Superposition states of ultracold bosons in rotating rings with a weak potential barrier

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We study ultracold bosons in a one-dimensional rotating ring lattice with a weak potential barrier well below unit filling. Due to the potential barrier the eigenstates are superpositions of different quasi-momenta. At the critical rotation frequency where the single-particle spectrum of the uniform system is doubly degenerate, the ground-state wave function is a condensate for weak interaction, a NOON-state for intermediate interaction, and a center-of-mass superposition for strong interaction. We demonstrate that the energy gap in the last regime is independent of the number of particles only if the barrier is sufficiently narrow, i.e. a single-site barrier, and decreases exponentially for more realistic barrier potentials that necessarily have finite widths. We also provide the signatures of the different superposition states in momentum distribution and noise correlation measurements.

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Ultracold bosons in rotating ring traps are a fascinating subject of research because the particles in this system can form various multi-particle superposition states. Some of these superposition states may play a central role in studies of the quantum-to-classical transition [1] or in applications such as entanglement-enhanced metrology [2].

Most of the work in this area has focussed on NOON-state production in uniform ring lattices [3, 4] and superlattices [5]. In these systems there are critical rotation frequencies at which the single-particle spectrum is degenerate so that even weak interactions lead to strong correlations between the particles. The energy gap between ground and excited states for these systems does, as one might expect for multi-particle transitions, decrease exponentially with the number of particles. This does, of course, limits the schemes proposed to generate these quasi-momentum NOON-states to operate with a modest number of atoms [4, 6].

Very recently, the authors of Ref. [7] showed that for strong interactions the ground state of a Lieb-Liniger model with a delta-function potential barrier is a superposition of states with different total (angular) momentum of the particles. As the energy gap in this model is independent of the number of particles involved, the production of superposition states with larger number of particles seems feasible. This is a remarkable result, and we wished to examine the extent to which the result would apply to systems with a more realistic potential.

With this in mind, we shall present our results for the nature of the different superposition states that occur for ultracold bosons in rotating ring lattices with a weak potential barrier. We focus on systems at a critical rotation frequency where the single-particle spectrum of the uniform ring is doubly degenerate. We study systems with less than one atom per site in order to avoid the superfluid-to-Mott-insulator transition for strong interactions and introduce a weak potential barrier that breaks rotational (or translational) invariance and leads to superposition states of different quasi-momenta.

We use both exact diagonalization of systems with small numbers of atoms and sites, along with the Bose-Fermi mapping in the Tonks-Giradeau regime to fully characterize the ground-state wave function of this many-body system. We find that the nature of the lowest-energy superposition state at the critical rotation frequency with a weak barrier potential depends on the strength of the interactions. For weak interactions it is a Bose-Einstein condensate. For intermediate strength it is a strongly-correlated NOON-state. For strong interactions, where the particles are locked together, it is superposition of two center-of-mass motional states.

The latter limit appears most attractive for generating superpositions with many particles as the energy gap is independent of the number of particles. This independence of the number of particles however depends critically on the large momentum transfer that a sharp potential barrier is able to provide. As soon as we consider a Gaussian potential with finite width, the energy gap decreases exponentially with increasing number of particles. Any real potential in an experiment will have a finite width and this gives a limit to the number of particles that can actually participate in the superposition state. Finally, we present the experimental signatures of the different superposition states in momentum distribution and noise correlations measurements.

Hamiltonian. We consider a system of N ultracold bosons with mass M confined in a 1D ring lattice of L sites with lattice constant d. The ring is rotated in its plane with angular velocity Ω. In the rotating frame the Hamiltonian is [4, 8]

$$\hat{H} = -J \sum_{j=1}^{L} \left(\mathrm{e}^{\mathrm{i}\theta} \hat{a}_{j+1}^\dagger \hat{a}_j + \mathrm{H.c.} \right) + \frac{U}{2} \sum_{j=1}^{L} \hat{n}_j (\hat{n}_j - 1) + \sum_{j=1}^{L} V_j \hat{n}_j \quad (1)$$

where $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$ and $\hat{a}_j$ are the number and bosonic annihilation operators of a particle at site j, $\theta = M\Omega L d^2/h$ is the phase twist induced by rotation, J is the hopping energy between nearest-neighbor sites, U the on-site interaction energy, and V_j describes the potential barrier at site j.

To understand the effect of rotation on the atoms in the ring lattice, we write the many-body Hamiltonian (1) in terms of the quasi-momentum operators $\hat{b}_q = \frac{1}{\sqrt{L}}\sum_{j=1}^{L}\hat{a}_j e^{-2\pi i q j/L}$, where $2\pi q/dL$ is the quasi-momentum and $q = 0, \dots, L-1$ an integer. In this basis the Hamiltonian (1) has the form [3, 4]

$$\hat{H} = \sum_{q=0}^{L-1} E_q \hat{b}_q^\dagger \hat{b}_q + \frac{U}{2L}\sum_{q,s,l=0}^{L-1}\hat{b}_q^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_{[q+s-l]\,\mathrm{mod}\,L} + \sum_{\{q,q'\}=0}^{L-1} V_{qq'}\hat{b}_{q'}^\dagger \hat{b}_q \tag{2}$$

where $E_q = -2J\cos(2\pi q/L - \theta)$ are the single-particle energies, $V_{qq'}$ is the Fourier transform of the single-particle potential $V_{qq'} = \frac{1}{L}\sum_j V_j e^{2\pi i(q-q')j/L}$, and the modulus is taken because in collision processes the quasi-momentum is conserved up to an integer multiple of the reciprocal lattice vector $2\pi/d$, i.e. modulo Umklapp processes. In absence of a potential barrier, i.e. $V_j = 0$, the single-particle spectrum is twofold degenerate for $\theta = \pi/L$ which we will refer to as the critical rotation frequency or critical phase twist.

Ground state at the critical phase twist. In the following we will focus on the ground state at the critical phase twist for a small single-site potential barrier ($V_j = 0$ for $j \neq 0$, i.e. $V_{qq'} = V_0 \ll J$). Note that a single-site barrier leads to constant momentum transfer in the first Brillouin zone.

In Fig. 1 we show our results for the many-body spectrum and detailed characterization of the ground-state wave function using exact diagonalization of a small system for $N = 3$ atoms on $L = 5$ lattice sites. We can clearly distinguish three regimes: weak, intermediate, and strong interactions.

In the non-interacting system, $U = 0$, all bosons occupy the lowest-energy single-particle state. In the presence of the potential barrier, $V_0 \neq 0$, translation symmetry is broken and quasi-momentum ceases to be good quantum number. For a weak barrier, $V_0 \ll J$, the ground state of the single-particle Hamiltonian is an equal superposition of the quasi-momentum states $|q = 0\rangle$ and $|q = 1\rangle$, and the many-body ground state is

$$|\psi_0\rangle = \left(\frac{\hat{b}_0^\dagger - \hat{b}_1^\dagger}{\sqrt{2}}\right)^N |0\rangle \tag{3}$$

where $|0\rangle$ is the many-body vacuum. This is corroborated by our exact-diagonalization results in the weakly-interacting regime: the momentum distribution is $\langle\hat{n}_q\rangle = \langle\hat{b}_q^\dagger\hat{b}_q\rangle = N/2$ for $q = \{0, 1\}$ and $\langle\hat{n}_q\rangle = 0$ otherwise. The distribution of total momentum $P(K)$, i.e. the probability that the many-body system has total quasi-momentum $2\pi K/dL$ is binomial. It can be calculated from $P(K) = \sum_n |K, n\rangle\langle K, n|$, where $|K, n\rangle\langle K, n|$ is the projector on the Fock state with K total quasi-momentum quantum number and n is a shorthand for the remaining quantum numbers [7]. Finally, the spectrum of the single-particle density-matrix (SPDM) $\langle\hat{a}_i^\dagger\hat{a}_j\rangle$ has one eigenvalue of size N which signals condensation.

As soon as the interactions overcome the energy splitting induced by the potential barrier, the almost degenerate many-body states are strongly mixed leading to correlations between the atoms. We discussed this mechanism in detail in the context of NOON-state production in rotating ring lattices and superlattices [9] as well as quantum vortex nucleation [10]. Neglecting the effect of the weak potential barrier, the non-interacting many-body spectrum at the critical phase twist is $N+1$-fold degenerate. Most of the degeneracy is lifted by the interactions in first order of perturbation theory, but the states $(\hat{b}_0^\dagger)^N|0\rangle$ and $(\hat{b}_1^\dagger)^N|0\rangle$ remain degenerate. In the presence of the potential barrier these two states are coupled at some higher order of perturbation theory (even if the system is non-commensurate), the degeneracy is lifted, and the ground state is the quasi-momentum NOON-state [7]

$$|\psi_1\rangle = \frac{(\hat{b}_0^\dagger)^N - (\hat{b}_1^\dagger)^N}{\sqrt{2}}|0\rangle. \tag{4}$$

While the momentum distribution is almost unchanged with respect to the non-interacting case, the momentum noise correlations $\langle\hat{n}_q\hat{n}_{q'}\rangle - \langle\hat{n}_q\rangle\langle\hat{n}_{q'}\rangle$ pick up the large fluctuations in the NOON-state (4). The distribution of total quasi-momentum $P(K)$ is bimodal, and the SPDM has two large eigenvalues of size $N/2$ indicating fragmentation of the condensate. Finally, the overlap with the many-body quasi-momentum basis states unambiguously proofs that the ground state is indeed the quasi-momentum NOON-state (4).

In passing we note that the presence of NOON-states can be observed in time-of-flight expansion after inducing many-body oscillations with a quench in the rotation frequency [5]. Their frequency is given by twice the energy gap which in the regime of intermediate interactions is exponentially small in the number of particles [3, 4].

Let us now discuss the novel strongly-interacting regime. In absence of the potential barrier, i.e. $V_0 = 0$, quasi-momentum is a good quantum number. Strong interactions ($U/J \to \infty$) lead to fermionization of the bosons within each subspace of total quasi-momentum K. In this regime the many-body energy spectrum is equal to the single-particle spectrum (with (anti-)periodic boundary conditions for (even) odd N [11]) which is degenerate at the critical phase twist. The potential barrier then breaks translation symmetry and couples the two degenerate ground states $|\psi_\infty^{K=0}\rangle$ and $|\psi_\infty^{K=N}\rangle$, which are the ground states of the quasi-momentum subspaces with $K = 0$ and $K = N$. We thus call the ground-state wave function a *center-of-mass superposition*

$$|\psi_\infty\rangle = \frac{|\psi_\infty^{K=0}\rangle - |\psi_\infty^{K=N}\rangle}{\sqrt{2}}. \tag{5}$$

Compared to the regime of intermediate interactions the two largest eigenvalues of the SPDM are smaller in the strongly-interacting limit pointing to the fact that the center-of-mass superposition (5) is only a partially-fragmented state. Since many quasi-momentum basis states contribute to (5) the overlap with a quasi-momentum NOON-state (4) is also smaller.

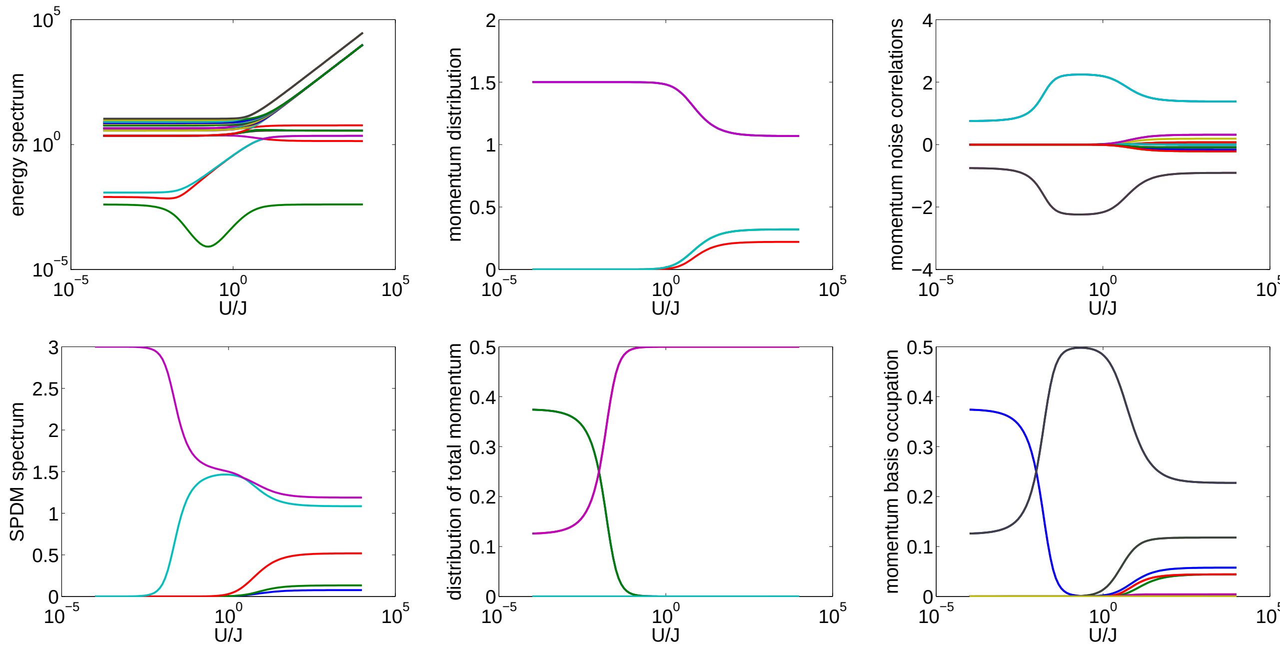

FIG. 1: Energy spectrum and characterization of the ground-state wave function for $N = 3$ particles on $L = 5$ sites at the critical phase twist as a function of the interaction parameter U/J: (a) many-body energy spectrum, (b) momentum distribution $\langle \hat{n}_q \rangle$, (c) momentum noise correlations $\langle \hat{n}_q \hat{n}_{q'} \rangle - \langle \hat{n}_q \rangle \langle \hat{n}_{q'} \rangle$, (d) spectrum of single-particle density matrix $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$, (e) distribution of total quasi-momentum $P(K)$ (as defined in the text), and (f) overlap with the many-body Fock states in the quasi-momentum basis $|n_{q=0}, \ldots, n_{q=L-1}\rangle$. Note that in (b), (c), (e) and (f) most curves are doubly degenerate.

The distribution of total quasi-momentum is not sensitive to the difference between the states (4) and (5). State (5) is a superposition involving the center-of-mass coordinate of N particles and might be valuable for studies of the quantum-to-classical transition, similar to experiments on the diffraction of large molecules [12], moving mirrors driven by radiatio-pressure force [13] and electrons in superconducting flux qubits [14]. However, state (5) does not possess the intriguing many-body correlations present in state (4) which are needed for application such as entanglement-enhanced metrology and other quantum-information tasks.

Larger systems in the Tonks-Giradeau limit. In the Tonks-Giradeau regime the strong repulsion between atoms mimics the Pauli exclusion principle and prevents two atoms from occupying the same lattice site. In this regime, the bosonic operators, $\hat{a}_j$, can be re-expressed using the Jordan-Wigner transformation (JWT) [11] in terms of fermionic ones, $\hat{c}_j$, fulfilling anti-commutation relations. Under the JWT, any correlation function of the bosonic system can be rewritten in terms of fermionic operators and computed for the corresponding non-interacting fermionic ground state by using Wick's theorem. Local observables, such as the density, or those involving only nearest-neighbor sites, such as the Hamiltonian (1), map directly to the corresponding fermionic observables. For example, the bosonic spectrum is exactly the same as the spectrum of the non-interacting fermionic system.

We use the Bose-Fermi mapping to calculate the energy gap in the strongly-interacting regime. We find consistently with Ref. [7] that it is almost independent of the number of particles, a consequence of the constant momentum transfer in the first Brillouin zone for a single-site barrier (see below).

On the contrary, non-local observables, such as the two-point correlator, $\langle \hat{a}_j^\dagger \hat{a}_i \rangle$, needed to compute the quasi-momentum distribution or SPDM, are mapped onto a string of fermionic operators $\langle \hat{a}_j^\dagger \hat{a}_i \rangle \to \langle \hat{c}_j^\dagger (-1)^{\sum_{j>k>i} \hat{c}_k^\dagger \hat{c}_k} \hat{c}_i \rangle$ for $j > i$. Making extensive use of Wick's theorem, one can re-express this quantity as a Töplitz determinant $\langle \hat{a}_j^\dagger \hat{a}_i \rangle = \frac{1}{2} \det[G_{j,i}]$, where $G_{j,i}$ is a $j-i$ by $j-i$ matrix with elements $(G_{j,i})_{l,l'} = 2\langle \hat{c}_{i+l'-1}^\dagger \hat{c}_{j+l} \rangle - \delta_{l,l'-1}$. We can compute these determinants numerically for relatively large system sizes.

In contrast to the energy gap which is almost independent of the number of particles, the SPDM spectrum and momentum distribution substantially change with the number of particles. In Fig. 2 we plot the spectrum of the SPDM for $L = 100$ sites as a function of the number of particles N. We see that fragmentation strongly decreases with increasing number of particles so that can infer that the ground state has a decreasing overlap with a quasi-momentum NOON-state (4). Moreover, the momentum distribution for $N = 20$ atoms on $L = 100$ sites shows that even at this small filling depletion is large.

Number scaling for finite-width potential barrier. In future experiments the barrier will most likely be provided by a blue-detuned laser beam with Gaussian beam waist. That is why we now generalize the case of a single-site potential barrier and consider a Gaussian potential barrier of finite width ξ, i.e. $V_j = \mathcal{N}^{-1} V_0 e^{-d^2 j^2 / 2\xi^2}$ with the normalization $\mathcal{N} = \sum_{j=1}^{L} e^{-d^2 j^2 / 2\xi^2}$. The matrix elements $V_{qq'}$ are given

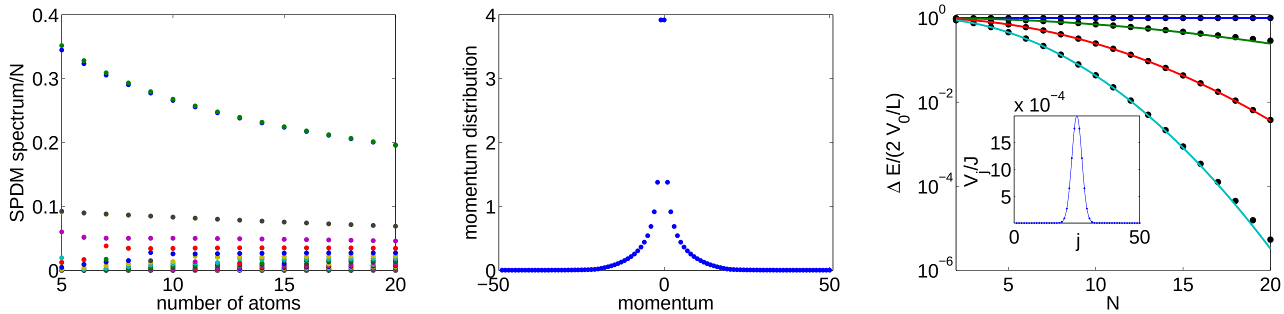

FIG. 2: Spectrum of the SPDM (left) versus number of atoms N for $L = 100$ sites and $V_0/J = 0.01$. Momentum distribution (middle) for $L = 100$, $N = 20$, and $V_0/J = 0.01$. Energy gap ΔE versus particle number N (right) for $L = 50$, $V_0/J = 0.01$, $\xi/d = 0$ (blue), $\xi/d = 2/3$ (green), $\xi/d = 4/3$ (red), and $\xi/d = 2$ (cyan). Points are the exact single-particle spectrum and lines from perturbative expression (6). Inset shows the barrier potential V_j for $L = 50$, $V_0/J = 0.01$, and $\xi/d = 2$.

by the discrete Fourier transform of the barrier potential V_j which for $d \ll \xi$ becomes the continuous Fourier transform $V_{qq'} = V_0 e^{-2\pi^2(\xi/dL)^2(q-q')^2}/L$ while for $\xi \to 0$ we recover the single-site barrier limit $V_{qq'} = V_0/L$.

We can get a perturbative expression for the energy gap using degenerate perturbation theory first order in V_0. The energy gap ΔE_N between the ground and first excited state in the Tonks limit for N particles is

$$\Delta E_N = 2\frac{V_0}{L} e^{-2\pi^2(\xi/dL)^2 N^2}. \tag{6}$$

We note that in this weak barrier limit the exponential scaling is independent of the barrier height.

In Fig. 2 we plot the energy gaps ΔE_N which open due to the potential barrier as a function of number of particles N for various barrier widths ξ/d. In the small barrier $V_0/J = 0.01$ the accuracy of the perturbative expression (6) is excellent. In contrast to the single-site potential barrier, i.e. $\xi \to 0$, a potential barrier with finite width ξ leads to exponentially small energy gaps for increasing number of particles N. The physical reason is that we need increasingly large momentum transfer to couple the center-of-mass momentum states. Since the matrix elements of a finite-width potential barrier decrease exponentially for increasing momentum transfer, we recover the exponential scaling of the energy gap ΔE_N similar of the weakly-interacting regime.

Summary. In conclusion, we have shown that a potential barrier in a rotating ring lattice loaded with ultracold bosons at low filling fraction supports several qualitatively very different superposition states of different total quasi-momentum: a condensate for weak, a NOON-state for intermediate, and a center-of-mass superposition for strong interactions. The energy gap in the strongly-interacting limit is only independent of the number of particles as long as one can neglect the width of the potential barrier. Otherwise one recovers the exponential scaling with increasing number of particles.

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