Adiabatic evolution of on-site superposition states in a completely-connected optical lattice

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Abstract. We analyze the dynamical melting of two-component atomic Mott-Insulator states in a completely-connected optical lattice within the adiabatic approximation. We examine in detail the effect of the dynamical phase acquired by the state during the adiabatic melting of the lattice potential. We show how for certain limits an on-site superposition state with two particles per site melts into a macroscopic superposition state, while an on-site superposition state with only one particle per site melts into a coherent state.

1. Introduction

The experimental realization of Bose-Einstein Condensation [1] in gases of alkali atoms has opened up a new area of research where quantum many-body theories can be tested in a clean way. One of the key ingredients contributing to the impressive advance in this research field has been the control of the trapping potentials. In particular, the use of optical lattices has provided an excellent playground for the quantum control of many-body quantum states. Several paradigm examples are the realization of the Mott-insulator (MI) to superfluid (SF) transition [2, 3], the Tonks gas and the Bose glass (for a review, see e.g. [4]). In a typical experimental setup the number of particles per site, the number and interactions between the different atomic species and the lattice potential barrier can be acutely controlled. The atomic interaction strength and the trapping potential can be changed dynamically on much shorter time scales than the experimental lifetime, making gases of ultracold atoms ideal systems to explore time-dependent quantum phenomena.

One of the most relevant dynamical process in a periodic potential is the MI-SF transition [5]. At zero temperature, the system undergoes a transition from a gapped many-body state where the particles are localized on each lattice site into a macroscopic wave function with long-range coherence. In [6] we have discussed possible applications of the MI-SF transition for a two-component system. We have shown that one could use the MI-SF transition to engineer atomic twin-Fock states if one starts from a MI state with two different atoms per site. Macroscopic twin-Fock states, with exactly the same number of particles in each of the modes, achieve the highest possible precision in atom-interferometric experiments [7]. Other states that have arisen much interest in quantum mechanics are the macroscopic superposition states or cat states. Such states could be obtained via the adiabatic melting of on-site superposition states with two particles per site in a completely connected lattice, as we indicate in [6].
In this paper we analyze in detail the adiabatic quantum melting of on-site superpositions in an optical lattice with infinite-range hopping [5, 8]. In this case the translational invariance symmetry is preserved during melting and within the adiabatic approximation, only the SF ground state is occupied. We can thus obtain an analytical expression for the melted states that allows us to analyze in detail the role of the relative phase acquired by the many-body state during the adiabatic evolution. The quantum melting in an optical lattice with only nearest neighbor hopping results in highly excited SF states and one can only calculate certain correlation functions [9, 10].

This paper is organized as follows. In section 2, we introduce the two-component Bose-Hubbard Model (BHM) and discuss its experimental feasibility. In section 3 we analyze the adiabatic melting of on-site superposition states with two particles per site and calculate the number and phase distributions to clarify the role of the dynamical phase acquired during the melting. In section 4 we analyze the melting of on-site superposition states with one particle per site. In section 5 we summarize our conclusions.

2. Two-component BHM

We use the two-component BHM [2] to describe atoms in two hyperfine states a and b that are trapped in the lowest Bloch band of a sufficiently deep optical lattice. The dynamics of this system is characterized by the following Hamiltonian \( (\hbar = 1) \)

\[
\hat{H} = -J \sum_{i,j>_<} (\hat{a}^\dagger_i \hat{a}_j + \hat{b}^\dagger_i \hat{b}_j) + U \sum_i \hat{n}^a_i \hat{n}^b_i + \frac{V}{2} \sum_i \hat{n}^a_i (\hat{n}^a_i - 1) + \frac{V}{2} \sum_i \hat{n}^b_i (\hat{n}^b_i - 1),
\]

where \( \hat{a}_i (\hat{b}_i) \) is the bosonic destruction operator for an a(b)-atom localized in lattice site i, \( \hat{n}^a_i = \hat{a}^\dagger_i \hat{a}_i \) and \( \hat{n}^b_i = \hat{b}^\dagger_i \hat{b}_i \) while \(< >\) denotes summation over nearest neighbors. The parameter J is the tunneling matrix element and V and U are the on-site intra- and inter-species interaction matrix elements, respectively. Based on the flexibility of these atomic systems, we make a simplification and consider a symmetric configuration for the a and b atoms. A crucial feature of the optical lattice setup is that the ratio between the tunneling and interaction matrix elements in Eq. (1) is experimentally controllable via the lattice laser intensities. The interaction matrix elements U, V can also be tuned with Feshbach resonances [11], or by shifting the a and b atoms away from each other using state-dependent lattices [12]. All of these methods of control can be exploited dynamically and one can connect via unitary evolution the MI regime where the on-site interactions dominate to the SF regime where the physics is characterized by the hopping between different sites. Combined with the long decoherence times of ultra-cold atoms this dynamical manipulation can often be implemented on near-adiabatic timescales [3, 13].

In this paper, we consider only infinitely connected lattices and thus the sum in the tunneling term of Hamiltonian Eq. (1) spans all lattice sites. This situation is very favorable theoretically because the Hamiltonian preserves the full permutational symmetry for all values of \( V/J \) and \( U/V \). In this case we obtain an exact analytical expression for the final SF state created via adiabatic evolution of a state created deep in the MI regime. In a typical experimental configuration where hopping takes place only between nearest neighbors the translational symmetry is broken for \( J \neq 0 \) and the final SF state is highly excited [9, 10]. For an infinitely connected lattice, the Hamiltonian can be rewritten as

\[
\hat{H} = -JM (\hat{A}^\dagger_0 \hat{A}_0 + \hat{B}^\dagger_0 \hat{B}_0) + U \sum_i \hat{n}^a_i \hat{n}^b_i + \frac{V}{2} \sum_i \hat{n}^a_i (\hat{n}^a_i - 1) + \frac{V}{2} \sum_i \hat{n}^b_i (\hat{n}^b_i - 1),
\]

where \( \hat{A}^\dagger_0 = 1/\sqrt{M} \sum_{i=1}^M \hat{a}^\dagger_i \) is the zero momentum mode for the a component and similarly for b. Off-resonant coupling to an external mode could lead to a term of this form in the Hamiltonian.
[14]. If one keeps the lattice very deep such that there is only infinitely connected tunneling, one could drive the transition using Feshbach resonances to tune down the interaction strengths $U$ and $V$.

3. Adiabatic evolution of $|\Psi_{aa+bb}\rangle$.

We consider the adiabatic melting of on-site superposition states of the form

$$|\Psi_{aa+bb}\rangle = \prod_{i=1}^{M} \frac{1}{\sqrt{2}} (|aa\rangle_i + |bb\rangle_i),$$

(3)

which can be created experimentally applying a rapid $\pi/2$-Raman pulse to a state with exactly two different particles per site [15]. This state is a binomial superposition of states with $n$ and $M - n$ pairs of particles of each species symmetrically distributed over $M$ lattice sites

$$|\Psi_{aa+bb}\rangle = \frac{1}{\sqrt{2^M}} \sum_{n=0}^{M} \binom{M}{n}^{1/2} |\Psi_{n}\rangle_{\text{sep}},$$

(4)

where $|\Psi_{n}\rangle_{\text{sep}} = \prod_{i<j<n} a_i^\dagger a_j^\dagger a_j a_i (\prod_{n<j} a_j a_j^\dagger) a_n$ and denotes symmetrization over lattice site configurations. We analyze the time evolution under Hamiltonian equation (2) for each term in the binomial distribution

$$i \frac{d}{dt} |\Psi_{\text{sep}}\rangle = \hat{H}(t) |\Psi_{\text{sep}}\rangle.$$  

(5)

We consider that $U/V$ is fixed during melting and thus $\hat{H}(t) = \hat{H}(V/J(t))$ where $V/J(t)$ is a smooth function of time that evolves from $J = 0$ in the MI regime to $V = U = 0$ in the SF regime as the one shown in the inset in Fig. 1. For $U > V$ and $J = 0$ the initial state $|\Psi_{\text{sep}}\rangle$ belongs to the degenerate ground state manifold with all phase-separated states. The ground state manifold becomes non-degenerate if we restrict ourselves to the permutationally symmetric subspace of the Hilbert space. Thus, at $t = 0$ $|\Psi_{\text{sep}}(t)\rangle = |0, V/J(0)\rangle_n$ where $|m, V/J(t)\rangle_n$ denotes the $m$-th eigenstate of $\hat{H}(t)$ in the permutationally symmetric subspace of the Hilbert space with $2n$ and $2M - 2n$ particles in the $a$ and $b$ modes. For $t > 0$ we expand the state in the instantaneous eigenbasis as

$$|\Psi_{\text{sep}}(t)\rangle = \sum_m c_m(t) |m, V/J(t)\rangle_n.$$  

(6)

The no-crossing rule [16] states that the eigenenergies $E_m^n(V/J) = V/J$ do not cross if the eigenstates $|m, V/J\rangle_n$ do have the same symmetry. The curves approach each other forming so-called avoided crossings. The speed of evolution determines whether an avoided crossing is traversed diabatically (impulse or sudden approximation) or adiabatically. For a sufficiently slowly-varying function $V/J(t)$ one can assume adiabatic evolution and only $c_0^m(t)$ is non-zero in Eq. (6). Plugging this state back in the Schrödinger equation (5), we obtain [17]

$$i \frac{d}{dt} c_0^m(t) = -c_0^m \left( i E_0^m(t) + \langle 0, V/J(t) | \frac{d}{dt} |0, V/J(t)\rangle_n \right),$$

(7)

which gives

$$c_0^m(t) = e^{-i \int_0^t E_0^m(t')dt'} e^{i \gamma_0^m(t)},$$

(8)

where

$$\gamma_0^m(t) = i \int_0^t \langle 0, V/J(t') | \frac{d}{dt'} |0, V/J(t')\rangle_n dt'.$$  

(9)
is the geometrical phase which is just a gauge if \( \hat{H} \) depends only on one parameter. In our case we have also a zero integrand in (9) and thus we only need to consider the dynamical phase \( \alpha_n(t) = \int_0^t E_0^n(V/J(t'))dt' \). Thus for \( t > 0 \) we can write down the evolved state

\[
|\Psi_{aa+bb}(t)\rangle = \frac{1}{\sqrt{2^M}} \sum_{n=0}^{M} \binom{M}{n}^{1/2} e^{-i\alpha_n(t)} |0, V/J(t)\rangle_n.
\]

(10)

In the SF limit \( V/J = 0 \) the ground state has all particles in the zero momentum mode

\[
|0,0\rangle_n \equiv |\Psi_{sf}\rangle = \frac{\hat{A}_0^1 |0\rangle + \hat{B}_0^1 |2M-2n\rangle}{\sqrt{(2n)!(2M-2n)!}} |\text{vac}\rangle \quad \text{(11)}
\]

and thus the final state reads

\[
|\Psi_f\rangle = \frac{1}{\sqrt{2^M}} \sum_{n=0}^{M} \binom{M}{n}^{1/2} e^{-i\alpha_n} |\Psi_{sf}\rangle_n.
\]

(12)

where \( \alpha_n = \int_0^t E_0^n(V/J(t'))dt' \). Note that the initial and final ground state energies are equal for all \( n \)-particle sectors although, in general and depending on the particular ramping function \( V/J(t) \), this is not true for intermediate values of \( t \). For example, we show in figure 1 the energy differences between the terms in equation (12) for \( M = 6 \). As expected, increasing numbers of pairs of different species result in higher energy differences. Due to the \( a-b \) symmetry, \( E_0^n = E_0^{M-n} \), for \( n = 0, .., M/2 \) and thus \( \alpha_n \) is always a symmetric function around \( M/2 \). We show in figure 2 the dynamical phase distribution \( \alpha_n \) of the melted state (12) using the particular ramping function shown in figure 1.

In next subsections we plot the phase and number probabilities of the final state \( |\Psi_f\rangle \). First, we assume that all the dynamical phases are equal, in which case we can show analytically that the final state is a macroscopic superposition state with 0.97 overlap with a rotated cat state. In the general case of non-vanishing ground energy differences between different \( n \)-particle sectors we can show that we still obtain cat state structures and even double cat states for symmetric phase distributions \( \alpha_n \).

3.1. Equal dynamical phases

For simplicity, we consider first the case \( \alpha_n = \alpha \) for all \( n \)-components in Eq. (12). This limit is achieved if we had \( \delta E_0^n t_f \ll \text{mod} (2\pi) \) for all \( n \) where \( \delta E_0^n \) is the variation of the ground state energy with \( n \).

We plot in figure 2 the number probability distribution in the \( \hat{J}_z \) eigenbasis such that \( \hat{J}_z |M, m_z\rangle = m_z |M, m_z\rangle \) with \( m_z = -M, .., M \) [18]. To give more insight into the properties of the final state \( |\Psi_f\rangle \) we plot the quasiprobability distribution \( Q(\theta, \phi) = |\langle \theta, \phi |\Psi\rangle|^2 \) obtained by projecting the state into the Bloch sphere [19]. Such a representation is the projection of the state into the coherent spin states (CSS) that read \( |\theta, \phi\rangle = e^{-i\theta \hat{J}_x} e^{-i\phi \hat{J}_y} |M, M\rangle \). The quasiprobability distribution for the melted state \( |\Psi_f\rangle \) is shown in figure 3 (a). After performing a single-particle operation \( \exp(i\pi \hat{J}_y/2) \) (realizable by Raman laser pulses) we find the rotated state \( \exp(i\pi \hat{J}_y/2) |\Psi_f\rangle \) (c.f. figure 3 (b)) to be nearly identical to the state

\[
|\Psi_{\text{max}}\rangle = \frac{1}{\sqrt{2}} (|\Psi_{sf}^0\rangle + |\Psi_{sf}^M\rangle)
\]

(13)

which is the maximally entangled macroscopic superposition (c.f. figure 3 (c)).
Figure 1. Ground energy differences for $M = 6$ for the particle sectors $n = 0, 1, 2$. Higher energy differences correspond to smaller $n$. Inset: ramping of $V/J(t)$ in Hamiltonian Eq. (2). $U/V = 3$ is fixed during the melting.

Figure 2. Dynamical phase $\alpha_n$ acquired by the melted state. Relative number probability distribution of the melted state (12). $M = 6$ sites.

We can calculate the overlap $O = |\langle \Psi_r | \Psi_{r_{\text{max}}} \rangle|$ where $| \Psi_{r_{\text{max}}} \rangle = e^{-i\pi \hat{J}_y} | \Psi_{\text{max}} \rangle$. In the $\hat{J}_z$ basis the states read

$$| \Psi_r \rangle = \frac{1}{\sqrt{2^M}} \sum_{n=0}^{M} \binom{M}{n}^{1/2} | M, M - 2n \rangle$$

and

$$| \Psi_{r_{\text{max}}} \rangle = \frac{\sqrt{2}}{2M} \sum_{n=0}^{M} \binom{2M}{2n}^{1/2} | M, M - 2n \rangle,$$

where we have used that

$$\langle m_z, M | \Psi_{r_{\text{max}}} \rangle = \frac{1}{\sqrt{2}} \left[ d_{m_z, M}^{M}(\frac{\pi}{2}) + d_{m_z, -M}^{M}(\frac{\pi}{2}) \right]$$

where $d_{m_z, M}^{M}$ is defined in [20] and

$$d_{m_z, M}^{M}(\frac{\pi}{2}) + d_{m_z, -M}^{M}(\frac{\pi}{2}) = 2^{-m_z} \left[ \binom{M-m_z}{M+m_z} \right]^{1/2} \binom{2M}{M-m_z} \frac{1}{2} \left[ \left( \frac{-1}{2} \right)^{M-m_z} + \left( \frac{1}{2} \right)^{M-m_z} \right].$$

The overlap $O$ can be calculated analytically in the limit of large $M$. We assume two gaussian distribution functions $f_{r_{\text{max}}}(x) = C_{r_{\text{max}}} e^{-2x^2/M}$ and $f_{r}(x) = C_{r} e^{-x^2/M}$ with

$$C_{r_{\text{max}}} = \frac{\sqrt{2(2M)!}}{2^M (M)!} \approx \left( \frac{16}{eM} \right)^{1/4}$$

$$C_{r} = 2^{-M/2} \sqrt{\frac{(M)!}{(M/2)!}} \approx \left( \frac{8}{eM} \right)^{1/4}$$

where we have used the Stirling formula. Then $\int_{-\infty}^{\infty} f_{r_{\text{max}}}(x)f_{r}(x)dx \approx \sqrt{8}/9$ and we obtain

$$O = |\langle \Psi_{\text{max}} | \exp(i\pi \hat{J}_y/2) | \Psi_r \rangle| = \sqrt{8}/9$$

for $M \to \infty$. This limit is monotonically attained with $O > 0.97$ for $M > 10$. 

5
3.2. General dynamical phase distribution $\alpha_n$

We now consider the case of non-equal dynamical phases $\alpha_n$ for the different $2n$-particle sectors. The exact shape of $\alpha_n$ depends on the particular melting process $V/J(t)$. If we take the dynamical phase distribution function shown in figure 2 which we obtained for the adiabatic melting of a state $M = 6$ sites we observe that the cat structure is preserved (figure 4 a)). There are again two shaded areas on opposite sites of the Bloch sphere which have changed the shape due to their dynamical phase factors.

We compute the quasiprobability distribution $Q(\theta, \phi)$ for different distributions $\alpha_n$. The actual shape of $E_n^0$ for $M = 6$ suggests (figure 1) that there is an algebraic relation between the ground energy differences. We assume a symmetric linear function $\alpha_n = \alpha |M/2 - n|$ for $n = 0, \ldots, M$. We always obtain catlike structures c.f. figure 4 b) and one can even obtain double cat structures as shown in figure 4 c).
4. Adiabatic melting of $|\Psi_{a+b}\rangle$.

Another MI state that can be easily experimentally obtained is

$$|\Psi_{a+b}\rangle = \prod_{i=1}^{M} \frac{1}{\sqrt{2}} (|a\rangle_i + |b\rangle_i)$$

which can be also written as a binomial superposition state of phase separated states $|\Psi_{a+b}^{\text{sep}}\rangle = \{\prod_{i=1}^{n} |a\rangle_i \prod_{j=n+1}^{M} |b\rangle_j\}$ with one particle per site. The final SF state can be written in the $\hat{J}_z$ basis as

$$|\Psi_c\rangle = \frac{1}{\sqrt{2^M}} \sum_{n=0}^{M} \binom{M}{n}^{1/2} e^{-i\alpha_n} \left| \frac{M}{2}, \frac{M-n}{2} \right\rangle.$$  

This state is a coherent state as one can observe from the number probability distribution in figure 5. For constant dynamical phases this is exactly a rotated SF

$$|\Psi_{\text{SF}}\rangle = \frac{1}{\sqrt{M!}} \left( \frac{\hat{A}_0^\dagger + \hat{B}_0^\dagger}{\sqrt{2}} \right)^M |\text{vac}\rangle.$$  

We plot in figure 6 the phase probability distribution for different linear symmetric $\alpha_n = \alpha |M/2 - n|$ and observe that the phase distribution distorts the coherent state into a gaussian state that can be squeezed (c.f. figure 6 a)) or even present double structures as the ones shown in figure 6 b).

![Figure 5](image1)

**Figure 5.** Number probability distribution of the state $|\Psi_c\rangle$.

![Figure 6](image2)

**Figure 6.** a) Q distribution for the melted $|\Psi_c\rangle$ with $\alpha_n = 3.5 |M/2 - n|$ and b) $\alpha_n = 1224 |M/2 - n|$.

5. Summary

We have calculated the phase and number probability distribution for the melted SF states obtained from on-site superposition states with one and two particles per site in the MI regime. We have considered an infinitely connected lattice where the full permutational symmetry is preserved during the dynamical evolution and no excitations are created within the adiabatic approximation. In this case we obtain a final superposition of ground SF states whose number distribution corresponds to a macroscopic coherent state and a macroscopic superposition state for the MI states with one and two particles per site respectively. However, each term in the final superposition acquires different dynamical phases which depend dramatically on the exact dynamical process under consideration. We have shown that for certain dynamical phase distributions one can obtain either squeezed melted states for the one-particle MI states or cat-like states for the two-particle Mott insulators.
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