Classical interpretation of dynamics of ultracold atoms in the titled optical lattice

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Abstract. In this paper, we study the dynamics of ultracold $^{87}$Rb under the influence of titled optical lattice via Bloch oscillation in the single-band regime. By simulating the intraband dynamics of wavepacket in position and momentum spaces, the dependences of amplitude and period of the oscillation on titled coefficient and lattice height are shown and compared with classical theory under tight-binding approximation. We also verify the limit of the single-band approximation where the Landau-Zener transition is neglected.

1. Introduction

The study of the ultracold atom has risen since the theoretical prediction of the fifth state of matter at extremely low temperatures in the 1920s, that is Bose-Einstein condensation (BEC). However, only after the invention of the laser in 1960, the interaction of atoms and laser has been rigorously studied leading to the introduction of various cooling methods such as the magneto-optical trap [1], evaporative cooling [2], Sisyphus cooling [3], etc. Among these techniques, optical lattice (OL) is considered as the most effective atomic trap with a perfect periodicity which enables us to observe the BEC in bosonic system. Nowadays, the role of OL in recent experiments is vital for inspiring the theoretical study of the behavior of trapped atoms [4]. In solid-state physics, the quantum system confined in a periodic potential is such a common problem whose unique features are band structures and periodic Bloch waves followed Blochs theorem. To expand the investigation, the static electric field is utilized for leading to the formation of a discrete energy spectrum called Wannier-Stark ladder [5]. Moreover, with the support of the external electric field, atoms located at a lower energy level can overcome the band gap and jump onto higher states. This phenomenon is named as Landau-Zener (LZ) transition which explicitly displays the interband dynamics [6]. This problem is firstly introduced by Bloch and Zener in the 1930s in terms of crystal electron trapped in a periodic potential in combination with the external electric field [7,8].

Besides the LZ transition and Wannier-Stark ladder, Bloch oscillation is also an attractive phenomenon associating with the examination of the ultracold system. In Bloch oscillation, the electrons perform an oscillation with the period $T_B = 2\pi\hbar/(Fd)$ with $F$ and $d$ are the field strength and periodicity of the potential, respectively. This oscillation contradicts the conventional idea that electrons are linearly accelerated by the external electric field. Despite the fact that the dynamics of ultracold system are clearly displayed via Bloch oscillation, this idea used to be a huge controversy for such a long time due to the decoherence of the system,
thus was not able to be experimentally observed. In 1992, Bloch oscillation was indirectly observed by Karl Leo with the help of superlattice conductor [9] ending this argument. Note that the superlattice conductor did not provide appropriate environment for Bloch oscillation to be well observed. The research was expanded to the system of neutral atoms where the linear accelerating potential was introduced to create the inertial force on the atoms [10]. In 1996, Dahan and colleagues followed this approach to observe of Bloch oscillation of $^{133}$Cs atoms in momentum space induced by adiabatic trapping method combining OL and linear potential [10]. This study led to the prominent study of Morsh on the observation of Bloch oscillation in the BEC of $^{87}$Rb [11]. Recently, this topic is still popular with the study of Bloch oscillation in the absence of a lattice [12] or improving the efficiency of Bloch oscillation in the limit of the tight-binding model [13]. In 2018, Geiger et al. for the first time proposed two procedures to directly observe Bloch oscillation in position space of $^7$Li atoms in tilted OL [14]. Therefore, the detailed analysis of Bloch oscillation in position space is well deserved.

In this work, we provide a comprehensive study of the intraband dynamics of ultracold $^{87}$Rb in OL with the linear potential using the solutions to the time-dependent Schrödinger equation (TDSE). The evolutions of the wavepacket are thoroughly examined for several representative lattice heights with fixed field strength and vice versa. Here, the experimental parameters in the work of Dahan [10] are adopted. We then analyze the property of wavepacket in position and quasimomentum space under the single-band approximation where the interband coupling is neglected. The comparison between classical perspective and quantum Bloch oscillation is also provided under the tight-binding model. Finally, the limit of the single-band approximation is evaluated.

This article is organized as follows: In Section 2, we illustrate the wavepacket in position and momentum configuration as well as the dependences of Bloch oscillation characteristics on the titled angle and lattice height. The comparison between the classical model and the quantum simulation is also given. Section 3 concludes the topic.

2. The dynamics of ultracold atoms confined in the tilted optical lattice

2.1. Experimental setup

The purpose of our paper is to simulate the Bloch oscillation in the BEC of $^{87}$Rb using the parameters provided in Ref. [10] in momentum and position spaces. Note that the investigation of the Bloch oscillation in position space is recently drawn much interest due to the first experimental observation in the work of Geiger et al. [14]. The parabolic potential is firstly introduced to propose a stable control of the observation. The advantages of this approach were rigorously discussed in the Refs. [15,16]. The initial Hamiltonian $H_0$ used to trap the atoms inside the parabolic optical potential has the form

$$H_0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_0 \sin^2(k Rx) + \frac{1}{2}m \omega^2 x^2,$$

(1)

where $k_R = 2\pi/\lambda$ is the recoil momentum with $\lambda$ is the wavelength of the laser pulses. Here $\omega$ and $m$ are the frequency of the parabolic trap and the mass of the $^{87}$Rb, respectively. Just after the stability of the system, the parabolic trap is switched off and the linear potential with the strength $F$ is turned on adiabatically. The Hamiltonian of the system is now changed to

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_0 \sin^2(k Rx) + F x.$$

(2)
The Hamiltonians are scaled by the recoil energy to its dimensionless form

\[ H_0 = -\frac{\partial^2}{\partial \chi^2} + \xi \sin^2(\chi) + \nu \chi^2, \] (3)

\[ H = -\frac{\partial^2}{\partial \chi^2} + \xi \sin^2(\chi) + \alpha \chi, \] (4)

where \( \nu = 0.5 m \omega^2 / (E_Rk_R^2) \), \( \xi = V_0 / E_R \) represents the height of OL and \( \alpha = F / (E_Rk_R) \) stands for the strength of external field. Here \( E_R = (\hbar k_R^2)/(2m) \) is the recoil energy. Throughout this paper, we adopt the parameters from the work of Dahan [10] for \(^{87}\)Rb including laser wavelength \( \lambda = 852 \) nm and the frequency of the parabolic trap \( \omega = 200 \pi \) rad/s.

2.2. The evolution of the wavepacket
We proceed to investigate the properties of the Bloch oscillation in BEC of \(^{87}\)Rb. Firstly, the wavepacket of ground band is considered for constant lattice height \( \xi = 2.0 \) and three representative values of linear force \( \alpha = 0.005, 0.05, \) and 0.1. The results are shown in figure 1. The left and right panels are the evolution of wavepacket in position and quasimomentum spaces, respectively. Note that the time of evolution is considered in terms of reduced time \( t_R = \hbar / E_R \) and is chosen such that the wavepackets are able to evolve in five periods.

![Figure 1](image-url) (Color online) The evolution of the ground-band wavepacket in position space (left panels) and momentum space (right panels) for fixed \( \xi = 2.0 \) and three representative values of \( \alpha = 0.005, 0.05, \) and 0.1.
From the left panels of figure 1, the $s$-band wavepacket obviously performs an oscillating pattern. To estimate the reliability of our numerical calculation, the tight-binding model is considered. In the limit of deep OL, the amplitude of Bloch oscillation is approximated by the Wannier-Stark localization length [14]

$$A = l_{WS} = 2J/\alpha,$$

(5)

with $J = 4\pi^{-0.5}\xi^{0.75}\exp(-2\sqrt{\xi})$ is the hopping parameter [17]. Moreover, the reduced period of Bloch oscillation is inversely proportional to $\alpha$ as

$$\tau = 2/\alpha.$$

(6)

Our TDSE results show perfect agreement between theoretical and numerical period. As stated in Eq. (5), the amplitudes of Bloch oscillations are inversely proportional to $\alpha$ for a fixed value of lattice height $\xi$ which is qualitatively consistent with our calculations. In cases of $\alpha = 0.005$ and 0.05, the oscillation in position space is well observed and not so robust. While for $\alpha = 0.1$, there exists splitting of the wavepacket with lower probabilities which can be detected as the faded structure at the end of each Bloch period in the lowest left panel of figure 1. In momentum space, the evolution of the wavepacket linearly develops in time as expected.

Starting from the origin, the wavepacket reaches the boundary of the first Brillouin zone (BZ) where it is Bragg-reflected to the opposite edge and repeatedly evolves linearly towards the positive boundary. It should be noted that the time duration when the position-configuration wavepacket reaches the lower boundary is coincident with the reflection event in momentum representation [14]. Again, in momentum space there exist several low-probability components which tend to linearly grow in the situation of $\alpha = 0.1$.

![Figure 2.](image)

Figure 2. (Color online) The LZ transition rates from the ground to the first three excited bands as a function of reduced time for $\alpha = 0.1$ and $\xi = 2.0$.

The interesting features seen in figure 1 are able to be discussed in terms of LZ transition. As the field strength increases up to a specific threshold, the atom absorbs enough energy and is able to tunnel into higher bands. For illustration the LZ transition process, the transition rates from the ground to the first three excited bands in the cases of $\alpha = 0.1$, $\xi = 2.0$ are calculated and presented in figure 2 as functions of time. The time duration considered is five Bloch periods as in the lower panels of figure 1. Here, the LZ transitions from the ground to first (solid red
curve) and second (dashed blue curve) bands are dominant and increase with time under the influence of the linear potential whose strength is sufficiently large. Meanwhile, the transition from the ground to the third excited band reaches to around 7% after the fifth Bloch oscillation. Thus the transitions to higher bands are negligible. Obviously, as evolution time increases, the LZ transition from the ground to the first and second excited bands are comparable and rise up to 65%. Therefore, the signals of secondary structure in figure 1 for $\alpha = 0.1, \xi = 2.0$ also emerges in both position and momentum representation as time grows. The analysis here is a firm evidence of the contribution from the first and second excited components to the ground band wavepacket when the field strength is considerably large.

We continue our investigation of the evolution of the wavepacket for constant field strength $\alpha = 0.01$. Now the lattice height takes three representative values $\xi = 0.5, 2.0$ and 4.0. The evolution of ground-band wavepackets is shown in figure 3.

![Figure 3](image.png)

**Figure 3.** (Color online) The evolution of the ground-band wavepacket in position space (left panels) and momentum space (right panels) at different values of lattice height $\xi = 0.5, 2.0$, and 4.0 for $\alpha = 0.01$ in five Bloch cycles.

Despite the constancy of the period of Bloch oscillation, the amplitude becomes smaller when extending the lattice depth which coincides with the prediction in Eq. 5. For a sufficiently large value of lattice height, the scenario of Bloch oscillation is clean and well observed as seen in the middle and lower panels of figure 3. However, in the case of shallow OL ($\xi = 0.5$), the picture showing the evolution of the wavepacket in Bloch and Wannier configurations is contaminated by several components as depicted in the upper panels of figure 3. We note that the feature in this situation is different from that of figure 1. Here, there exist the evolutions in which the wavepackets have constant quasimomenta $q = \pm 1$ as the obscure horizontal lines in the upper right panel of figure 3. Instead of continuing being accelerated after making the transition to
the higher band as in figure 1, the wavepackets in this case just gain enough energy to jump to the first excited band and are trapped within this band. The reason is straightforward since the external force now is sufficiently small $\alpha = 0.01$ and is not enough to further excite and accelerate these wavepackets.

Figure 4 depicts the structure of the ground and first excited bands of the system in the first BZ for $\alpha = 0.01$ and three representative OL height $\xi = 0.5, 2.0, \text{and } 4.0$. It is obvious that even the field strength is small, the band gap is still minimized by decreasing the height of OL. Therefore the band-gap minimization is considered as an alternative approach to enable the interband coupling besides applying strong external electric field. Figure 4 also indicates that the higher the lattice, the broader the band gap. Hence, in the cases of $\xi \leq 0.5$, the LZ transition occurs due to a small band gap, thus breaks the single-band approximation [11].

![Figure 4](image-url)

**Figure 4.** (Color online) The structures of ground and first excited bands of the system in the OL for $\alpha = 0.01$ and for (a): $\xi = 0.5$; (b): $\xi = 2.0$ and (c): $\xi = 4.0$.

2.3. Classical interpretation of Bloch oscillation

In this subsection, the Bloch oscillation is explained from the viewpoint of classical mechanics combining with the single-band and tight-binding approximation [18]. The classical Hamiltonian of the ground-state system in the tilted lattice is given by

$$H = E^m_n + \alpha \chi$$  \hspace{1cm} (7)

where $E^m_n$ is the energy dispersion of the ground band approximately calculated by the tight-binding approximation [17]

$$E^m_n = \sqrt{\xi - 2J \cos(\pi q)}$$  \hspace{1cm} (8)

Supposed that the system obeys the canonical equations [16]
\[ \dot{x} = \frac{\partial H}{\partial q}, \] (9)

\[ \dot{q} = -\frac{\partial H}{\partial x}. \] (10)

A pair of equations describing the motion of the system is derived by solving Eqs. (9) and (10) as

\[ \chi(t) = -\frac{2J}{\alpha} \sin\left(\frac{\pi\alpha}{2}t\right) \sin\left[\frac{\pi\alpha}{2}t + \pi q(0)\right], \] (11)

\[ q(t) = q(0) - \alpha t, \] (12)

This classical model is proposed by Heinze and colleagues in 2013 [19] resembling the dynamics of a nonlinear pendulum. Classical equations (11) and (12) are referred to the Ref. [18] with the initial conditions that the system starts at the origins in both position and momentum representations, means \( \chi(0) = 0 \) and \( q(0) = 0 \). The dependences of \( \chi(t) \) and \( q(t) \) on reduce time are illustrated in figure 5 for OL with height \( \xi = 2.0 \) and external field strength \( \alpha = 0.01 \) as in the middle panels of figure 3. In figure 5, the quantum results are also plotted as dotted lines. The numerical values used in figure 5 are extracted from the middle panels of figure 3 by choosing the ones with maximum probability at a specific time.

Figure 5. (Color online) The motion of the system in position (left panel) and momentum (right panel) spaces using Eqs. (10) and (11) is illustrated in red solid line whereas the blue squares represent the numerical simulation.

There are some differences should be noticed while comparing the classical interpretation with those obtained from TDSE calculation. Firstly, in the position space, even though the classical result perfectly matches that of TDSE in terms of Bloch period, the whole oscillating pattern of classical one does not coincide with the extraction from TDSE as seen in the left panel of figure 5. Moreover, in the momentum space, the system is linearly accelerated towards infinity since there is no Bragg reflection at the edge of the first BZ in the classical regime.

To provide quantitative evaluation, the relative error between the classical model and numerical result defined as

\[ \sigma = \frac{|\chi_{\text{model}} - \chi_{\text{TDSE}}|}{|\chi_{\text{TDSE}}|}, \] (13)
Figure 6. (Color online) The relative error of Bloch oscillation for $\alpha = 0.01$ and $\xi = 2.0$ provided by tight-binding model and by TDSE, respectively.

is plotted in Figure 6 in the position space. The result shows that the maximum deviation is about 20%. The explanation for this difference is proposed: the Eq. (6) is a result of the tight-binding model where energy dispersion of the ground state is approximated by the cosine function of quasimomentum. Despite these differences, it is obvious that the classical interpretation is still acceptable to describe the Bloch oscillation in specific conditions such as sufficiently high OL and weak external electric field.

3. Conclusion

In this paper, we have simulated the evolution of the wavepacket in the position and momentum spaces under the single-band approximation. By adjusting the lattice height and/or the strength of linear force, the dependences of the oscillatory properties on these factors are introduced. When increasing the lattice height and the tilted potential, the amplitude of the oscillation is decreased while the Bloch period is inversely proportional to the parameter $\alpha$ defining the strength of the external force. In the case of $\xi \geq 2.0$ and $\alpha < 0.1$, the evolution of the ground-band wavepacket is well-observed. The validity of the single-band approximation is examined by altering two factors associating with the tilted lattice potential to eliminate the LZ transition. Based on our investigation, the single-band model is broken for sufficiently shallow OL about $\xi \leq 0.5$ and/or strong external linear field $\alpha \geq 0.1$. In these cases, the wavepacket is provided enough energy to overcome the band gap for making the LZ transition. Then, the classical Bloch oscillation under the single-band tight-binding approximation is compared with the precisely TDSE results showing good agreement with 20% of maximum relative error. For the sake of simplicity, the classical approach is still applicable for specific ranges of parameters so that the OL is sufficiently high and the external field is sufficiently weak.

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References

[1] Petrich W, Anderson M H, Ensher J R and Cornell E A 1994 Behavior of atoms in a compressed magneto-optical trap JOSA B 11 1332.

[2] Davis K B et al 1995 Bose-Einstein condensation in a gas of sodium atoms Phys. Rev. Lett. 74 5202
[3] Zeppenfeld M et al 2012 Sisyphus cooling of electrically trapped polyatomic molecules Nature 491 570.
[4] Bloch I 2005 Ultracold quantum gases in optical lattices Nat. Phys. 1 23.
[5] Glück M, Kolovsky A R and Korsch H J 2002 Wannier-Stark resonances in optical and semiconductor superlattices Phys. Rep. 366 103.
[6] Bharucha C F et al 1997 Observation of atomic tunneling from an accelerating optical potential Phys. Rev. A 55 R857.
[7] Bloch F 1928 Quantum mechanics of electrons in crystal lattices Z. Phys. 52 555.
[8] Zener C 1934 A theory of the electrical breakdown of solid dielectrics P. R. Soc. Lond. A-ContA. 145 523.
[9] Leo K et al 1992 Observation of Bloch oscillations in a semiconductor superlattice Solid State Commun. 84 943.
[10] Dahan M B, Peik E, Reichel J, Castin Y and Salomon C 1996 Bloch oscillations of atoms in an optical potential Phys. Rev. Lett. 76 4508.
[11] Morsch O, Müller J H, Cristiani M, Ciampini D and Arimondo E 2001 Bloch oscillations and mean-field effects of Bose-Einstein condensates in 1D optical lattices Phys. Rev. Lett. 87 140402.
[12] Meinert F et al 2017 Bloch oscillations in the absence of a lattice Science 356 945.
[13] Clade P, Andia M and Guellati-Khelifa S 2017 Improving efficiency of Bloch oscillations in the tight-binding limit Phys. Rev. A 95 063604.
[14] Geiger Z A et al 2018 Observation and uses of position-space Bloch oscillations in an ultracold gas Phys. Rev. Lett. 120 213201.
[15] Kolovsky A R and Korsch H J 2004 Bloch oscillations of cold atoms in optical lattices Int. J. Mod. Phys. B 18 1235.
[16] Yamakoshi T and Watanabe S 2015 Wave-packet dynamics of noninteracting ultracold bosons in an amplitude-modulated parabolic optical lattice Phys. Rev. A 91 063614.
[17] Morsch O and Oberthaler M 2006 Dynamics of Bose-Einstein condensates in optical lattices Rev. Mod. Phys. 78 179.
[18] Hartmann T, Keck F, Korsch H J and Mossmann S 2004 Dynamics of Bloch oscillations New J. Phys. 6 2.
[19] Heinze J et al 2013 Intrinsic photoconductivity of ultracold fermions in optical lattices Phys. Rev. Lett. 110 085302.