Nature of intrinsic relation between Bloch-band tunneling and modulational instability

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On examples of Bose-Einstein condensates embedded in two-dimensional optical lattices we show that in nonlinear periodic systems modulational instability and inter-band tunneling are intrinsically related phenomena. By direct numerical simulations we found that tunneling results in attenuation or enhancement of instability. On the other hand, instability results in asymmetric nonlinear tunneling. The effect strongly depends on the band gap structure and it is especially significant in the case of the resonant tunneling. The symmetry of the coherent structures emerging from the instability reflects the symmetry of both the stable and the unstable states between which the tunneling occurs. Our results provide an evidence of profound effect of the band structure on superfluid-insulator transition.

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Bose-Einstein condensate (BEC) embedded in an optical lattice represents a remarkable laboratory for study of the interplay among various physical phenomena, having general physical nature. One of such phenomena—the modulational instability—is a characteristic feature of nonlinear systems\cite{1}. For BECs (where it is also referred to as dynamical instability) it has been described theoretically in\cite{2,3,4,5} and observed experimentally in\cite{1}. Another phenomenon, which is typical for linear periodic systems, is the Landau-Zener tunneling. It was also discussed in the context of the BEC applications\cite{6,8} and explored in a series of experiments\cite{10}, where the phenomenon was implemented in one-dimensional (1D) optical lattices and was stimulated by the effective linear force created by the lattice acceleration. The existing theoretical descriptions, based on two-level models, however, are not unanimous about how Landau-Zener tunneling occurs, except one point: two-body interactions (i.e. the nonlinearity) make the tunneling asymmetric. It was suggested in Ref.\cite{9}, that asymmetry stems from the fact that the Landau-Zener tunneling in a nonlinear system is intimately related to the instability. Indeed, tunneling couples two band edges with the eigenstates that acquire different stability properties in the presence of the nonlinearity, one of them being unstable. In this case the initial atomic distribution turns out to be of crucial importance. Recently, Landau-Zener tunneling and modulational instability have been explored within the unique experimental setting\cite{11}. However, the data available so far, are not conclusive about the reasons for asymmetry of nonlinear Landau-Zener tunneling. Among the other reasons, it is due to the fact that to stimulate the tunneling a linear force is necessary. Such a force gives rise to other phenomena, such as, for example, Bloch oscillations\cite{12}, which in turn, can also imply the asymmetry.

¿From the point of view of understanding the fundamental relation between tunneling and modulational instability, flexibility of multidimensional lattices in general\cite{11}, and 2D lattices, in particular, open new perspectives, offering diversified possibilities of the observing tunneling and instabilities, without any use of external forces, namely, that of the lattice acceleration. For systems of cold noninteracting atoms this has already been discussed in\cite{12}. Moreover, within the framework of a different system, which is a beam propagation through an optically induced 2D lattice, nonlinear tunneling has been observed experimentally in\cite{13}. In what follows tunneling without external forces is referred to as Bloch-band tunneling and is subject of our principal concern.

Our main goal is to explore intrinsic relation between Bloch-band tunneling and modulational instability. We show that tunneling can either enhance of attenuate instability, as well as instability can result in asymmetry of tunneling with respect to initial population of stable and unstable states. Experimentally such states can be created by manipulating with noninteracting atoms and subsequent switching in the nonlinearity, what can be managed by means of Feshbach resonance. We argue that the band structure is the most relevant characteristic governing the dynamics and supports resonant exchange of the atoms between bands. As an important physical application of our results, we notice that instability of Bloch waves, with subsequent emergence of coherent localized structures, implies the superfluid-insulator transition (see e.g.\cite{2}, as well as\cite{14} for discussion in the tight-binding approximation, and\cite{15} for experimental observation). We thus provide an evidence of profound influence of the band structure on the superfluid-insulator transition and suggest a possibility of its managing by simple control of parameters of an optical lattice.

We consider an effectively 2D BEC, with a positive
scattering length, governed by the Gross-Pitaevskii equation

\[ i \frac{\partial \Psi}{\partial t} = -\Delta \Psi + V(\mathbf{r})\Psi + |\Psi|^2 \Psi. \]  

(1)

Here time is measured in the units of \( 2\hbar/E_R \), where \( E_R = \hbar^2 k^2/(2m) \) is the recoil energy, \( k = 2\pi/\lambda \) is the wave vector of the laser beams considered equal in all directions, and coordinates \( \mathbf{r} = (x, y) \) are measured in the units of \( k^{-1} \). We restrict our consideration to the potential

\[ V(\mathbf{r}) = V_0 [\cos(2x) + \cos(2y) - \cos(2x)\cos(2y)] \]  

(2)

where \( V_0 \) is measured in the units of \( 2E_R \).

When the nonlinearity is weak enough and the lattice amplitude is of order of the recoil energy, the underlying band structure makes possible local additional external factors are involved. The nonlinearity couples modes in different bands making possible local transfer atoms among them.

When Bloch bands overlap in different directions (Case I in Fig. 1), the linear tunneling between states with the same energy is possible. It turns out, however, that the most intensive exchange of atoms between the bands occurs not in this case, but in the case of a resonant tunneling, when matching conditions are satisfied, i.e., when four waves satisfy simultaneously the energy and momentum conservation laws (see e.g. [10]). Such a lattice can be created by adjusting the laser intensity as it is shown in Case II of Fig. 1. The states in points M (of the first band) and X (of the second band) possess not only the same energy \( E_M = E_X \) [hereafter \( E_\alpha = E(q_\alpha) \) with \( E(q) \) being the eigenvalue of the operator \( -\Delta + V(x, y) \); explicit forms of the dependence \( E(q) \) are shown in Fig. 1], but also satisfy the conservation of the quasi-momentum. By denoting an arbitrary vector of the reciprocal lattice by \( \mathbf{Q} \), the last condition can be expressed either as \( q_M = q_X + q - q_M + Q \) if one considers tunneling from initial state X to the state M or as \( q_X = q_M + q_M - q_X + Q \) if one considers tunneling from M to X. A process where the majority of particles is initially concentrated in the state A from where they tunnel into the state B will be referred to as A→B tunneling.

Resonant wave interactions available in Cases I and III, are those conventionally referred to as self-phase and cross-phase modulations and governed by the integrals

\[ \chi_{X,M} = 4 \int \Psi_X^* \Psi_M \mathbf{d} \mathbf{r} \]  

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respectively [hereafter \( \Psi_{X,M} \) are the Bloch states, real for the points X and M, and \( V_0 = (0, \pi) \times (0, \pi) \) is a volume of the unit cell of the lattice]. In the two-mode approximation one can introduce slowly varying modulations \( A_{X,M} \) of the states \( \Psi_{X,M} \) and represent (in the leading order)

\[ \Psi = A_X(\mathbf{r}, t) \Psi_X(\mathbf{r}) e^{-iE_Xt} + A_M(\mathbf{r}, t) \Psi_M(\mathbf{r}) e^{-iE_Mt}. \]  

(3)

Then, following the standard steps (see e.g. [11]), one deduces the Hamiltonian governing the dynamics slow amplitudes (\( \partial A_\alpha/\partial t = -i\delta H/\delta A_\alpha \)):

\[ H = \frac{1}{2} \int d\mathbf{r} \left\{ |\hat{M}^{-1} \nabla A_X|^2 + |\hat{M}^{-1} \nabla A_M|^2 + \chi_X |A_X|^4 + \chi_M |A_M|^4 + 4\chi |A_X|^2 |A_M|^2 \right\}. \]  

(4)

Here \( \hat{M}^{-1} (\alpha = X,M) \) is a \( 2 \times 2 \) tensor of the inverse effective mass in a point \( q_\alpha \), whose entries are defined by \( M^{-1}_{\alpha} (q_\alpha) = \partial^2 E(q_\alpha)/(\partial q_{\alpha,i} \partial q_{\alpha,j}) \). The introduced dynamics preserves the averaged number of atoms in each band, i.e. \( N_{X,M} = \int |A_{X,M}|^2 d\mathbf{r} \) are constants.

If, however, the matching conditions are met, then the other types of the resonant four-wave interactions, resulting in change of the average number of atoms in the bands, can occur. Now the Hamiltonian governing evolution of the modulation of the Bloch states reads

\[ H = \frac{1}{2} \int d\mathbf{r} \left\{ |\hat{M}^{-1} \nabla A_X|^2 + |\hat{M}^{-1} \nabla A_M|^2 + \chi_X |A_X|^4 + \chi_M |A_M|^4 + 4\chi |A_X|^2 |A_M|^2 \right\}. \]  

(5)

The resonant processes occur simultaneously with the nonresonant transitions between states in different bands but with the same wavevector (as those observed in [12]). The latter, however, are negligible in our configuration.
This was proved numerically by evaluating projections of the obtained distributions into the states $\Psi_{M,X}$.

It follows from (3) and (4) that stability of initial distributions is determined by the signs of $M_{jj}^{-1}$ [4]. Since we consider the condensate with a positive scattering length, and $M_{jj}(q_x) > 0$ and $M_{jj}(q_M) < 0$ ($j = x,y)$, in both cases the states $\Psi_M$ and $\Psi_X$ are unstable and stable, respectively, since one of the stability conditions of a band $\alpha$ populated with the density $\rho_\alpha$ reads $Z(Z + 2x_\alpha\rho_\alpha) < 0$ with $Z = q_x^2/M_x + q_y^2/M_y$. Meantime, in the resonant case (3) there exists an additional domain of instability defined by the condition $[Z + \rho_\alpha^2(3 - \chi_\alpha)][Z + \rho_\alpha^2(1 - \chi_\alpha)] < 0$, what results in faster development of instability, reported in numerical simulations below. Thus, tunneling can either stabilize or destabilize the dynamics of the wave function depending on the direction of the tunneling that corresponds to $M\rightarrow X$ and $X\rightarrow M$ processes, respectively.

To inspect the interplay between tunneling and instability, we carried out direct numerical simulations of Eq. (1), subject to periodic boundary conditions and initial condition in a form $r_X(0)\Psi_M + r_X(0)\Psi_X$ [c.f. (4)] where the factors $\alpha$ determine the distribution of atoms between the states. Simultaneous use of smooth initial perturbation allowed us to accelerate the development of the instability (c.f. time scales in Fig. 2 where no initial perturbation is applied and Fig. 3 where initial states were perturbed).

For quantitative analysis we computed the occupation rates $r_{X,M} = N_{X,M}/N$, where $N = N_X + N_M$ is the total number of atoms. When the two states have nonzero initial population, the nonlinearity results in periodic particle exchange between these states. When tunneling is nonresonant (Cases I and III in Figs. 2 and 3) this exchange is relatively weak; it is caused by wave interactions of higher orders not accounted by the Hamiltonian (4). Exchange of atoms between the bands becomes the leading order phenomenon when tunneling is resonant (Case II) what is described by additional hopping integrals in (6).

Let us consider $X\rightarrow M$ process shown in Fig. 2. Period of oscillations $T$ decreases as amplitude potential $|V_0|$ increases: from the top to bottom $T \approx 560, 362, 116$. This is explained by growth of the cross-phase modulation: (from top to bottom) $\chi \approx 6.4; 6.8; 7.6 \times 10^{-3}$. When the gap is opened (Case III) the system stays for a long time in a stable position due to low occupation of the unstable state $M$. Nevertheless, because of periodic increase of the population of the state $M$ the instability is developed at $t \approx 3100$. Possibility of tunneling accelerates this process: in the Case I the instability is developed at $t \approx 2500$. The most substantial enhancement of the instability is observed when the tunneling becomes resonant: in the Case II the instability occurs at $t \approx 2050$.

The development of the instability results in emergence of coherent structures. If tunneling is resonant (Case II) atomic distribution displays asymmetric peaks, which evolve in time. The peaks are elongated in $x$-direction, what seems to contradict to an intuitive assumption that the symmetry of the developed coherent structure resembles the symmetry of the unstable state, from which they are evolved [4]. Such an interpretation well corroborates with the results shown below in the Cases I and III of Fig. 4. In the case at hand, however, one has to keep in mind that, while the tensor of the inverse effective mass is symmetric at the unstable point $M$, it is not symmetric any more at the point $X$. Specifically, for the Case II in Fig. 2 $M_{XX}^{-1} = \text{diag}(3.03)$. Since $M_{xx}^{-1} > M_{yy}^{-1}$, when the atoms are at the $X$-point, dispersion of the wave along the $x$-direction is stronger than the dispersion along $y$-axis.

Since instability is developed due to particle exchange between the two states, this explains elongation of the emerging excitations along the $x$-axis.

Now we turn to the situation when initially the most of particles occupy unstable state $M$, i.e. to the $M\rightarrow X$ process, illustrated in Fig. 3. In the configuration where there is no linear tunneling (Case III) the instability is developed at $t \approx 270$. Nonresonant tunneling (Case I) leads to some attenuation of the instability that starts at $t \approx 370$. In the both cases the developed coherent

FIG. 2: [Color online] (a) Dynamics of the density maximum; (b) Time evolution of the occupation rates $r_X(t)$ (red lines) and $r_M(t)$ (blue lines). (c) Snapshots of the atomic density distributions after instability is developed. All simulations are done with the initial distributions $r_M(0) = 0.2$ and $r_X(0) = 0.8$. The cases I, II, and III correspond to those in Fig. 4.
structures resemble those observed in Ref. [4] for a separable square lattice and reflect the symmetry of the lattice. Dramatical changes occur in the case of the resonant Bloch-band tunneling (the Case II). Besides significant attenuation of instability, which now occur at $t \approx 450$, one observes change of the symmetry of the developed structure. Like in the case of $X \rightarrow M$ tunneling, the emerging pulses are strongly localized along $y$-axis and elongated along $x$-axis, what corroborates with the fact that the attenuation of the instability has occurred due to tunneling into the stable state $X$.

Different symmetries of the emerging structures, that can be identified e.g. by means of diffraction imaging, provide a possibility for the experimental observation of the phenomenon and identification of the type of the process. We also mention that although the time difference in development of instability differs in our numerics only by $10\% \div 30\%$ for different processes, this is experimentally observable time. Indeed, for condensed rubidium atoms in calculations 50 units of the dimensionless time correspond to $2 \, \text{ms}$, what means that time difference in instability of different regimes is of order of $8 \div 20 \, \text{ms}$.

The results shown in Figs. 2, 3 reveal a common feature, namely that until the instability is developed the atoms are mainly distributed between the two interconnected states $\Psi_M$ and $\Psi_X$. This is a strong support of the validity of a two-mode approximation suggested in [8], and in this Letter defined by the Hamiltonians [11] and [9]. However, after the instability is developed, we observed transfer of atoms to states other than $\Psi_{X,M}$ (see panels (b) in Figs 2, 3). When such transfer takes place the two-mode approach is not applicable any more.

To conclude, we have shown that two-body interactions in a BEC loaded in a two-dimensional orthogonal nonseparable optical lattice result in a strong interplay between the phenomena of Bloch-band tunneling and modulation instability. As a consequence, tunneling appears to be one of the key factors for the superfluid-insulator transition, especially in the case of lattices with negligible gap, where matching conditions for the four wave interactions are provided. The gap width, meantime, is an easily changeable lattice parameters and can be controlled by the laser intensity. Specifically we found that the atoms, initially loaded in a stable state, due to inter-band exchange develop instability, which is significantly enhanced when the matching conditions are satisfied. On the other hand resonant tunneling attenuates the instability when atoms are initially loaded in an unstable state. We also found that the instability makes the Bloch-band tunneling strongly asymmetric in the sense of dependence of developed patterns on initial atomic distribution.

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