangle_P \tilde{G}^{-1} + \Sigma \langle \delta_S \tilde{h} \rangle_P - \tilde{h}
$$

and therefore

$$
\delta_{\Sigma} \tilde{T}_P = \delta_{\Sigma} \tilde{T}_P = \frac{1}{2} \left( \tilde{h} \tilde{h}^\dagger + \frac{1}{2} \left( \tilde{h} \tilde{h}^\dagger \right)_P + \frac{1}{2} \langle \tilde{G} \rangle_P - \frac{1}{2} \tilde{G} \right)
$$

Using the definitions of the averaged propagators (equation (31)) this reduces to

$$
\delta_S \tilde{T}_P = \tilde{h}, \quad \delta_{\Sigma} \tilde{T}_P = -\frac{1}{2} \left( \tilde{h} \tilde{h}^\dagger + \frac{1}{2} \left( \tilde{h} \tilde{h}^\dagger \right)_P + \frac{1}{2} \langle \tilde{G} \rangle_P - \frac{1}{2} \tilde{G} \right)
$$

where

$$
Q_\eta \equiv S + \frac{1}{2} \tilde{G}^{-1} + \Sigma \tilde{h} - \eta \tilde{h}
$$

The term $Q_\eta$ corresponds to $Q_\eta = F - F = 0$ when the one-point Dyson equations (equations (27) and (14)) are fulfilled. Hence, the $\delta \tilde{h}$ variations in equations (A.7) and (A.8) vanish at stationarity (i.e. at the physical self-energies).

Appendix B. Canceling functional derivatives of $\tilde{T}_P$

At stationarity the expression of the $\tilde{T}_P$ functional in equation (A.1) contains expressions in terms of $G_{00}$ and $F$, so one might wonder if there is no implicit dependence on the free propagators of the system. In order to check that this is not the case, we rewrite equation (A.1) in terms of $G_{00}$ and $F$ as
\[
\hat{T}_{PV}[\mathbf{S}_{PV}], \Sigma_{PV}, \{\mathbf{S}_{F_{PV}}, \Sigma_{F_{PV}}\}] = \frac{1}{2} (\text{Tr} \ln [(\mathbf{G}^{-1}_{00} - \mathbf{1})])_P - \frac{1}{2} (F - \mathbf{S}_{PV})^\dagger \mathbf{G}_{00}(F - \mathbf{S}_{PV})
\]

The variation in \(\mathbf{G}_{00}\) yields

\[
\frac{\delta \hat{T}_{PV}[\mathbf{S}_{PV}], \Sigma_{PV}, \{\mathbf{S}_{F_{PV}}, \Sigma_{F_{PV}}\}]}{\delta \mathbf{G}_{00}} = \frac{1}{2} (\text{Tr} \mathbf{G}_{00}^{-1} \mathbf{G}_{00}^{-1})_P - \frac{1}{2} (F - \mathbf{S}_{PV})^\dagger \mathbf{G}_{00}(F - \mathbf{S}_{PV})_P
\]

which by the short-hand notations introduced in equations (26) and (31) can be rewritten as

\[
\frac{\delta \hat{T}_{PV}[\mathbf{S}_{PV}], \Sigma_{PV}, \{\mathbf{S}_{F_{PV}}, \Sigma_{F_{PV}}\}]}{\delta \mathbf{G}_{00}} = \frac{1}{2} \text{Tr} (\mathbf{G}_{00})_P - \frac{1}{2} (\Phi_\eta^\dagger \Phi_\eta)_P
\]

where we have used that the trace and the arithmetic average commute, i.e. \(\frac{1}{2} (\text{Tr} \mathbf{G}_{00}) = \frac{1}{2} \text{Tr} (\mathbf{G}_{00})_P\). Note that — as opposed to the geometrical average — the geometrical average used in the context of fermionic DMFT [36–39] would not commute with the trace operator \(\text{Tr}\) in equation (B.3) and therefore break the universality of the functional \(\hat{T}_{PV}\). As pointed out in [51] for fermions, the geometrical average introduced in DMFT, therefore appears to be incompatible with SFT.

The variation of \(\hat{T}_{PV}\) in \(F\) yields

\[
\frac{\delta \hat{T}_{PV}[\mathbf{S}_{PV}], \Sigma_{PV}, \{\mathbf{S}_{F_{PV}}, \Sigma_{F_{PV}}\}]}{\delta \mathbf{F}^\dagger} = \mathbf{G}_{00}(F - \mathbf{S}_{PV}) - (\mathbf{G}_{00}(F - \mathbf{S}_{PV}))_P
\]

which using equation (31) can be rewritten as

\[
\frac{\delta \hat{T}_{PV}[\mathbf{S}_{PV}], \Sigma_{PV}, \{\mathbf{S}_{F_{PV}}, \Sigma_{F_{PV}}\}]}{\delta \mathbf{F}^\dagger} = \Phi - (\Phi_\eta)_P = 0.
\]

\(\hat{T}_{PV}\) is therefore completely independent of both \(F\) and \(\mathbf{G}_{00}\) also at stationarity.

**Appendix C. Disorder-averaged bosonic dynamical mean-field theory (BDMFT) limit**

Disorder-averaged SFT for bosons has disorder-averaged BDMFT as a certain limit. In its simplest form, disorder-averaged BDMFT is restricted to site-local disorder \(\eta\) and site-local interaction \(\hat{V}\).

In this case, disorder-averaged BDMFT is obtained from SFT by restricting the reference systems free propagator to be site-local, i.e.

\[
\Delta_{ij}^{(n)}(\tau, \tau') = \delta_{ij}[\Delta_{ij}^{(n)}(\tau, \tau')],
\]

where \(i, j\) are the site-, and \(\nu, \nu'\) the Nambu indices. The imaginary time retardation in \(\Delta(\tau, \tau')\), however, remains completely general.

The reference systems local bare propagator \(\mathbf{G}_{\Delta_{00}}\) and interaction give rise to a purely local self-energy

\[
[\mathbf{\Sigma}_{\nu, \nu'}^{\Delta_{00}}]_{ij} = \delta_{ij}[\mathbf{\Sigma}_{\nu, \nu'}^{\Delta_{00}}]_{ij}, \quad \mathbf{[\Sigma}_{\nu, \nu'}^{\Delta_{PV}}]_{ij} = \delta_{ij}[\mathbf{\Sigma}_{\nu, \nu'}^{\Delta_{PV}}]_{ij},
\]

and the self-energy variations of \(\hat{T}_{PV}^{\text{(SFT)}}\) (equations (45) and (46)) reduce to the disorder-averaged BDMFT self-consistency conditions

\[
\mathbf{G}_{\Delta_{00}}(F' - \mathbf{S}_{\Delta}) - \mathbf{G}_{00}(F - \mathbf{S}_{\Delta}) = \mathbf{G}_{00}[(\mathbf{G}_{00}^{-1} - \mathbf{G}_{\Delta_{00}}^{-1}) \Phi_{\Delta} + F' - F] = 0,
\]

\[
[(\mathbf{G}_{\Delta_{00}}^{-1})_{ii} - \mathbf{\Sigma}_{\nu, \nu'}^{\Delta_{00}}]^{-1} - [\mathbf{G}_{00}^{-1} - \mathbf{\Sigma}_{\nu, \nu'}^{\Delta_{PV}}] = 0,
\]

which can be fulfilled exactly by the retarded \(\Delta(\tau, \tau')\), and can be simplified to

\[
\hat{G}_{\nu} = \hat{G}_{\Delta_{PV}}, \quad \Phi = \Phi_{\Delta_{PV}},
\]

where \(\Phi\) and \(\hat{G}_{\nu}\) are the disorder-averaged condensate and local connected Green’s function of the lattice, while \(\Phi_{\Delta_{PV}}\) and \(\hat{G}_{\Delta_{PV}}\) are the disorder-averaged condensate and connected Green’s function of the reference
system. This is therefore the standard BDMFT self-consistency condition of clean systems [33, 34], where the propagators of the clean system have been replaced by their disorder-averaged counterparts, which for the case of uncorrelated disorder discussed in appendix D are translationally invariant.

Appendix D. Uncorrelated disorder: translational invariance of the arithmetic average

In the following we will specialize the formalism derived in section 2 by assuming that the disorder is distributed according to an uncorrelated and translationally invariant probability distribution, i.e.

\[ P(\eta) = \prod_{i,j} p_{i-j}(\eta_{i,j}), \quad (D.1) \]

where the product goes over all site-indices \( i, j \), and the distribution \( p_{i-j} \) depends only on the relative distance between the sites \( i \) and \( j \). As we will see this enables us to simplify the reference system considerably due to the translational invariance of disorder-averaged observables.

The interacting propagators at a given disorder configuration \( \eta \) can be computed directly by

\[ G^{\Delta \eta}_{F}(\tau - \tau') = - \langle \mathbf{b}(\tau) \mathbf{b}^{\dagger}(\tau') \rangle_{\eta} + \langle \mathbf{b}^{\dagger}(\tau) \mathbf{b}(\tau') \rangle_{\eta}, \quad \Phi^{\Delta \eta}_{F} = \langle \mathbf{b}^{\dagger} \rangle_{\eta}, \quad (D.2) \]

where \( \mathcal{T} \) is the time-ordering operator and \( \langle \ldots \rangle_{\eta} \) means taking the expectation value with respect to the reference system with disorder configuration \( \eta \).

Using equation (D.2) further enables the computation of the fixed-disorder self-energies through equation (14). The propagators \( G^{\Delta \eta}_{F}, \Phi^{\Delta \eta}_{F} \), and the corresponding self-energies \( S^{\Delta \eta}_{F}, \Sigma^{\Delta \eta}_{F} \), are not translationally invariant and can therefore be very hard to handle numerically.

If we now assume that we average over an infinite number of disorder configurations, the reference system’s propagators will be translationally invariant, since due to the translational invariance of the uncorrelated disorder probability distribution of equation (D.1) all values \( \eta_{ij} \) will occur with the same weights for each pair of sites \( (i, j) \) with the same distance \( i - j \), i.e.

\[ G^{\Delta \eta}_{F}\left( x_{i}, x_{j}, \tau - \tau' \right) = G^{\Delta \eta}_{F}(x_{i} - x_{j}, \tau - \tau'), \quad (D.3) \]

with a translationally invariant condensate

\[ \Phi^{\Delta \eta}_{F}(x_{i}) = \Phi^{\Delta \eta}_{F}(x_{i}), \quad (D.4) \]

According to equation (14) this implies that also the average self-energies will be translationally invariant with

\[ \Sigma^{\eta}_{F}(i \omega, k) = G^{-1}_{D}(i \omega, k) - G^{-1}_{D}(i \omega, k) \Phi^{\eta}_{F}(i \omega, k), \quad (D.5) \]

and

\[ S^{\eta}_{F}(x_{i}) = F(x_{i}) - G^{-1}_{D}(i \omega, k = 0) \Phi^{\eta}_{F}(x_{i}) = S^{\eta}_{\Delta}(x_{i}), \quad (D.6) \]

Finally, \( \Omega^{\eta}_{F\rho} = \langle \Omega^{\eta}_{F\rho} \rangle_{\rho} \) can be computed directly from averaging over the fixed-disorder systems.

As no fixed-disorder quantities are needed in order to evaluate the functional in equation (47), the evaluation of the self-energy functional has now the same complexity as the disorder-free case of [48], where the self-energies and propagators were translationally invariant by definition. The only difference lies in the treatment of the reference system, which has to be averaged over all disorder configurations \( \eta \).

Appendix E. Lattice observables

Once a stationary solution fulfilling equation (52) has been found, the corresponding lattice observables can be computed using the self-energies

\[ \Sigma_{\eta} \approx \Sigma^{\eta}_{F\eta}, \quad S_{\eta} \approx S^{\eta}_{F\eta}, \quad \Sigma \approx \Sigma^{\eta}_{\Delta}, \quad S \approx S^{\eta}_{\Delta}, \quad (E.1) \]

In particular, the disorder-averaged propagators \( G \) and \( \Phi \) can be computed using the self-energies \( \Sigma \) and \( S \) and the free propagator \( G_{0\rho} \) in the Dyson equations of equation (14). The fix-disorder propagators \( G_{\eta \rho} \) and \( \Phi_{\eta \rho} \), on the other hand, can be computed using \( \Sigma_{\eta} \) and \( S_{\eta} \) and the free propagator \( G_{0\rho} \) in equation (14). As the latter are not translational invariant, however, they can only be computed on a finite-sized lattice, as equation (14) requires the inversion of a matrix in position space. It is therefore preferable to use the translationally invariant averaged propagators \( G \) and \( \Phi \) in the thermodynamic limit.

As the arithmetic averaging is a linear operation, disorder-averaged observables of the lattice system which can be expressed as linear terms of one- and two-point quantities without any disorder-dependent prefactors, can be directly evaluated from the average propagators \( \Phi \) and \( G \). This is trivially the case for the disorder-averaged condensate through equation (31), while for the particle density we have
where we have used equation (31) in the last step and the same definition of the trace operator \( \text{Tr} \) as in [48]. The same is true for the kinetic energy
\[
E_{\text{kin}} = \frac{1}{2L} \langle \text{Tr}[g(i\omega_n - \Phi^\dagger \Phi)] \rangle_p = \frac{1}{2L} \langle \text{Tr}[g_\eta] \rangle_p + \langle \Phi^\dagger \Phi \rangle_p.
\]
(E.2)

The interaction energy, on the other hand, cannot be directly evaluated from the averaged propagators as [48]
\[
E_{\text{int}} = \frac{1}{L} \sum_i \langle (n_i^2 - n_i) \rangle_p = -\frac{1}{4L} \langle \text{Tr}[\Sigma_\eta G_\eta] \rangle_p \approx -\frac{1}{4L} \langle \text{Tr}[\Sigma G] \rangle.
\]
(E.4)

However, as the SFT functional is equal to the free energy at stationarity, we have direct access to the disorder-averaged free energy of the lattice \( \Omega_{\text{p}PV} \), from which we can compute the interaction energy by the numerical derivative
\[
E_{\text{int}} = \frac{U}{L} \frac{\partial \Omega_{\text{p}PV}}{\partial U}.
\]
(E.5)

Appendix F. Poles in the connected Green’s function

The arithmetically averaged connected Green’s function of the lattice, \( \tilde{G} \), depends on momentum \( k \) only through the non-interacting dispersion \( \epsilon_k \) and can thus be parametrized in the single-particle energy \( \epsilon \) as \( \tilde{G}(i\omega_n, \epsilon) = \tilde{G}(i\omega_n', \epsilon = \epsilon_k) \). In terms of a local disorder-averaged self-energy \( \Sigma \) (such as the one used in the SFA3 reference system) it can be written as
\[
\tilde{G}(i\omega_n, \epsilon) = [\sigma^2(i\omega_n + (\mu - \epsilon))I - \Sigma(i\omega_n)]^{-1}.
\]
(F.1)

The inversion in equation (F.1) results in simple poles of \( \tilde{G} \) whenever \( \det[\tilde{G}^{-1}(i\omega_n, \epsilon)] = 0 \), i.e., when
\[
\epsilon = \mu - \text{Re} \left[ \Sigma_{00}(i\omega_n) \right] = A[\Sigma, i\omega_n] \equiv e^p (i\omega_n),
\]
(F.2)

where \( A[\Sigma, i\omega_n] = \sqrt{[\Sigma_{00}(i\omega_n)]^2 - \omega_n^2} - \text{Im} \left[ \Sigma_{00}(i\omega_n) \right]^2 \) and \( \Sigma_{ij} \) are the Nambu-components of the \( 2 \times 2 \) local self-energy. In other words, the lattice Green’s function \( \tilde{G} \) develops a pole if for some \( i\omega_n \)
\[
\min_k \epsilon_k \leq e^p (i\omega_n) \leq \max_k \epsilon_k,
\]
(F.3)

while the determinant of \( \tilde{G} \) can be expressed as
\[
\det[\tilde{G}^{-1}(\epsilon, i\omega_n)] = (\epsilon - e^p (i\omega_n)) (\epsilon - e^{-p} (i\omega_n)).
\]
(F.4)

In the absence of \( U(1) \) symmetry breaking \( \Sigma_{00}(i\omega_n) = 0 \), and \( \tilde{G} \) can only have a simple pole at \( i\omega_n = 0 \), since \( e^p (i\omega_n) = e^p (i\omega_n) \) and \( A[\Sigma, i\omega_n] = 0 \) is always imaginary. In the superfluid phase, where \( |\Sigma_{00}(i\omega_n)| > 0 \), the poles \( e^p \) of \( \tilde{G} \) can be located at any Matsubara frequency.

However, the superfluid SFT groundstates we observe only develop simple poles at zero frequency (in specific parameter ranges). This happens in the superfluid phase for strong disorder \( D \gtrsim W \) and in the Bose glass phase close to the superfluid phase boundary, see the gray regions in figures 2 and 5. In the clean system, such a pole signals an instability towards \( U(1)-\)symmetry breaking and arises only in the metastable Mott insulator phase. In the case studied here, which is no longer homogeneous, as discussed in section 4, the pole is related to the appearance of isolated quasi-condensates on the lattice.

Remarkably, although the poles make non-local quantities such as, e.g., \( n_k = -\sum_n \text{Tr} \tilde{G}(i\omega_n, k) / 2\beta \) diverge at certain values of \( k \), the pole can be treated semi-analytically in the computation of local quantities, as we will show in the following.

The central quantity where the lattice Green’s function enters in the SFT functional of equation (47) is the trace-log term \( \text{Trln}[\tilde{G}^{-1}] \), which—as shown in [48]—is only defined up to a regularization factor \( C_\infty \) and can be evaluated as
\[
\frac{1}{2} \text{Trln}[\tilde{G}^{-1}] = C_\infty = \ln \left[ \frac{\det \sqrt{-\tilde{G}^{-1}}}{\det \sqrt{-R^{-1}}} \right].
\]
(F.5)
where $R$ is the regularization function

$$
R(\omega_n) = \begin{cases} 
-i\sigma_\epsilon/\omega_n & n \neq 0, \\
-\beta 1, & n = 0.
\end{cases}
$$

By $\text{Tr} \ln [-\tilde{G}^{-1}] = \text{Tr} \ln [-\tilde{G}^{-1}]/4$, we therefore can evaluate the trace-log term as

$$\frac{1}{2} \text{Tr} \ln [-\tilde{G}^{-1}] - C_\infty = \frac{1}{4} \sum_n \int d\epsilon \ D(\epsilon) \ln [Q(\omega_n) \det [\tilde{G}^{-1}(\epsilon, \omega_n)]^2],$$

(7)

where $D(\epsilon)$ is the single-particle density of states, and $Q(\omega_n)$ is the regularization function

$$Q(\omega_n) = \begin{cases} 
\omega_n^\beta & n \neq 0, \\
\beta^{-4}, & n = 0.
\end{cases}
$$

In order to evaluate the integral in equation (7) numerically, the dispersion is discretized on the energy grid $\epsilon = \epsilon_m$. Using the linear interpolation

$$\tilde{D}_m(\epsilon) = \frac{D(\epsilon_{m+1}) - D(\epsilon_m)}{\epsilon_{m+1} - \epsilon_m} \epsilon + D(\epsilon_m),$$

(9)

of the density of states, and inserting the explicit expression for the determinant from equation (4) gives

$$\int d\epsilon D(\epsilon) \ln [Q(\omega_n) \det [\tilde{G}^{-1}(\epsilon, \omega_n)]^2] \approx \sum_m \int_{\epsilon_m}^{\epsilon_{m+1}} d\epsilon \ I_m(\epsilon, \omega_n),$$

(10)

where the integrand is given by

$$I_m(\epsilon, \omega_n) \equiv \tilde{D}_m(\epsilon) \ln [Q(\omega_n)(\epsilon - \epsilon^F(\omega_n))^2(\epsilon - \epsilon^F(\omega_n))^2].$$

(11)

If the interval $[\epsilon_m, \epsilon_{m+1}]$ does not contain the poles $\epsilon^F(\omega_n)$, the $m$th summand of equation (10) can be straight-forwardly integrated analytically. Also in the presence of a pole, $\epsilon_m < \epsilon^F < \epsilon_{m+1}$, this term is integrable, and can be computed analytically by dividing the interval into two pieces as

$$\int_{\epsilon_m}^{\epsilon_{m+1}} d\epsilon \ I_m = \int_{\epsilon_m}^{\epsilon^F} d\epsilon \ I_m + \int_{\epsilon^F}^{\epsilon_{m+1}} d\epsilon \ I_m.$$

(12)

Also in the presence of poles (i.e. quasi-condensates) in the connected Green’s function, the SFT functional therefore remains well-defined.

A central local observable that is directly computed from $\tilde{G}$ is the density per site $n$, given by equation (2) and thereby by the sum

$$n = -\frac{1}{\beta} \sum_n \int d\epsilon D(\epsilon) G_{00}(\omega_n, \epsilon) \approx -\frac{1}{\beta} \sum_{n,m} \int_{\epsilon_m}^{\epsilon_{m+1}} d\epsilon \ {\tilde{D}_m}(\epsilon) G_{00}(\omega_n, \epsilon),$$

(13)

where in the last step we have used equation (9). Using equation (4) the Green’s function component $G_{00}$ can be expressed as

$$G_{00}(\omega_n, \epsilon) = \frac{\omega_n - \epsilon + \mu - \tilde{S}_{00}(\omega_n)}{(\epsilon - \epsilon^F(\omega_n))(\epsilon - \epsilon^F(\omega_n))},$$

(14)

Again, if $[\epsilon_m, \epsilon_{m+1}]$ does not contain $\epsilon^F(\omega_n)$, the $m$th summand of equation (13) can be integrated analytically. If a pole $\epsilon^F$ is present, the expression (13) is an integral over a simple pole, which however can be integrated analytically using the limit

$$\int_{\epsilon_m}^{\epsilon_{m+1}} d\epsilon \ {\tilde{D}_m}(\epsilon) G_{00}(\epsilon, \omega_n) = \lim_{\gamma \to 0} \left(\int_{\epsilon^F + \gamma}^{\epsilon_{m+1}} d\epsilon + \int_{\epsilon_m}^{\epsilon^F - \gamma} d\epsilon \right) \{\tilde{D}_m(\epsilon) G_{00}(\epsilon, \omega_n),$$

(15)

which ensures that the two divergent parts of the integrals cancel each other out, giving a finite result.

The same procedure can also be applied when computing the kinetic energy, which by equation (3) is given by

$$E_{\text{kin}} = -\frac{1}{\beta} \sum_n \int d\epsilon D(\epsilon) \epsilon G_{00}(\omega_n, \epsilon),$$

(16)

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