Many-site coherence revivals in the extended Bose-Hubbard model and the Gutzwiller approximation

Uwe R. Fischer and Bo Xiong
Seoul National University, Department of Physics and Astronomy
Center for Theoretical Physics, 151-747 Seoul, Korea

We investigate the collapse and revival of first-order coherence in deep optical lattices when long-range interactions are turned on, and find that the first few revival peaks are strongly attenuated already for moderate values of the nearest-neighbor interaction coupling. It is shown that the conventionally employed Gutzwiller wavefunction, with only onsite-number dependence of the variational amplitudes, leads to incorrect predictions for the collapse and revival oscillations within the extended Bose-Hubbard model. We provide a modified variant of the Gutzwiller ansatz, reproducing the analytically calculated time dependence of first-order coherence in the limit of zero tunneling.

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I. INTRODUCTION

The Hubbard model describes interacting particles in sufficiently deep periodic lattice potentials, so that the tight-binding approach applies, and the Wannier functions form the basis of the bosonic or fermionic field operator expansion \[ [1] [3]. It was realized about a decade ago that in optical lattices, generated by counterpropagating laser beams, a clean and highly controllable implementation of the Hubbard model can be obtained [4]. Initially, attempts to achieve a precise understanding of the collective behavior of atoms or molecules trapped in the lattice was concentrated on the classic version of the model with onsite interactions only. However, a zoo of quantum phases beyond the superfluid and Mott phases, like various supersolid and charge-density wave phases, emerges when long-range interactions are turned on [5]. The most prominent and (for electrically neutral atoms/molecules) physically realizable examples of the latter are magnetic and electric dipole-dipole interactions [6]. The so-called extended Hubbard model which incorporates the long-range character of the interactions [7]. It is crucial for the determination of possible phases to obtain information on the interaction parameter values in the extended Bose-Hubbard model, and we suggest, in the following, experimental means to measure them by using the temporal variations of first-order coherence.

Collapse and revival oscillations are familiar from quantum optics [8] as a sensitive measure for the spectrum of the Hamiltonian and the many-body dynamics of the system. In ultracold bosonic quantum gases, collapse and revival oscillations were experimentally observed both on the two- and multi-body interaction level [8] [10], when switching quasi-instantaneously from the superfluid to the Mott side in a dynamical quantum phase transition, a quench [11]. Rapid experimental progress in the meantime even allows for the single-site and single-atom resolution of the time evolution of the site occupation number [12] [13].

In the optical lattice realization of collapse and revival of coherence, effectively many small samples on the various sites are prepared, which are independent of each other when only contact interactions are present. When the particle numbers in individual sites are small, i.e. at small filling, the revival times are short enough for observing the collapse and revival phenomenon [14]. The collapse and revival times have in addition been demonstrated to be sensitive to the effective dimension of a single well and its trap power law [14].

It has been previously shown that a sensitive measure of the many-body dynamics due to collapse and revival dynamics in optical lattices may be experimentally accessible when tunneling across different sites is included [16] [18]. Furthermore, significant effects on collapse and revival can be expected when effective three-body interactions [19] as well as the number squeezing of an initial state with finite interactions on the superfluid side are taken into account [20]. In addition, the number squeezing of an initial state can be caused by finite sweep rates, when quenching from the superfluid to the localized Mott phase [21].

We explore in the following effects which are intrinsically beyond the familiar purely onsite collapse and revival evolution in optical lattices and come from long-range interactions (that is not those, e.g., coming from an additional external confinement potential [22]). The extended Hubbard model provides nearest-neighbor (NN) coupling of sites on the two-body interaction level, so that the Hamiltonian converts the onsite phenomenon collapse and revival obtained for contact interactions into a genuine many-body–many-site effect. We demonstrate that an attenuation of the first few phase coherence revivals takes place in a range of the ratio of onsite and NN interaction couplings relevant to the predicted quantum phases of the extended Bose-Hubbard model [5] [23]. It is shown that, as opposed to the reduction of the coherence signal by the (phase-sensitive) tunneling term in the Hamiltonian, no real damping takes place due to a NN interaction coupling, instead there are two distinct revival scales related to onsite and NN interaction couplings \( U \) and \( V \), respectively. The consequent effective attenuation of the first few revival peaks due to \( V \) is...
much stronger than those to tunneling damping, increasing with filling rather than decreasing, and can easily overcome inhomogeneity (external trapping) effects. We therefore propose a sensitive measure of the value of \( V \) realizable in current optical lattice experiments.

The modulation of the first-order coherence signal with frequency \( V/h \), taking as in Sec. II below a coherent product state as the initial state after a quench into a deep lattice, does not occur in the conventional time-dependent Gutzwiller approach. This approach employs a product state of purely onsite-occupation dependent variational wavefunctions, and is indeed widely used for ground-state calculations in the extended Bose-Hubbard model, cf. e.g. [24, 26]. As we will show below, it however leads at least in dynamical situations (i.e. with explicit time dependence of correlation functions) to in general grossly incorrect predictions and hence needs modification. We will devise a variant of the Gutzwiller product state with the variational amplitudes depending on the NN-coupling-induced attenuation of the coherence signal will completely dominate the damping caused by residual tunneling.

II. COHERENT INITIAL STATE

The Hamiltonian of the single-band extended Bose-Hubbard model is assumed to be of the form

\[
\hat{H} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{V}{2} \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j
\]  

where \( \langle ij \rangle \) indicates summation over NN, and \( M \) is the number of lattice sites. We consider here the most general situation that the parameters \( J, U, V \) can be controlled independently of each other, e.g. by optical lattice depth and the ratio of contact and long-range interactions. Their values are determined by overlap integrals of Wannier functions incorporating single-particle energy operators and two-body interaction power laws and effective ranges, respectively. The two-body interaction terms correspond to density-density type interactions with on-site (\( U \)) and NN (\( V \)) parts.

We take in this section the initial state to be the product of onsite coherent (superfluid) states with Poissonian probability distribution of site occupation

\[
|SF\rangle = \prod_{i=1}^{M} e^{-|\alpha_i|^2/2} \sum_{n_i=0}^{\infty} \frac{\alpha_i^{n_i}}{\sqrt{n_i!}} |n_i\rangle
\]

where \( |n_i\rangle \) are local number eigenstates, \( \hat{n}_i |n_i\rangle = n_i |n_i\rangle \) and \( \hat{a}_i |\alpha_i\rangle = \alpha_i |\alpha_i\rangle \) with average \( \langle \hat{n}_i \rangle = \langle \hat{\alpha}_i \rangle = |\alpha_i|^2 \). Such a state is for example physically realizable with a quasi-instantaneous sweep across the superfluid–Mott transition starting from (deep inside) the superfluid phase, in which \( J \gg U, V \) [9, 10]. We note that finite \( M \) corrections due to a particle-number-conserving initial state and the resulting time evolution were investigated for the Bose-Hubbard model in [18]. However, they became negligible for a number of sites \( M \gtrsim 5 \), so that we can expect to be able to safely neglect them for sufficiently large \( M \) also with nonvanishing off-site interaction coupling.

The limits of either \( U \) and \( J \) being dominant over the other couplings are well known, and lead to the (deep) Mott phase (at commensurate filling in the present homogeneous case \( N/M = \bar{n} \) integer, where \( N \) is the total number of particles) and the superfluid phase of weakly noninteracting bosons, respectively. We choose \( U \equiv 1 \) as the unit of energy and \( 2\pi U \) as the unit of time (\( \hbar = 1 \)).

We first derive an analytical result for the exact time evolution of first-order coherence when \( J = 0 \) in [11]. Because the energy is expressible in the number (i.e. Fock space) basis when \( J = 0 \), the first order correlation function can be analytically determined. Calculating with the initial coherent product state [2] the off-diagonal elements of the single-particle density matrix, one obtains

\[
\langle SF | e^{iHt} \hat{a}_i^\dagger \hat{a}_j e^{-iHt} | SF \rangle = \prod_{l} \exp(-\bar{n}_l) \sum_{n_i, n_i'} \frac{\alpha_i^{n_i} \alpha_j^{n_i'}}{\sqrt{n_i! n_i'!}} \sqrt{n_i n_i'} \delta_{n_i-1, n_i} \delta_{n_j, n_j'} \exp \left[ i t (E_{n_i'} - E_{n_i}) \right]
\]

\[
= \alpha_i^{*} \alpha_j \prod_{k=i,j, NN} \exp[-\bar{n}_k] \sum_{n_i, n_j=0}^{\infty} \frac{\bar{n}_i^{n_i}}{n_i!} \frac{n_j^{n_j}}{n_j!} \sum_{n_l=0}^{\infty} \frac{\bar{n}_l^{n_l}}{n_l!} \exp \left[ i t U (n_i - n_j) + i t V \left( \sum_{|il|} n_l - \sum_{|jl|} n_j \right) \right]
\]

\[
= \bar{n} \exp[i\theta_{ij}] \exp \left[ 2\bar{n} (\cos[U t] - 1) \right] \exp \left[ 2\bar{n} v (\cos[V t] - 1) \right]
\]

where the site-occupation-dependent interaction energy reads \( E_{n_i} = \frac{U}{2} \sum_i n_i (n_i - 1) + \frac{V}{2} \sum_{\langle ij \rangle} n_i n_j \), and \([il]\)
and \([jl]\) indicate sums over all NNs \(l\) of \(i\) and \(j\) at fixed \(i\) and \(j\), respectively. We assume for simplicity in \([9]\) that \(|i − j| > 2\), for which the coherence signal becomes independent of distance \(|i − j|\) (expressions when \(|i − j| \leq 2\) can easily be derived as well). The last line is valid for homogeneous filling \(\bar{n}\). Finally, \(\nu\) is the number of NN, i.e. \(\sum_{[kl]} = \nu\), and \(\theta_{ij} = \arg[|\alpha_{i}|] − \arg[|\alpha_{j}|]\) describes a possible initial phase offset between sites.

A significant attenuation of the revival peaks occurs already for moderate values of \(V/U\), which exceeds the experimentally observed damping in the \(V \to 0\) (contact interaction) limit caused, e.g., by external trapping and finite temperature \([8, 10]\). Hence the presently obtained homogeneous system result should readily be observable in experiments like \([10]\), which aim at the minimization of external trapping (inhomogeneity) effects, and can sensitively detect even small dipole strengths of particles trapped in an optical lattice.

The attenuation of \(2\pi/U\) oscillations between revivals at \(2\pi/V\) increases with the product \(\bar{n}\nu\), cf. Fig. 1. We take as a measure of the attenuation the value of \(\Delta_V\) at the first onsite revival \(t_V = 2\pi/U\),

\[
\Delta_V = 1 − \exp\left[2\bar{n}\nu\left(\cos\left(\frac{2\pi V}{U}\right) − 1\right)\right]
\]  

\((5)\)

The overdamped limit corresponds to \(\Delta_V \to 1\). For small \(V/U\), the attenuation is given by \(\Delta_V = \bar{n}\nu(2\pi V/U)^2\).

We now compare our attenuation result \((4)\) above with the real damping of the revival amplitude due to single-particle tunneling coupling between sites. In contrast to the small \(J\) result \(\Delta_J = (2\pi J)^2 \left[\nu(2\nu − 1)e^{−4\pi J^2(2\bar{n})} + \nu e^{−36 J^2(1,1)(2\bar{n})}\right]\) (where \(I_0, F_{1,1}\) are modified Bessel and hypergeometric functions, respectively \([10]\)), the small \(V\) result from \([8]\) is linear in \(\nu\) instead of quadratic. More importantly, the \(J\) damping decreases exponentially with filling \(\bar{n}\), while the \(V\) attenuation effect increases with the filling. However, while \(J/U\) will be necessarily small in the Mott phase (it is exponentially decreasing with increasing laser intensity), \(V/U\) can be of order unity \([27]\), so that the effect of \(V\) can be very pronounced while that of \(J\) will be subdominant, cf. Fig. 3 below. For \(V > U\), the period of the first full-amplitude coherence revival is \(2\pi/V\) instead of \(2\pi/U\). When \(U/V\) is not a rational number, no full height revival occurs, and so-called fractional revivals are obtained instead \([8]\).

Due to the long-range nature and slow fall-off of the dipolar interaction with distance \(\propto 1/r^3\), the next-nearest and next-to-next-nearest neighbors etc. add other coupling terms of the form \(V_{NNNN}N\nu\sum_{i\neq j} \bar{n}_i \bar{n}_j\) to the Hamiltonian \([11]\), where \(\{ij\}\) indicates a sum over next-nearest neighbors and \(\lambda\) is their number, \(\sum_{i\neq j} = \lambda\) at fixed \(k\). Therefore, additional (slower) oscillation factors will be added in \([3]\). We take as a concrete example to illustrate this a 2D square lattice, with dipoles oriented perpendicular to the 2D plane. This geometry implies that the closest next-nearest neighbors are a distance \(\sqrt{2a}\) from a given site, such that the associated coupling \(V_{NNN}/V = 1/\sqrt{8}\), and the following next-to-next-nearest-neighbor sites at a distance \(2a\), giving a coupling \(V_{NNNN}/V = 1/8\). Therefore, while the revival at integer multiples of \(2\pi/V\) occurs with the full initial height when only nearest neighbors would be taken into account (i.e. for perfectly screened interactions at the NN distance), adding further next-nearest couplings, etc., makes the first full height revival peak occur much later. The full height revivals related to truly long-range interactions thus occur at a very late and hence not experimentally observable stage after the sweep. The influence of the
\( V_{NN\mu} \) on the experimentally most relevant quantity, the attenuation of the first few revivals, is however small as long as \( V/U \ll 1 \). Our further discussion is based on the assumption that the Hamiltonian (1) with only nearest-neighbor couplings describes the system, keeping in mind the above limitation.

### III. MODIFYING THE GUTZWILLER APPROACH

Conventionally, the equations of motion resulting from (1) are solved (numerically) with a Gutzwiller mean-field product state variational ansatz for the many-body wavefunction, cf., e.g. [28, 29]

\[ |GW \rangle = \prod_{i=1}^{M} \sum_{n_i} f_i(n_i, t) |n_i\rangle = \sum_{n_1} \cdots \sum_{n_M} \left\{ \prod_{i=1}^{M} f_i(n_i, t) \right\} |n_1, \ldots, n_M\rangle \quad (6) \]

with \( f_i(n_i, t = 0) = e^{-|a_i|^2/2\alpha_i^2}\alpha_i^{n_i}/\sqrt{n_i!} \) for a coherent state and \( |n_1, \ldots, n_M\rangle = |n_1\rangle \otimes \cdots |n_i\rangle \otimes \cdots |n_M\rangle \) is the number basis state corresponding to noninteracting bosons occupying Wannier orbitals at each site. The above variational wavefunction ansatz is a bosonic version of the fermionic product state wavefunction originally proposed by Gutzwiller [1].

The mean-field theory implicit in the Gutzwiller ansatz for the wave function is expected to be exact for the standard onsite interaction Bose-Hubbard model when either \( \bar{n} \) or \( \nu \) [21, 34, 51] are large; thus the “mean-field parameter” \( \bar{n}\nu \), characterizing the validity of mean-field theory, should be sufficiently large. The Gutzwiller ansatz then becomes exact for contact interactions in infinite dimension [22]. Another extreme case of exact validity is a fully connected lattice [33]. The Gutzwiller wavefunction, in the ground state and for contact interactions, has been argued to be qualitatively correct for lower, and hence easily experimentally realized, dimensions as well [34]. The Gutzwiller ansatz is however widely used for ground-state calculations also in the extended Bose-Hubbard model [8, 22, 26], where its rigorous validity for large mean-field parameter \( \bar{n}\nu \) is much less obvious than in the onsite interaction case. As we will now argue, the extended Bose-Hubbard Hamiltonian cannot be decoupled (in a nontrivial manner) into the sum of single-particle Hamiltonians, like the Hubbard model with contact interactions, where mean-field decoupling and the Gutzwiller ansatz have been shown to be equivalent [35].

The mean-field decoupling for the tunneling term, in the homogeneous case, \( \phi \equiv \langle \hat{a}_i \rangle \), leads from (1), when \( V = 0 \), to a sum of single-particle Hamiltonians, \( \hat{H}_i = -J(\hat{a}_i^\dagger \phi + \phi^* \hat{a}_i - |\phi|^2) + \frac{U}{2} \bar{n}_i(\bar{n}_i - 1) \). On the other hand, the nonlocal interaction term \( \propto V \), after applying mean-field decoupling, just shifts the chemical potential, and thus remains dynamically ineffective. In particular, while the Gutzwiller wavefunction (6) reproduces the on-site-interaction modulations with period \( 2\pi/U \), no modulations of \( g_1 \) with period \( 2\pi/V \) are created after mean-field decoupling has been performed. Note that the (instantaneously) vanishing order parameter does not cause the failure of the conventional Gutzwiller wavefunction ansatz. For local interactions, collapse and revival are captured accurately by the Gutzwiller wavefunction, even though the mean-field amplitude vanishes when first-order coherence collapses. The inadequacy of the Gutzwiller ansatz for the time evolution of coherence in the extended Bose-Hubbard model thus is much stronger than that caused by the tunneling term \( \propto J \) [16, 17]. The tunneling term can (at least in large dimensions) be accurately decoupled in mean-field, while this is not possible in a nontrivial way for the \( V \) term in (1), as argued above. We also observe in this regard that the expression (3) for the collapse and revival oscillations of \( g_1 \) is nonperturbative in either \( 1/\bar{n} \) or \( 1/(\bar{n}\nu) \), so that there is no obvious mean-field limit of the exact quantum evolution of first-order coherence in deep optical lattices. The quantum evolution of coherence can therefore serve as a sensitive probe of various time-dependent ansätze.

**FIG. 2.** (Color online) Time evolution of \( g_1 \) with an initial coherent state for \( V/U = 0.05, 0.1, 0.3 \), from top to bottom, with filling \( \bar{n} = 2 \). Solid line using the Gutzwiller variant (4), dotted blue line using the conventional Gutzwiller ansatz, Eq. (6).
that the on-site distribution function depends on the particle numbers in neighboring sites for the extended Bose-Hubbard model (1) when Eq. (A.3) in the appendix.

the analytical result \( \Psi \) is reproduced and hence the exact quantum evolution in the limit of zero tunneling. We illustrate this by comparing \( \Psi \) with the evolution using either \( \Psi_0 \) or \( \Psi_1 \), see Fig.2. The evolution according to \( \Psi_0 \) is identical with \( \Psi \), while propagating the initial coherent state with the conventional Gutzwiller ansatz \( \Psi_1 \) shows no modulation of the revival peaks with period \( 2\pi/V \) at all.

We anticipate that the Gutzwiller variant (GWV) ansatz \( \Psi_0 \) will also be a good approximation of the dynamical many-body state for a given \( U, V \) when the tunneling rate \( J \) is sufficiently small. We illustrate the effect of finite \( J \) by numerically computing in a 1D lattice the time evolution of an initially coherent state, using the GWV tunneling energy functional \( \mathcal{A}_V \) derived in the appendix. We show the results in Fig.3. There is the expected (real) damping occurring for finite \( J \) in addition to the attenuation of the first few coherence revivals obtained by finite \( V \). When \( \bar{n}V \gtrsim J \) (assuming \( U \gtrsim V \)), which is the regime of validity for the ansatz \( \Psi_1 \), the \( V \) attenuation will dominate the \( J \) damping; cf. Fig.2. Conversely, for \( J \gtrsim \bar{n}V \), the conventional Gutzwiller ansatz \( \Psi_0 \) will again be applicable, i.e., yield in this regime a better approximation than the GW ansatz \( \Psi_0 \).

Finally, coherent state amplitudes \( \Psi_1 \) apply in \( \Psi_0 \) when one is entering deep into the superfluid phase, which has \( J \gtrsim \bar{n}U, \bar{n}V \).

IV. NUMBER SQUEEZED INITIAL STATE

To employ our variant of the Gutzwiller ansatz for a less simple initial state than the coherent state \( \Psi_0 \), we now investigate the NN coupling effect on collapse and revival when finite number squeezing is present in the initial state. We take as the initial state the numerically determined ground state of the Hamiltonian (1) in one dimension for finite \( J/U \) and small system sizes \((M = 7)\), by exact diagonalization (ED), so that the initial state is determined as the ground state of (1) for a number-squeezed state.

We evolve this number-squeezed initial state within the GWV wavefunction ansatz \( \Psi_1 \) in a 1D lattice. To implement GWV propagation, we proceed by the following prescription. We convert the number basis amplitudes \( \Psi \) of the general many-body wavefunction obtained from ED, \( |\Psi\rangle = \sum_{n_1,\ldots,n_M} f(n_1,\ldots,n_M) |n_1,\ldots,n_M\rangle \) into real amplitudes of an initial product state of the GW type, and then propagate this initial state by the equations of motion of the GWV wavefunction, Eq. (8).

A comparison we made with the ED propagation of the full initial data shows that similar results are obtained as long as \( \eta = U/(\mu J) \) does not become too large [i.e., larger than \( \mathcal{O}(\bar{n}) \)], in which case both initial coherences \( q_i(0) \) are sufficiently close to the coherent state value \( \Psi_{\Omega} \).
approach also fails to reproduce that, for larger $\eta$, cf. Fig. 4. We note, in particular, that the Gutzwiller height is observed in distinction to the GWV evolution initial state (6), but like for the coherent ansatz (6), but like for the coherent initial state, no attenuation of the revival peak height is observed in distinction to the GWV evolution (7), cf. Fig. 4. This opens up the possibility of probing the existence and time development of coherence revivals, and thus the interplay of quantum fluctuations and order parameter value, for various initial data sampled from around the transition point between superfluid and localized phases. The collapse and revival phenomenon ultimately owes its existence to the granularity of matter, i.e. the fact that particle number is quantized in integer multiples. Measuring the collapse and revival oscillations around the transition point with single-atom resolution [12] should therefore afford interesting insights into the microscopic physics, that is the many-body wavefunction describing the transition.

V. CONCLUSION

The collapse and revival oscillations of first-order coherence were shown to be a sensitive measure of the NN couplings in the extended Bose-Hubbard model. After a rapid quench from the superfluid side, the first few revival peaks are significantly attenuated for moderate NN couplings. Even relatively small dipole moments of molecules stored in optical lattices can thus be detected by the attenuation of the height of the first few revival peaks. The attenuation effect is strong enough to overcome masking inhomogeneity effects like those caused by the external harmonic trapping, in distinction to the weak real damping caused by residual tunneling between deep wells in the localized phases. The Gutzwiller variant ansatz we determined from the exact collapse and revival quantum evolution in the limit of zero tunneling is also potentially relevant for exploring the phase boundaries in the ground state of the extended Bose-Hubbard model. A particular example are supersolid phases in the limit of large NN coupling $V$, where a comparison should be instructive to those obtained by the standard Gutzwiller approach [20].

We expect the morphology of quantum phase revivals to be a valuable future tool for both the quantitative analysis of interaction couplings of Hamiltonians of atoms/molecules with long-range interactions stored in deep optical lattices, as well as a sensitive test-bed for the validity of various approximation schemes for the many-body wavefunction. Finally, a possible extension of the present work is to include pair-exchange terms between lattice sites, i.e., by adding a contribution $\hat{H}_{\text{pair}} \propto \sum_{<ij>} \langle \hat{a}_i^\dagger \hat{a}_j^\dagger \rangle^2 \hat{a}_i \hat{a}_j^\dagger$ to the Hubbard Hamiltonian (1), see e.g. [38], from which novel interaction-induced effects on the dynamical evolution of first- and second-order coherence can be expected [39].

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Appendix: Equations of motion from the GWV ansatz

We delineate here the derivation of the equations of motion for the GWV wavefunction (7). For clarity and simplicity of notation, we restrict ourselves to a one-dimensional lattice; generalizations to higher lattice dimensions are straightforward.
We deduce the equations of motion variationally, starting from the functional
\[ \mathcal{E} = \langle \text{GWV} | i \partial_t - \sum_i \left\{ \hat{H}_i - \mu \hat{n}_i \right\} | \text{GWV} \rangle , \quad (A.1) \]
where \( \hat{H}_i = -J \sum_{j=1,\pm} \hat{a}_j^\dagger \hat{a}_j + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + \frac{V}{2} \hat{n}_i \hat{n}_{i+1} + \frac{V}{2} \hat{n}_i \hat{n}_{i-1} \).

We first consider the case with no tunneling, \( J = 0 \), for which (7) reproduces the exact quantum evolution. Due to the fact that the GWV wavefunction (7) is still a product state ansatz like the original Gutzwiller wavefunction, the energy functional (A.1) decomposes into contributions of a given site:
\[ \mathcal{E}_i = \sum_{n_i,n_{i+1},\cdots} f_i^*(n_i,n_{i+1},n_{i-1},t) f_{i-1}^*(n_{i-1},n_i,n_{i-2},t) f_{i+1}^*(n_{i+1},n_i+1,n_i,t) \cdots \]
\[ \times \left[ i \partial_t \hat{g}_i(n_i,n_{i+1},n_{i-1}) + \mu n_i \right] f_i(n_i,n_{i+1},n_{i-1},t) f_{i-1}(n_{i-1},n_i,n_{i-2},t) f_{i+1}(n_{i+1},n_i+1,n_i,t) \cdots \quad (A.2) \]

where \( i \partial_t \hat{g}_i(n_i,n_{i+1},n_{i-1}) \) now acts on \( f_i(n_i,n_{i+1},n_{i-1},t) \) only. Furthermore, when \( J = 0 \), the phase factors of e.g. the functions \( f_{i+1}(n_{i+1},n_{i+2},n_i,t) \) and \( f_{i-1}(n_{i-1},n_i,n_{i-2},t) \), containing all their time and NN particle number dependence, cancel with those of their conjugates in \( \mathcal{E}_i \), so that they can be replaced by the onsite distributions of the initial state, \( f_{i\pm 1}(n_{i\pm 1},n_i,n_{i\pm 2},t) \rightarrow f_{i\pm 1}(n_{i\pm 1}) \). The equations of motion then are
\[ [i \partial_t \hat{g}_i(n_i,n_{i+1},n_{i-1},t) + \mu n_i] f_i(n_i,n_{i+1},n_{i-1},t) = 0, \quad (A.3) \]
with the normalization condition \( \sum_{n_i} \langle f_i(n_i,n_{i+1},n_{i-1},t) \rangle^2 = 1 \), leading to number conservation in the form \( \sum_{n_i} n_i \langle f_i(n_i,n_{i+1},n_{i-1},t) \rangle^2 = \bar{n} \). The above equations of motion give the exact time evolution when \( J = 0 \).

Due to \( \left\{ \hat{H}_i(n_i,n_{i\pm 1}), \hat{g}_i(n_i,n_{i\pm 1}) \right\} = 0 \), where \( \hat{g}_i(n_i,n_{i\pm 1}) \) is an arbitrary operator function, a number of additional conserved quantities can be constructed. One such quantity is, choosing \( \hat{g}_i(n_i,n_{i\pm 1}) = \hat{n}_i + \hat{n}_{i+1} + \hat{n}_{i-1} \),
\[ \langle \text{GWV} | \hat{n}_i + \hat{n}_{i+1} + \hat{n}_{i-1} | \text{GWV} \rangle = \sum_{n_i,n_{i\pm 1}} (n_i + n_{i+1} + n_{i-1}) | F_i \rangle^2 = C, \quad (A.4) \]

where the threefold product amplitude \( F_i \) is defined by
\[ F_i(n_i,n_{i+1},n_{i-1},t) \equiv f_i(n_i,n_{i+1},n_{i-1},t) f_{i+1}(n_{i+1},n_i,n_{i-1},t) f_{i-1}(n_{i-1},n_i,n_{i-2},t) \quad (A.5) \]

\[ -J \langle \hat{a}_{i+1}^\dagger \hat{a}_i \rangle \simeq -J \sum_{n_i,n_{i\pm 1}} \sqrt{(n_i + 1)n_{i\pm 1}} F_i^*(n_i,n_{i+1},n_{i-1},t) F_i(n_{i+2},n_{i+1},n_i,n_{i-1},t) \sum_{n_{i\pm 2}} |f_{i\pm 2}(n_{i\pm 2})|^2 \exp(iVn_{i\pm 2}t), \quad (A.6) \]

with similar expressions for the other three terms. In the short time domain \( t < 2\pi/V \), we are interested in [cf. the final paragraph of section II], the oscillating factor at the end of the right-hand side can be omitted, so that collecting all four terms, the tunneling contribution to the functionals (A.1) respectively (A.2) becomes...
where the normalization condition now reads
\[ \sum_{n_i, n_{i+1}} |F_i(n_i, n_{i+1}, t)|^2 = 1. \]
Writing the interaction part as well in the product amplitudes (A.5), the equations of motion can then be derived from the functional derivative \( \delta \mathcal{E}_i / \delta F_i^*(n_i, n_i+1, n_i-1, t) = 0. \)

Finally, one can easily verify that the tunneling term preserves the conservation of the sum of onsite and NN numbers, \([ -J(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_i \hat{a}_{i-1} + \hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_{i-1}^\dagger \hat{a}_{i+1}) ] = 0, \) so that the conservation law (A.4) still holds, providing a benchmark for the accuracy of numerical calculations.

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