Bloch waves and bloch bands of Bose-Einstein condensates in optical lattices

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Bloch waves and Bloch bands of Bose-Einstein condensates in optical lattices are studied. We provide further evidence for the loop structure in the Bloch band, and compute the critical values of the mean-field interaction strength for the Landau instability and the dynamical instability.

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I. INTRODUCTION

Bose-Einstein condensates (BECs) in optical lattices have been attracting increasing attention from both theorists [1–7] and experimentalists [8,9]. People are interested in how the interaction and coherence of this system affect the interesting phenomena observed with dilute cold atoms in optical lattices [10], such as Landau-Zener tunneling and Bloch oscillations. Recent studies have shown that these phenomena are indeed strongly influenced by the interaction between atoms. A series of effects have been discovered, including nonlinear Landau-Zener tunneling [1], the breakdown of Bloch oscillations [2,3], and dynamical instability [2,4]. There are similar nonlinear periodic systems in other fields, for example, the system of nonlinear guided waves in a periodically layered medium [11].

In a one-dimensional optical lattice created by two counterpropagating off-resonance laser beams, a BEC is essentially a one-dimensional system when the lateral motion can be either neglected [6] or confined [9]. Its grand canonical Hamiltonian is

$$H=\int_{-\infty}^{\infty}dx\left\{\psi^*\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}+v\cos x\right)\psi+\frac{c}{2}|\psi|^4-\mu|\psi|^2\right\},\tag{1.1}$$

where ψ is the macroscopic wave function of the BEC. In the above equation, all the variables are scaled to be dimensionless using the system's basic parameters: the atomic mass m, the wave number k_L of the two laser lights, and the average density n_0 of the BEC. The strength of the periodic potential v is in units of $4\hbar^2k_L^2/m$, the wave function ψ in units of $\sqrt{n_0}$, x in units of $1/2k_L$, and t in units of $m/4\hbar k_L^2$. The coupling constant $c=\pi n_0 a_s/k_L^2$, where $a_s>0$ is the s-wave scattering length. A two-dimensional version of this system has also received some attention [12].

In this Brief Report, we study the Bloch bands and Bloch waves of a BEC in an optical lattice, and present additional results that we were unable to obtain in our previous studies in Refs. [1,2]. These results are possible now due primarily to the development of an exact solution in Ref. [4]. As Bloch bands and Bloch waves are the two most important concepts in understanding a linear periodic system, they will also play crucial roles in the physics of the nonlinear periodic system (1.1). Bloch waves are the extremum states of the Hamiltonian (1.1) of the form

$$\psi(x,t)=e^{ikx}\phi_k(x),\tag{1.2}$$

where $\phi_k(x)$ is a periodic function of period 2π and k is the Bloch wave number. Each Bloch wave state (1.2) satisfies the time-independent Gross-Pitaevskii equation

$$-\frac{1}{2}\left(\frac{\partial}{\partial x}+ik\right)^2\phi_k+c|\phi_k|^2\phi_k+v\cos(x)\phi_k=\mu\phi_k,\tag{1.3}$$

as can be verified by variation of the Hamiltonian (1.1). Bloch bands are given by the set of eigenenergies $\mu(k)$.

II. BLOCH BANDS

In Ref. [1], we studied the tunneling between the two lowest bands to see how it is affected by the interaction. We found that the tunneling is described by a revised Landau-Zener model, which we call the nonlinear Landau-Zener model. This model predicts a dramatic change in the band structure, a loop appearing at the Brillouin zone edge $k=\pm 1/2$ for $c/v>1$ (see Fig. 1). A direct consequence of this loop structure is the breakdown of the Bloch oscillations due to the nonzero adiabatic tunneling into the upper band.

The loop structure is confirmed by an exact solution found recently by Bronski *et al.* [Eq. (10) of Ref. [4]], which assumes a much simpler form in terms of our notations:

$$\psi_B(x)=a_+e^{ix/2}+a_-e^{-ix/2},\tag{2.1}$$

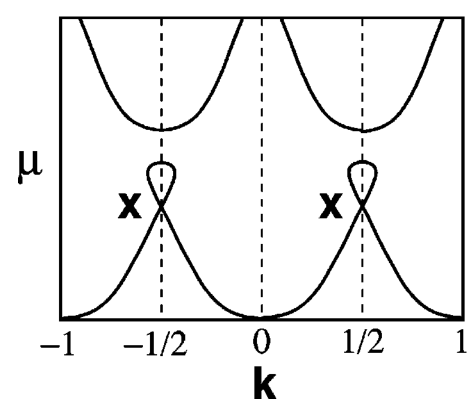

FIG. 1. Schematic drawing of the first and second Bloch bands of a BEC in an optical lattice when $c>v$. μ is in units of $4\hbar^2k_L^2/m$; k in units of $2k_L$.

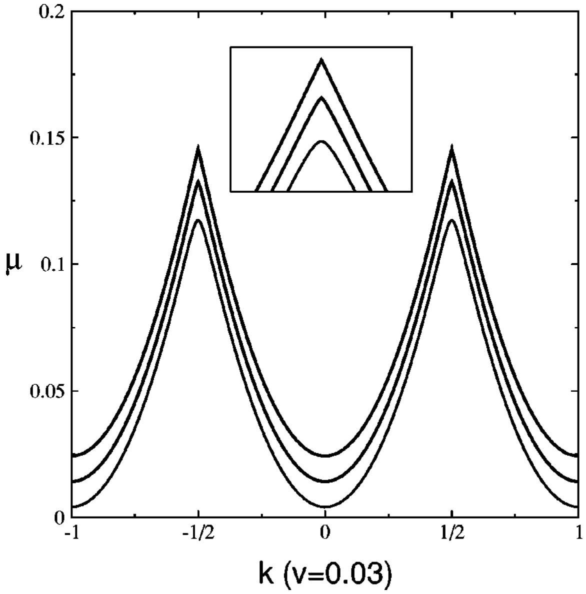

FIG. 2. The lowest Bloch bands of BECs in an optical lattice obtained by numerical calculation. Top curve is for $c=0.05>v$; middle curve for $c=0.03=v$; bottom curve for $c=0.01<v$. The inset is an enlarged version of the tips. The units are the same as in Fig. 1.

where $a_\pm=(\sqrt{c-v}\pm\sqrt{c+v}/2\sqrt{c}$. Substituting it into Eq. (1.3), we have $\mu=\frac{1}{8}+c$. This solution exists only when $c \geqslant v$, and is a Bloch wave at the edge of the Brillouin zone, $k=1/2$. This Bloch wave carries a nonzero velocity $\sqrt{c^2-v^2}/2c$, while its complex conjugate has an opposite velocity. This is in sharp contrast with the behavior in a linear periodic system, in which Bloch waves at the zone edge always have zero velocity. This difference confirms the looped band structure. The solution ψ_B and its complex conjugate are the two degenerate states at the crossing point X (Fig. 1). The nonzero velocity carried by this Bloch wave is a manifestation of the superfluidity of the BEC. For free particles, the flow $e^{ix/2}$ is stopped completely by Bragg scattering from the periodic potential; for the BEC, the flow can no longer be stopped when the superfluidity is strong, that is, $c>v$.

This loop structure is further supported by our numerical calculation of the lowest band $\mu(k)$, as shown in Fig. 2. It is evident that the slope $d\mu/dk$ at the zone edge $k=\pm 1/2$ becomes nonzero as the interaction strength c is increased over the periodic potential strength v, a clear indication of the loop structure. However, due to the limitation of our numerical method [2], we are unable to produce the loop directly. An improved numerical method is being developed to calculate the loop and the higher Bloch bands.

III. STABILITY OF BLOCH WAVES

In our second paper [2], we studied the superfluidity and stability of the Bloch waves in the lowest band (excluding the loop). We found that the Bloch waves in the middle of the Brillouin zone represent superflows, and the other Bloch waves toward the zone edge have both a Landau instability and a dynamical instability. Moreover, we found that these instabilities can disappear from all these Bloch waves when the atomic interaction is beyond certain critical values for a fixed lattice strength. For easy reference, we call the critical value for the Landau instability c_L, and the critical value for the dynamical instability c_d. In that work, we were unable to find these two critical values because our numerical method was not good enough to find accurate Bloch waves at the zone edge. Now the exact solution ψ_B allows us to overcome the difficulty and calculate these two critical values c_L and c_d. It is done by studying the stabilities of the Bloch wave ψ_B. Since the Bloch wave at the zone edge is the last one to become stable either in terms of the Landau instability or dynamically, the critical values of c for ψ_B to become stable are just c_L and c_d.

The physical significance of the two critical values c_L and c_d of ψ_B lies in the way the Bloch states at $k\neq 0$ are achieved experimentally: the Bloch state at $k=0$ is first prepared and then driven to the desired Bloch states at $k\neq 0$ by accelerating the optical lattice [10]. Therefore, as the only point connecting the loop to the rest of the Bloch band, a stable ψ_B means that the Bloch states on the loop can be accessed and studied experimentally by accelerating the optical lattice.

We first study the Landau instability by analyzing how the energy of the system deviates under a small perturbation. Since the system is periodic, we are allowed to write the perturbation as

$$\psi=\psi_B+e^{ix/2}[u(x,q)e^{iqx}+v^*(x,q)e^{-iqx}], \tag{3.1}$$

where q ranges between $-1/2$ and 1/2, labeling the perturbation mode, and the perturbation functions u and v have a periodicity of 2π in x. Then the energy deviation caused by this perturbation is

$$\delta E=\int_{-\infty}^{\infty}dx(u^*,v^*)M(q)\begin{pmatrix}u\\ v\end{pmatrix}, \tag{3.2}$$

where

$$M(q)=\begin{pmatrix}\mathcal{L}(1/2+q) & c\phi_B^2\\ c\phi_B^{*2} & \mathcal{L}(-1/2+q)\end{pmatrix}, \tag{3.3}$$

with

$$\mathcal{L}(k)=-\frac{1}{2}\left(\frac{\partial}{\partial x}+ik\right)^2-v\cos(x)+c-\frac{1}{8} \tag{3.4}$$

and

$$\phi_B^2=c+\sqrt{\frac{c^2-v^2}{2c}}-\frac{v}{c}e^{-ix}+c-\sqrt{\frac{c^2-v^2}{2c}}e^{-2ix}. \tag{3.5}$$

If $M(q)$ is positive definite for all $-1/2\leqslant q\leqslant 1/2$, the Bloch wave ψ_B is a local minimum and a superflow. Otherwise, δE can be negative for some q; the Bloch wave is a saddle point and has a Landau instability. As already noticed in Ref. [2], the positive definiteness of the matrices $M(q)$ for all q's is

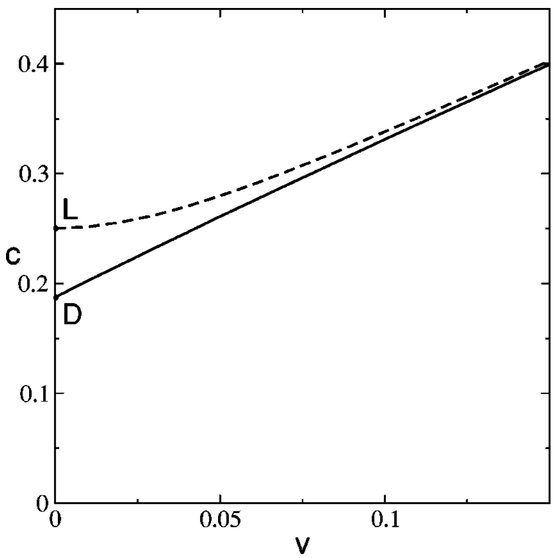

FIG. 3. The critical values of c. The dashed line is c_L, the critical value of c for all the Bloch waves in the lowest band being superflows; the solid line is c_d, above which all the Bloch waves in the lowest band are dynamically stable. $c=\pi n_0 a_s/k_L^2$, and v is in units of $4\hbar^2 k_L^2/m$.

guaranteed by the positive definiteness of $M(0)$. Diagonalizing $M(0)$ for different values of c with a fixed v, we obtain the critical value c_L, which is shown as a dashed line in Fig. 3. For the intersection point L at $v=0$, we have $c_L=1/4=(k=1/2)^2$.

The dynamical stability of the Bloch wave ψ_B is studied by linearizing the Gross-Pitaevskii equation:

$$i\frac{\partial\psi}{\partial t}=-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}+c|\psi|^2\psi+v\cos(x)\psi. \tag{3.6}$$

With a procedure similar to the above, we arrive at the linearized dynamical equation

$$i\frac{\partial}{\partial t}\begin{pmatrix}u\\ v\end{pmatrix}=\sigma M(q)\begin{pmatrix}u\\ v\end{pmatrix},\quad \sigma=\begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix}. \tag{3.7}$$

The dynamical stability is determined by the matrix $\sigma M(q)$. If all $\sigma M(q)$ for $-1/2\leqslant q\leqslant 1/2$ have no complex eigenvalues, then ψ_B is dynamically stable; otherwise, it is unstable. However, as pointed out in Ref. [2], the dynamical instability always starts at the perturbation mode $q=1/2$. Therefore, we need to diagonalize only $\sigma M(1/2)$ to find the critical value c_d. The results are shown as the solid line in Fig. 3, where the intersection D at $v=0$ is precisely $c_d=3/16$. This lower bound of the critical value c_d simply means that when $c<3/16$ any periodic potential brings the dynamical instability into the system.

The value of c_d at point D is confirmed by analyzing the limiting case $v\ll c$, where the matrix $\sigma M(1/2)$ can be approximated with a 4×4 matrix:

$$\sigma M(1/2)\approx\begin{pmatrix} c-\frac{1}{8} & 0 & c & -v\\ 0 & c+\frac{3}{8} & 0 & c\\ -c & 0 & -\frac{3}{8}-c & 0\\ v & -c & 0 & \frac{1}{8}-c\end{pmatrix}. \tag{3.8}$$

The eigenvalues of this matrix can be found exactly; all of them are real only when $c>3/16$. Note that the point D must be understood in the sense that $c_d\rightarrow 3/16$ as $v\rightarrow 0$ since precisely at $v=0$ the system has no dynamical instability. As one may get an impression from Fig. 3 that the asymptotic behavior of the two curves at large v is linear, we want to stress that it is not. Our numerical results show that the asymptotic behavior undergoes very small oscillations along a straight line, of which we have no complete understanding at this moment.

Finally, we make two remarks. First, the method of defining Bloch waves and Bloch bands for the nonlinear system (1.1) at the beginning is a natural generalization from the linear periodic system. Nevertheless, there is an essential difference due to the nonlinearity. In the linear system $(c=0)$, the Bloch waves are the only extremum states of the Hamiltonian or the only eigenfunctions of Eq. (1.3); for the nonlinear system (1.1), there are possible extremum states that are not Bloch waves.

Second, it is interesting to put the dynamical instability that is discussed in this report and in Refs. [2,4,5] into perspective. Usually, quantum dynamics is a regular motion because it has discrete eigenvalues and thus an almost periodic motion regardless of whether its corresponding classical dynamics is chaotic or not. In this sense, quantum chaos has been called "pseudochaos" [13]. In contrast, the dynamical instability that we have discussed is "true" quantum dynamical chaos that deserves more attention in the future. On the other hand, with the Madelung transformation $\psi(x,t)=\rho(x,t)e^{iS(x,t)}$, the nonlinear Schrödinger equation (3.6) can be turned into a set of equations of fluid dynamics. In this regard, the quantum dynamical instability should be related to the turbulence in fluid dynamics, and we may call it "quantum turbulence."

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[1] Biao Wu and Qian Niu, Phys. Rev. A **61**, 023402 (2000); O. Zobay and B. M. Garraway, *ibid.* **61**, 033603 (2000).
[2] Biao Wu and Qian Niu, Phys. Rev. A **64**, 061603(R) (2001).
[3] A. Trombettoni and A. Smerzi, Phys. Rev. Lett. **86**, 2353 (2001).
[4] J. C. Bronski, L. D. Carr, B. Deconinck, and J. N. Kutz, Phys. Rev. Lett. **86**, 1402 (2001).
[5] J. C. Bronski, L. D. Carr, B. Deconinck, J. N. Kutz, and K. Promislow, Phys. Rev. E **63**, 036612 (2001).
[6] Kirstine Berg-Sørensen and Klaus Mølmer, Phys. Rev. A **58**, 1480 (1998); D. Choi and Qian Niu, Phys. Rev. Lett. **82**, 2022 (1999).
[7] M. Halthaus, J. Opt. B: Quantum Semiclassical Opt. **2**, 589 (2000).
[8] B. P. Anderson and M. A. Kasevich, Science **282**, 1686 (1998).
[9] S. Burger, F. S. Cataliotti, C. Fort, F. Minardi, M. Inguscio, M. L. Chiofalo, and M. P. Tosi, Phys. Rev. Lett. **86**, 4447 (2001).
[10] C. F. Bharucha, K. W. Madison, P. R. Morrow, S. R. Wilkinson, B. Sundaram, and M. G. Raizen, Phys. Rev. A **55**, R857 (1997); K. W. Madison, C. F. Bharucha, P. R. Morrow, S. R. Wilkinson, Q. Niu, B. Sundaram, and M. G. Raizen, Appl. Phys. B: Lasers Opt. **65**, 693 (1997).
[11] A. A. Sukhorukov and Y. S. Kivshar, e-print nlin.PS/0105073.
[12] B. Deconinck, B. A. Frigyik, and J. N. Kutz Phys. Lett. A **283**, 177 (2001).
[13] G. Casati and B. Chirikov, Physica D **86**, 220 (1995).