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 populates 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 tunnelling time, a prediction that has recently been experimentally corroborated by the Mainz group [11]. In this Letter, 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 tunnelling 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]

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

Here, $k_L = 2\pi/\lambda$ is the magnitude of the laser wave vector, $V_0 = -|V_0| < 0$ (red-detuned lattice), while $r \equiv I_z/I_{xy}$ 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 $H_0 = -(\hbar^2/2m_b)(\partial_x^2 + \partial_y^2) + V(x, y)$ (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

$$\begin{aligned}
\langle \mathbf{k} + \mathbf{G}_{m,n}|H_0|\mathbf{k} + \mathbf{G}_{m,n}\rangle &= E_R\{[(k_x/k_L) + m + n]^2 + [(k_y/k_L) + m - n]^2\},\\
\langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{\pm1,0}\rangle &= \langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{0,\pm1}\rangle = 2rV_0,\\
\langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{\pm1,\pm1}\rangle &= (r - 1)V_0,\\
\langle \mathbf{k}|H_0|\mathbf{k} + \mathbf{G}_{\pm1,\mp1}\rangle &= (r + 1)V_0,
\end{aligned} \quad (2)$$

where $\mathbf{k} = (k_x, k_y)$ is the wave vector, $\mathbf{G}_{m,n} \equiv m\mathbf{b}_1 + n\mathbf{b}_2$ (m, n-integers) are the reciprocal-lattice vectors [with basis $\mathbf{b}_{1,2} = k_L(\hat{\mathbf{e}}_x \pm \hat{\mathbf{e}}_y)$], 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 $\mathbf{k} = (\pm1, 0)k_L$ and $(0, \pm1)k_L$. However, for optical lattice depths smaller (in absolute value) than some r-dependent threshold value, i.e., for $|V_0| < V_{\text{th}}(r)$, these minima occur at wave vectors $\mathbf{K}$ that

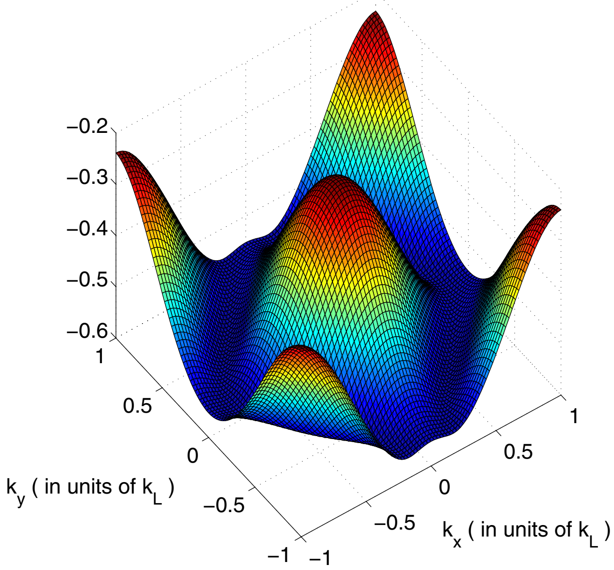

FIG. 1 (color online). Excited-band dispersion for $V_0/E_R = -1.0$, $r = 0.08$.

are incommensurate with the lattice period in both x- and y-directions and independent of V_0: $K_x = \pm 0.5k_L$, $K_y = \pm 0.5k_L$. For example, the threshold value for $r = 0.08$ is $V_{\rm th} \approx 1.08E_R$, while for $r = 0.15$ it is $V_{\rm th} \approx 0.83E_R$. Contour plot of the excited-band dispersion for $V_0/E_R = -1.0$ and $r = 0.08$ is displayed in Fig. 2. The band minima are only twofold degenerate, related by a mirror symmetry, because $(\pm\frac{1}{2}k_L, \pm\frac{1}{2}k_L)$ are equivalent to each other and so are $(\pm\frac{1}{2}k_L, \mp\frac{1}{2}k_L)$.

The two relevant bands originate from the lowest-energy states of a DW: the lowest $(+)$ band from the DW ground state (even parity), the excited $(-)$ band from the first

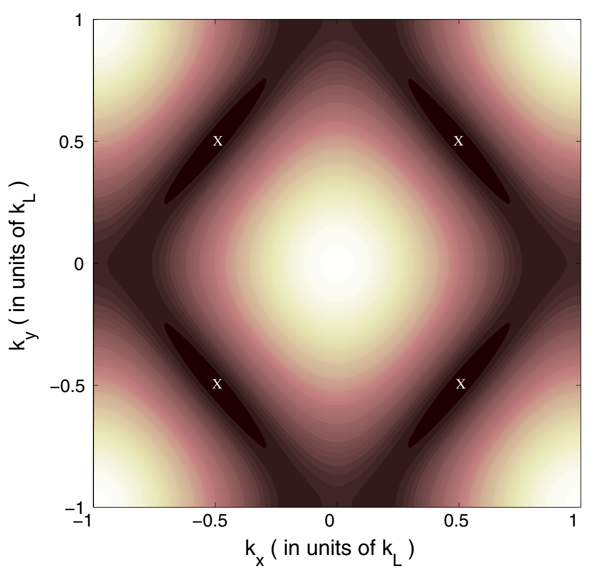

FIG. 2 (color online). Contour plot of the excited-band dispersion for $V_0/E_R = -1.0$, $r = 0.08$. Band minima are marked by "×."

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_2^+ molecular ion. For the DW comprising potential-minima at $(x_1, 0)$ and $(x_2, 0)$,

$$\Phi_\pm(x, y) = \frac{\varphi(x - x_1, y) \pm \varphi(x - x_2, y)}{\sqrt{2(1 \pm S)}}, \tag{3}$$

where $\varphi(x, y) = (\pi\sigma^2)^{-1/2}e^{-(x^2+y^2)/(2\sigma^2)}$ is a 2D Gaussian and $S = \int \varphi^*(x - x_1, y)\varphi(x - x_2, y)d^2\mathbf{r} = e^{-b^2/(4\sigma^2)}$ is the overlap integral of two such Gaussians, a distance $b \equiv x_2 - x_1$ apart. Optimal value σ_0 of the Gaussian-width σ 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 σ_0 becomes larger with decreasing lattice depth (i.e., for decreasing $|V_0|$). In particular, our calculation shows that for $|V_0|/E_R \lesssim 1.0$, one has $\sigma_0 \gtrsim 0.39b$. 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 $|V_0| \gtrsim 0.4E_R$, 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 ξ_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 $U_\pm = (g/\xi_z\sqrt{2\pi})\int\Phi_\pm^4(x, y)d^2\mathbf{r}$ and $U_{+-} = (g/\xi_z\sqrt{2\pi})\int\Phi_+^2(x, y)\Phi_-^2(x, y)d^2\mathbf{r}$, respectively, where $g \equiv 4\pi\hbar^2 a_s/m_b$. Calculation yields

$$\frac{U_{+-}}{E_R} = \frac{2(a_s/\xi_z)}{\sqrt{2\pi}(\sigma_0 k_L)^2}, \tag{4}$$

$$\frac{U_\pm}{U_{+-}} = \frac{1 + 3e^{-b^2/2\sigma_0^2} \pm 4e^{-3b^2/8\sigma_0^2}}{(1 \pm e^{-b^2/4\sigma_0^2})^2}. \tag{5}$$

These interaction energies are proportional to the ratio a_s/ξ_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 $|V_0| \lesssim 2.2E_R$, 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 $a_s/\xi_z = 0.06$, values of Hubbard parameters are $U_+ = 0.0426E_R$, $U_- = 0.0498E_R$, $U_{+-} = 0.0420E_R$. Unlike the situation in ordi-

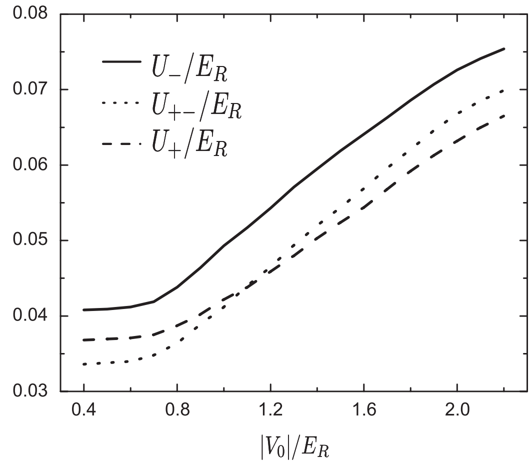

FIG. 3. Hubbard interaction parameters (in units of E_R) for $r = 0.08$, $a_s/\xi_z = 0.06$, and different lattice depths.

nary (single-well) optical lattices, where the Hubbard energy of the excited (p) band is smaller than that of the lowest (s) band, here we find that $U_- > U_+$.

While the "$-$"-band minima are degenerate, condensate fragmentation [15] in momentum space is prevented by the presence of interactions, no matter how weak. It is also easy to check that condensation into any state that is a linear superposition of two different band minima has higher energy than in a single minimum. Therefore, our state is a "simple" BEC [16] at wave vector denoted with $\mathbf{K}$. It is interesting to note that "$-$"-band has nearly flat dispersion around the minima, which may pose a challenge to the experimental realization of this state.

Our primary objective is to study the influence of interactions on the lifetime of bosons in a band minimum of the excited band. Thus, it is essential to elucidate the dominant decay process involved. It is worthwhile noting that the DW-type systems have asymmetric level-spacings, with energy levels appearing in pairs and the energy gap between the "$-$"-band and the second-excited band (W_{32}) being much greater than the one between the "$+$"- and "$-$"-bands (W_{21}); for instance, for $V_0/E_R = -1.0$ and $r = 0.08$, our band-structure calculation yields $W_{32} = 1.52E_R$, $W_{21} = 0.079E_R$. Therefore, promotion of particles from the "$-$"-band to the yet higher one, relevant for the decay channel studied in Ref. [5], is energetically very costly. Thus, the dominant decay process we need to consider is the one where two bosons decay from the "$-$"-band minimum to the "$+$"-band. The increase in the interaction energy, which is predominantly due to the exchange-energy contribution (interband interactions, here described by U_{+-}), compensates for the decrease in the single-particle band energy.

We recall the expression for the interaction energy

$$V_{\text{int}} = \frac{1}{2N_0} \sum_{n,m;\mathbf{k},\mathbf{k}',\mathbf{q}} U_{m'n',mn} a^\dagger_{n',\mathbf{k}+\mathbf{q}} a^\dagger_{m',\mathbf{k}'-\mathbf{q}} a_{m,\mathbf{k}'} a_{n,\mathbf{k}}, \quad (6)$$

where m, n, m', n' are band indices, and N_0 is the number of unit cells in the system. For the first two bands, interaction parameters are $U_{++,++} = U_+$, $U_{--,--} = U_-$, and $U_{++,--} = U_{--,++} = U_{+-,-+} = U_{+-,+-} = U_{-+,-+} = U_{-+,+-} = U_{+-}$. Let us assume that the initial state is $|\psi_i\rangle = (a^\dagger_{-,\mathbf{K}})^N|\text{vac}\rangle$, where N is the number of particles in the condensate and $|\text{vac}\rangle$ stands for the boson vacuum, while the final state is $|\psi_f\rangle = a^\dagger_{+,\mathbf{k_1}} a^\dagger_{+,\mathbf{k_2}} (a^\dagger_{-,\mathbf{K}})^{N-2}|\text{vac}\rangle$. The change of the interaction energy between $|\psi_i\rangle$ and $|\psi_f\rangle$ is $\Delta E_{\text{int}} = E_{\text{int},f} - E_{\text{int},i} = 4\nu U_{+-} - 2\nu U_-$, where $\nu = N/N_0$ is the average filling per DW. The energy-conservation condition reads $\Delta E_{\text{int}} + \Delta E_{\text{kin}} = 0$, i.e.,

$$2\varepsilon_-(\mathbf{K}) - \varepsilon_+(\mathbf{k_1}) - \varepsilon_+(\mathbf{k_2}) = \mathbf{4\nu U_{+-} - 2\nu U_-}. \quad (7)$$

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:

$$w = \frac{1}{\hbar}\left(\frac{4\pi\nu\hbar^2 a_s}{m_b \xi_z}\right)^2 {\sum_{\mathbf{k_1},\mathbf{k_2}}}' \frac{|\int d^2\mathbf{r}\Psi^*_{+,\mathbf{k_1}}\Psi^*_{+,\mathbf{k_2}}\Psi^2_{-,\mathbf{K}}|^2}{\rho[\varepsilon_+(\mathbf{k_1})]^{-1} + \rho[\varepsilon_+(\mathbf{k_2})]^{-1}}. \quad (8)$$

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

To quantify the stability of bosons in the excited band, it is pertinent to compare it with the time scale corresponding to the hopping amplitude $t_h = \langle\Phi^i_-|H_0|\Phi^{i+1}_-\rangle$, where Φ^i_-, Φ^{i+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 $t_h = -0.1007E_R$. With the choice of ^{87}Rb atoms and $\lambda = 810$ nm ($E_R \approx h \times 3.5$ kHz), the hopping time scale is $\hbar/|t_h| \approx 0.45$ 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 $2(\varepsilon^{\min}_- - \varepsilon^{\max}_+)$] and from below [by $2(\varepsilon^{\min}_- - \varepsilon^{\min}_+)$], while the change in the interaction energy is linear in the filling factor [recall Eq. (7)].

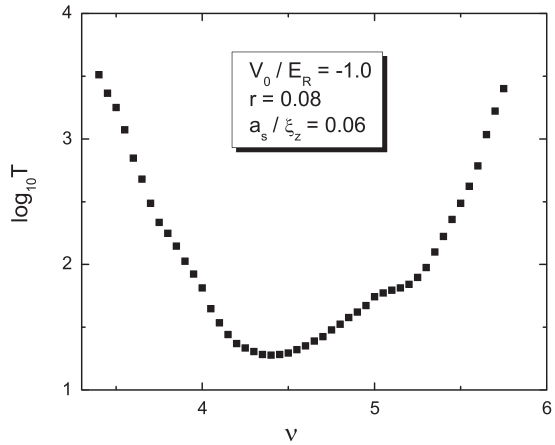

FIG. 4. Boson lifetime in the first excited band for different filling factors ν. Values of parameters are indicated.

The predicted superfluid phase can be experimentally identified from the time-of-flight density distribution $\langle n(\mathbf{r})\rangle_t \propto \sum_{\mathbf{G}} |\tilde{\Phi}_-(\mathbf{k})|^2 \delta^2(\mathbf{k} - \mathbf{K} - \mathbf{G})$, where $\mathbf{k} = m_b \mathbf{r}/(\hbar t)$ and $\tilde{\Phi}_-(\mathbf{k})$ 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 $\mathbf{K}$ 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 $\mathbf{k} = \mathbf{K}$ and $\mathbf{k} = \mathbf{0}$. 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] $\mathcal{J}_{ij} \propto \langle \Psi | a_i^\dagger a_j - a_j^\dagger a_i | \Psi \rangle \propto \sin(\mathbf{K} \cdot \mathbf{R}_{ij})$ between sites i and j with relative position vector $\mathbf{R}_{ij}$. 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].

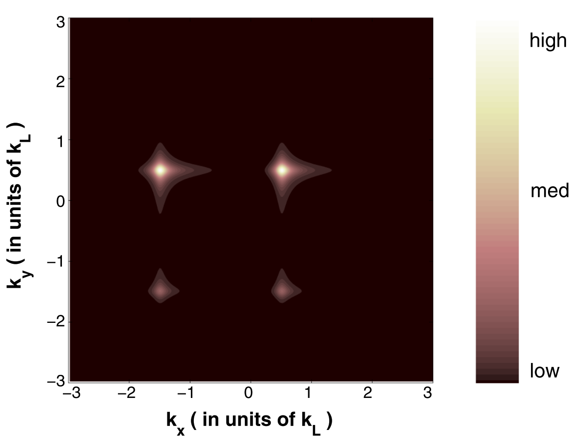

FIG. 5 (color online). Prediction of the density distribution in a time-of-flight experiment, for $V_0/E_R = -1.0$, $r = 0.08$, and condensate wave vector $\mathbf{K} = (0.5, 0.5)k_L$.

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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