Incommensurate Superfluidity of Bosons in a Double-Well Optical Lattice

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We study bosons in the first excited Bloch band of a double-well optical lattice, recently realized at NIST. By calculating the relevant parameters from a realistic nonseparable lattice potential, we find that in the most favorable cases, the boson lifetime in the first excited band can be several orders of magnitude longer than the typical nearest-neighbor tunneling time scales, in contrast with that of a simple single-well lattice. In addition, for sufficiently small lattice depths, the excited band has minima at nonzero momenta incommensurate with the lattice period, which opens a possibility to realize an exotic superfluid state that spontaneously breaks the time-reversal, rotational, and translational symmetries. We discuss possible experimental signatures of this novel state.

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Optical lattices provide an exquisite tool for controlled exploration of novel types of order in cold atomic gases [1]. In particular, realization of a (quasi-)two-dimensional (2D) double-well (DW) optical lattice at NIST was one of the latest major developments in the experimental cold-atom physics [2], motivating further experimental [3] and theoretical [4] efforts.

Ultracold atoms, either fermionic or bosonic, in higher Bloch bands have recently ignited a great deal of interest [5–13]. In the fermion case, Pauli blocking enables one to populate high Bloch bands by simply increasing the atomic density [8]. By contrast, the true ground-state condensation of bosons only occurs in the lowest s-orbital band even for high boson densities. When the majority of bosons populate a higher band, bosons are in excited states with a finite lifetime. Isacsson et al. [5] have studied bosons in the first excited band of 1D optical lattice and found lifetimes that are on the order of 10–100 times longer than the typical nearest-neighbor tunneling time scales, in contrast with that of a simple single-well lattice.

We study weakly interacting cold bosons populating the first excited band of a quasi-2D DW optical lattice.

We show that in the superfluid regime, Bose-Einstein condensation (BEC) takes place at an incommensurate nonzero momentum, which spontaneously breaks time-reversal, rotational, and translational symmetries. We further demonstrate that, due to vastly reduced available phase space for the decay to the lowest band, the lifetime of a Bose gas in the first excited band of a DW lattice can be several orders of magnitude longer than the inverse tunneling rate, which in turn sets the characteristic time needed to establish phase coherence in the system [14].

The DW lattice consists of a nonseparable optical potential in the x-y plane and a conventional optical potential in the z-direction. In the case with DWs oriented in the x-direction, in a coordinate system with the origin at a maximum point of the “in-plane”-lattice light intensity, the optical potential in the x-y plane is given by [2]

$$V(x, y) = 2V_0\left[(\cos(2k_L y) - \cos(2k_L x)) + 2r(\cos(k_L x) + \cos(k_L y))^2\right].$$  (1)

Here, $k_L = 2\pi/\lambda$ is the magnitude of the laser wave vector, $V_0 = -|V_0| < 0$ (red-detuned lattice), while $r = I_x/I_{xy}$ stands for the relative intensity of two components of light with the in-plane and out-of-plane polarizations. The band structure of the single-particle Hamiltonian $H_0 = -(\hbar^2/2m_b)(\vec{a}_x^2 + \vec{a}_y^2) + V(x, y)$ (m_b-boson mass) in the x-y plane can be solved by using the plane-wave basis. The corresponding matrix elements of $H_0$ read

$$\langle \mathbf{k} + \mathbf{G}_{m,n}|H_0|\mathbf{k} + \mathbf{G}_{m,n}\rangle = E_R[\langle k_x/k_L + m + n \rangle^2 + \langle k_y/k_L + m - n \rangle^2],$$

$$\langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{\pm 1,0}\rangle = \langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{0,\pm 1}\rangle = 2rV_0,$$

$$\langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{\pm 1,\pm 1}\rangle = (r - 1)V_0.$$  (2)

where $\mathbf{k} = (k_x, k_y)$ is the wave vector, $\mathbf{G}_{m,n} = m\mathbf{b}_1 + n\mathbf{b}_2$ (m, n-integers) are the reciprocal-lattice vectors [with basis $\mathbf{b}_{1,2} = k_L(\hat{\mathbf{x}} \pm \hat{\mathbf{y}})$], and $E_R = \hbar^2k_L^2/(2m_b)$ is the recoil energy.

The dispersion of the first excited band is depicted in Fig. 1, where the energies are expressed in units of $E_R$. While the lowest band has minimum at $\mathbf{k} = 0$, the first excited band has maximum at $\mathbf{k} = 0$ and minima for $\mathbf{k} \neq 0$. For larger values of $|V_0|$, these minima occur at commensurate wave vectors of $\mathbf{k} = (\pm 1, 0)k_L$ and $(0, \pm 1)k_L$. However, for optical lattice depths smaller (in absolute value) than some $r$-dependent threshold value, i.e., for $|V_0| < V_0(r)$, these minima occur at wave vectors $\mathbf{K}$ that
excited state (odd parity) of a DW. These two states can be sought in the form of “bonding” and “antibonding” linear combinations of single-well Gaussians, respectively, similar to the Heitler-London variational approach to the $H^*_0$ molecular ion. For the DW comprising potential-minima at $(x_1,0)$ and $(x_2,0)$,

$$
\Phi_\pm(x,y) = \frac{\varphi(x-x_1,y) \pm \varphi(x-x_2,y)}{\sqrt{2(1 \pm S)}},
$$

(3)

where $\varphi(x,y) = (\pi\sigma^2)^{-1/2}e^{-(x^2+y^2)/(2\sigma^2)}$ is a 2D Gaussian and $S = \int \varphi^*(x-x_1,y)\varphi(x-x_2,y)d^2r = e^{-b^2/(4\sigma^2)}$ is the overlap integral of two such Gaussians, a distance $b \equiv x_2 - x_1$ apart. Optimal value $\sigma_0$ of the Gaussian-width $\sigma$ is obtained by minimizing the expectation value $\langle \Phi_+(x,y)|H_0|\Phi_+(x,y) \rangle$ of the DW ground-state energy over this parameter. The value of $\sigma_0$ becomes larger with decreasing lattice depth (i.e., for decreasing $|V_0|$). In particular, our calculation shows that for $|V_0/E_R| \approx 1.0$, one has $\sigma_0 \approx 0.39b$. Strictly speaking, the Wannier functions are well described by the ansatz in Eq. (3) only for not-too-small $|V_0|$ (implying that the midbarrier between single wells is sufficiently high). By comparing the variational ground state energies of a DW corresponding to different lattice depths with band-structure calculations, we can estimate that this approach is accurate for $|V_0| \approx 0.4E_R$, which puts the lower bound on the lattice depths that will hereafter be discussed.

The $z$-dependent part of the full 3D Wannier functions $\Phi_\pm(x,y,z) = \Phi_\pm(x,y)\phi(z)$ takes on the standard Gaussian form $\phi(z) = (\pi \xi_z^2)^{-1/4}e^{-z^2/(2\xi_z^2)}$, where $\xi_z$ is the effective harmonic “zero-point” length in the $z$-direction, characterizing the transverse confinement of the system.

The intraband and interband Hubbard interaction parameters are given by $U_\pm = \langle g/\xi_z^2\sqrt{2\pi}\rangle \int \Phi_\pm^*(x,y)\Phi_\pm(x,y)d^2r$ and $U_{+-} = \langle g/\xi_z^2\sqrt{2\pi}\rangle \int \Phi_+^*(x,y)\Phi_-^2(x,y)d^2r$, respectively, where $g = 4\pi \hbar^2 a_s/m_b$. Calculation yields

$$
\frac{U_{+-}}{E_R} = \frac{2(\alpha_s/\xi_z)}{\sqrt{2\pi}(\sigma_0 k_L)^2},
$$

(4)

$$
\frac{U_\pm}{U_{+-}} = \frac{1 + 3e^{-b^2/2\sigma_0^2} \pm 4e^{-3b^2/8\sigma_0^2}}{(1 \pm e^{-b^2/4\sigma_0^2})^2}.
$$

(5)

These interaction energies are proportional to the ratio $\alpha_s/\xi_z$, the realistic values of which can be estimated to be between 0.03 and 0.07 [2]. Evaluation of Hubbard $U$’s, displayed in Fig. 3, shows that they are smaller than the bandgap between the lowest and the excited band for $|V_0| \approx 2.2E_R$, the latter being the largest optical lattice depth that we shall be concerned with in what follows.

[It is useful to note, however, that parameter $V_0$ here does not have entirely the same meaning as lattice depth in the case of conventional optical lattices.] For instance, for $V_0/E_R = -1.0$, $r = 0.08$, and $\alpha_s/\xi_z = 0.06$, values of Hubbard parameters are $U_+ = 0.0426E_R$, $U_- = 0.0498E_R$, $U_{+-} = 0.0420E_R$. Unlike the situation in ordi-
of unit cells in the system. For the first two bands, interaction parameters are \( U_{+,++} = U_+ \), \( U_{++,--} = U_-- \), and \( U_{+-,+-} = U_{++} + U_{-} + U_+ = U_{+} + U_0 = U_-- = U_+ \). Let us assume that the initial state is \( |\psi_i\rangle = (a_{-k}^\dagger)^N |\text{vac}\rangle \), where \( N \) is the number of particles in the condensate and \(|\text{vac}\rangle\) stands for the boson vacuum, while the final state is \( |\psi_f\rangle = a_{+k}^\dagger a_{+k}^\dagger (a_{-k}^\dagger)^2 |\text{vac}\rangle \). The change of the interaction energy between \(|\psi_i\rangle\) and \(|\psi_f\rangle\) is \( \Delta E_{\text{int}} = E_{\text{int},f} - E_{\text{int},i} = 4U_0 U_+ - 2U_0 + 2U_0 \), where \( \nu = N/N_0 \) is the average filling per DW. The energy-conservation condition reads \( \Delta E_{\text{kin}} + \Delta E_{\text{int}} = 0 \), i.e.,

\[
2e_-(K) - e_+(k_1) - e_+(k_2) = 4\nu U_+ - 2\nu U_0. \tag{7}
\]

By employing the Fermi Golden Rule and the tight-binding condition in the \( z \)-direction, in which the system is tightly confined, we arrive at the expression for the transition rate per DW:

\[
w = \frac{1}{\hbar} \left( \frac{4\pi \hbar^2 a_i}{m_p \xi_z} \right)^2 \sum_{k_1, k_2} |\int d^2r \Psi^*_{+k_1} \Psi^*_{+k_2} \Psi_{-k}^2|^2 \rho(e_+(k_1))^{-1} + \rho(e_+(k_2))^{-1}. \tag{8}
\]

Here, \( \Psi_{\pm k}(r) = e^{i k \cdot r} u_k^\pm(r) \) are the Bloch wave functions for the two bands \([u_k^\pm(r)\text{ being their corresponding lattice-periodic parts}], \rho(e) = \sum_{k \in \mathbb{B} \mathbb{Z}} \delta(e - e_+(k)) \) is the density-of-states for the \( '-' \)-band, and the prime indicates that the momentum summation is restricted to the pairs \((k_1, k_2)\) that satisfy both the energy-conservation condition in Eq. (7) and momentum conservation up to a reciprocal-lattice vector \((k_1 + k_2 = 2K + G)\). The transition rate is calculated by way of numerical evaluation of the \( '+' \)-band density-of-states \( \rho(e) \) and the spatial integral \( \int d^2r \Psi^*_{+k_1} \Psi^*_{+k_2} \Psi_{-k}^2 \) in Eq. (8). The latter is based on the eigenvectors obtained in the band-structure calculation, that is, coefficients in the Fourier expansion \( u_k^\pm(r) = \sum_{G} C_{k;G} e^{i G \cdot r} \) over reciprocal-lattice vectors.

To quantify the stability of bosons in the excited band, it is pertinent to compare it with the hopping time scale corresponding to the hopping amplitude \( t_h = \langle \Phi_i | H_0 | \Phi^{(+1)} \rangle \), where \( \Phi_i^*, \Phi^{(+1)} \) are the Wannier functions corresponding to a pair of adjacent (in the \( x \)-direction) DWs. For \( V_0/E_R = -1.0, r = 0.08 \), we obtain \( t_h = -0.1007 E_R \). With the choice of 87Rb atoms and \( \lambda = 810 \text{ nm} \) \((E_R \approx h \times 3.5 \text{ kHz})\), the hopping time scale is \( t_h/|t_h| = 0.45 \text{ ms} \). The logarithm of the dimensionless lifetime \( T = |t_h|/(\hbar w) \), depicted with varying filling factor in Fig. 4, exhibits nonmonotonic dependence on the filling. The salient feature is that the lifetime is very long for fillings smaller than some critical value and also for fillings larger than some higher critical value. This is easy to understand from the energy-conservation requirement: namely, the change in band energy in the decay process of interest is bounded both from above [by \( 2(\varepsilon_{\text{min}} - \varepsilon_+ \)] and from below [by \( 2(\varepsilon_{\text{min}} - \varepsilon_- \)], while the change in the interaction energy is linear in the filling factor [recall Eq. (7)].
The predicted superfluid phase can be experimentally identified from the time-of-flight density distribution 
\[ \langle n(r) \rangle \sim \sum |\Phi_-(k)|^2 \delta^2(k - K - G), \]
where \( k = m_b r/(\hbar t) \) and \( \Phi_-(k) \) is the Fourier transform of the Wannier function \( \Phi_-(x, y) \). The resulting density distribution, displayed in Fig. 5, has Bragg peaks at the condensate wave vector \( K \) and some of the wave vectors related to it by a translation through a reciprocal-lattice vector. Importantly, this distribution is asymmetric with respect to both \( k = K \) and \( k = 0 \). This is a combined effect of the odd parity of the Wannier function \( \Phi_-(x, y) \) and its extended character in real space (that is, localized in momentum space) in the regime of interest.

The resulting many-body state \( |\Psi\rangle \) spontaneously breaks the time-reversal and lattice translational symmetries, with circulating bond currents [17] \( J_{ij} \propto \langle \Psi | a_i^\dagger a_j^\dagger - a_j a_i |\Psi \rangle \propto \sin(K \cdot R_{ij}) \) between sites \( i \) and \( j \) with relative position vector \( R_{ij} \). Unlike the supersolid phase [6], which has the superfluid and density-wave orders, our state besides the superfluid order supports a current order. This state does not carry a net current since the group velocity corresponding to a band minimum equals zero; yet, it can potentially have anomalous transport properties resulting from breaking the time-reversal symmetry (i.e., violation of the Onsager reciprocity relations) [18].

In summary, we have found that a long-lived nonequilibrium superfluid state with broken time reversal and translational symmetries can be realized with cold bosons in the first excited Bloch band of a double-well optical lattice. The lifetime of this metastable state is shown to be several orders of magnitudes longer than the typical tunnelling time. Experimental realization using, for example, stimulated Raman transitions [11] or a similar method, is clearly called for.

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