Dirac Point Structure in a Bose-Einstein Condensate in a Honeycomb Optical Lattice

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We study the Bose-Einstein condensate in a honeycomb optical lattice within Bogoliubov theory and find that for a $k = 0$ condensate, the Dirac points appear in the Bogoliubov excitation spectrum when $0 < \beta < 2$, which illustrates that the Bose-Bose interaction does not change the Dirac point structure but only give a modification of the velocity of the Dirac cone. When the bosons are driven to condense at $k = K$, however, we find that the topology of the Dirac points will be altered by arbitrary weak interaction. Furthermore, we find that the next-nearest-neighbor hopping in an isotropic and an anisotropic lattice has different effects to the dynamics of the condensate and it should be taken into account when the lattice is not sufficiently deep.

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In recent years, the Dirac point structure has arisen a lot of interests in condensed matter physics\cite{1-3}, nonlinear optics\cite{4-6} and cold atomic physics\cite{7, 8}. The Dirac point structure corresponds to many important phenomena in physics, such as the room-temperature quantum Hall effect in graphene\cite{9}, topological edge state in topological insulator\cite{10}, and conical diffraction in honeycomb photonic lattices\cite{4}. To realize such a structure in a cold atomic system, several groups proposed to load fermions on different optical lattices\cite{11-13} and recently, in experiment, L. Tarruell et al has realized it in a tunable honeycomb lattice\cite{15}. Before this realization of Dirac point structure with Fermi gas, the honeycomb lattice was first investigated with Bose-Einstein condensates\cite{16, 17}, although new quantum phases were observed, no signatures of Dirac points were observed.

In this paper, we study the Bose condensates in a honeycomb optical lattice and find that in the tight-band limit, for a $k = 0$ condensate, stable Dirac points appear in the two lowest bands even in the presence of the interaction if the anisotropy $\beta$ (the meaning of $\beta$ is given in the following) is within the region $(0, 2)$. However, if the bosons are condensed at $k = K$, where $K$ is the momentum where the two bands touch, even within Bogoliubov theory, we find that no matter how weak the interaction is, the Dirac points will be altered by the interaction, which agrees with the conclusions obtained in Refs.\cite{6, 18} by numerical methods. Furthermore, we find that for a lattice that is isotropic but not sufficiently deep, the next-nearest-neighbor (NNN) hopping effectively affects the dynamics of the condensate but nearly does not affect the dynamics around the Dirac points. However, for an anisotropic lattice, the NNN hopping will alter the topology of the Dirac points and make the Dirac points no longer well defined. Therefore, to observe the Dirac points, it’s better to use an isotropic lattice.

Model—The honeycomb optical lattice, which consists of two sublattices A and B, can be realized by three detuned standing-wave lasers, with the optical potential given by\cite{11}

$$V(x, y) = \sum_{i=1, 2, 3} V_i \sin^2[k_L(x \cos \theta_i + y \sin \theta_i + \pi/2)],$$

where $\theta_1 = \pi/3$, $\theta_2 = 2\pi/3$, $\theta_3 = 0$, and $k_L$ is the optical wave vector. With different $V_i$, the honeycomb lattice can be either isotropic or anisotropic\cite{19}. In this work, we consider single-component bosonic atoms in this lattice. For bosons, the intra-species collisions is dominated by s-wave scattering. In the following, we consider $r_0 << k^{-1} a_s$, where $r_0$ is the effective interaction length, $k = \frac{\pi}{L}$ is the wave vector, and $a_s$ is the s-wave scattering length. Furthermore, we first assume the lattice is deep, therefore, the effective Hamiltonian is given as the Bose-Hubbard model

$$H = -\sum_{<ij>} \left( t_{ij} \hat{a}_i^\dagger \hat{b}_j + h.c. \right) - \sum_{i \in A} \mu \hat{a}_i^\dagger \hat{a}_i - \sum_{i \in B} \mu \hat{b}_i^\dagger \hat{b}_i + \frac{U}{2} \left[ \sum_{i \in A} \hat{n}_i^a \hat{n}_i^a + \sum_{i \in B} \hat{n}_i^b \hat{n}_i^b \right],$$

where $<ij>$ represents the nearest neighbor (NN) sites, $\hat{a}_i$ and $\hat{b}_i$ denote the bosonic mode operators for the sublattices A and B, respectively. $\mu$ is the chemical potential and $U$ describe the on-site interaction between bosons. The tunnelling rates $t_{ij}$, in general, depend on the tunnelling directions in an anisotropic honeycomb lattice. In this paper, both the isotropic case and the anisotropic case are analyzed in detail.

First, we make a Fourier transformation for the Hamiltonian. With $\hat{a}_i^\dagger = \frac{1}{\sqrt{N}} \sum_k \exp(i \mathbf{k} \cdot \mathbf{A}_i) \hat{a}_k^\dagger$, $\hat{b}_i^\dagger = \frac{1}{\sqrt{N}} \sum_k \exp(i \mathbf{k} \cdot \mathbf{B}_i) \hat{b}_k^\dagger$, where $N$ is the number of sites of the sublattice A (or B).
and the Hamiltonian can be given as
\[
H = \sum_k \left[ \phi(k) \hat{a}_k^\dagger \hat{b}_k + \text{h.c.} - \mu \hat{a}_k^\dagger \hat{a}_k - \mu \hat{b}_k^\dagger \hat{b}_k \right] + \frac{U}{2N} \sum_q \left[ \hat{\rho}^a_q \hat{\rho}^a_{-q} + \hat{\rho}^b_q \hat{\rho}^b_{-q} \right],
\]
where \( \hat{\rho}^a_q = \sum_{p} \hat{\alpha}^a_{p-q} \hat{\alpha}^a_p \) (\( \alpha = a, b \)). \( \phi(k) = \sum_{s=1}^{3} t_s \exp(i k \cdot b_s) \), with \( b_1 = (1/\sqrt{3}, 1/2) \), \( b_2 = (1/\sqrt{3}, -1/2) \), and \( b_3 = (-a/\sqrt{3}, 0) \), \( a \) is the lattice spacing. In this paper, we set \( t_1 = t_2 = t \) and \( t_3 = \beta t \). Furthermore, we set \( t \) and \( a \) as the energy unit and length unit, respectively.

For the free case, i.e. \( U = 0 \), this Hamiltonian can be rewritten in a 2 \( \times \) 2 matrix form,
\[
H = \sum_k \left( \begin{array}{cc} -\mu & \phi(k) \\ \phi^*(k) & -\mu \end{array} \right) \left( \begin{array}{c} \hat{a}_k \\ \hat{b}_k \end{array} \right),
\]
by making a transformation \( (\hat{\alpha}_k, \hat{\beta}_k)^T = V(\alpha_k, \beta_k)^T \), where the matrix \( V \) takes the form
\[
V = \frac{1}{\sqrt{|\phi(k)|}} \left( \begin{array}{cc} |\phi(k)| & -\phi(k) \\ -\phi^*(k) & |\phi(k)| \end{array} \right),
\]
the Hamiltonian is diagonalized and the energy eigenvalues are
\[
\varepsilon_{\pm}(k) = -\mu \pm |\phi(k)|.
\]
Since the bosons are condensed into the zero crystal momentum, \( \varepsilon_{-}(0) \) should take zero, and therefore \( \mu = |\phi(0)| \). Such a non-zero value of chemical potential is common in lattice models and it guarantees the energy of excitations to be positive, which is necessary for the condensates to be stable.

The dispersion relations are determined by \( |\phi(k)| \), which is directly related to the hopping amplitude and it guarantees the energy of excitations to be positive, which is necessary for the condensates to be stable.

The two bands no longer touch with each other and they are gapped.

When the interaction is tuned on, the chemical potential has a shift: \( \mu = -|\phi(0)| \to -|\phi(0)| + U n \), where \( n \) is the density of the system. In the Bogoliubov approximation and neglecting the constant condensation energy, the Hamiltonian can be written as
\[
H_{BG} = \frac{1}{2} \sum_k B^\dagger_k H_k B_k,
\]
where \( B^\dagger_k = (a^\dagger_k, a^-k, b^-k, b^\dagger_k) \) and
\[
H_k = \begin{pmatrix}
\varepsilon_0 + U & U & \phi(k) & 0 \\
U & \varepsilon_0 + U & 0 & \phi(k) \\
\phi^*(k) & 0 & \varepsilon_0 + U & U \\
0 & \phi^*(k) & U & \varepsilon_0 + U
\end{pmatrix}.
\]
Here we assume the filling factor of bosons is unit and \( \varepsilon_0 = |\phi(0)| \) just for convenience. Based on this Hamiltonian, we find that the dispersion relations are
\[
\varepsilon_{\pm}(k) = \sqrt{\varepsilon_0^2 + 2U\varepsilon_0 + |\phi(k)|^2 \pm 2(\varepsilon_0 + U)|\phi(k)|}.
\]
If we take \( U \) to be zero in Eq.(6), it is same as Eq.(4).

For the free case, i.e. \( \beta = 1 \), the two bands keep touching and the Dirac point structure is not destroyed by the interaction, which is shown explicitly in the following.

For \( 0 < \beta < 2 \), there are two regions which we are interested in. The first one is around the \( k = 0 \), by expanding the momentum \( k \) around \((0, 0)\) and up to the second order of \( k_x \) and \( k_y \), the dispersion relation (6) becomes
\[
\varepsilon_{-}(k) = \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2},
\]
where \( v_x = \sqrt{3U/\beta^2 \varepsilon_0} \) and \( v_y = \sqrt{U/\beta^2} \). The sound velocity is anisotropic and dependent on the anisotropy that is characterized by \( \beta \) of the lattice. The second region is around the Dirac points. Following the same procedure, we obtain
\[
\varepsilon_{\pm}(q) = \varepsilon_0 \pm \sqrt{v_x^2 q_x^2 + v_y^2 q_y^2}, \quad (8)
\]
\[
\varepsilon_{\pm}(q) = \sqrt{\varepsilon_0^2 + 2U\varepsilon_0} \pm \frac{\varepsilon_0 + U}{\sqrt{\varepsilon_0^2 + 2U\varepsilon_0}} \sqrt{v_x^2 q_x^2 + v_y^2 q_y^2}, \quad (9)
\]
where \( q \) is a small momentum away from the Dirac points \( K = (k_x^0, k_y^0) \), i.e. \( (k_x, k_y) = (k_x^0 + q_x, k_y^0 + q_y) \). \( \tilde{v}_x = \sqrt{3\beta^2 / 2} \) and \( \tilde{v}_y = \sqrt{1 - \beta^2/4} \). The anisotropy of the velocity is a consequence of the anisotropy of the lattice. Removing the constant energy, we see that \( \varepsilon_{\pm}(q) \) from Eqs.(4), (5) and Fig.1, we see, for \( 0 < \beta < 2 \), the two bands touch at several points and Dirac points appears. In particular for the isotropic case where \( \beta = 1 \), the dispersion has the same Dirac structure as the graphene material (as shown in Fig.1). The Dirac points are purely due to the structure of the honeycomb lattice, without any relation to the quantum statistics. For \( \beta > 2 \), the two bands no longer touch with each other and they are gapped.

FIG. 1: (Color online) (Right) the isotropic case, i.e. \( \beta = 1 \). The two bands touch at six points, with two different kind of Dirac points. (Left) the anisotropic case with \( \beta = 3 \), the bands are gapped.
represents the standard energy-momentum relation for the relativistic Dirac particles, with $v_x$ and $v_y$ replacing the light velocity. Therefore, there is real Dirac structure around the touching points. Furthermore, compared Eq.(9) to Eq.(8), we see that the interaction has only modified the velocity of quasiparticles around the Dirac points.

Before discussing how to detect the Dirac point structure in experiments, we have to realize that here the physics is dominated by the condensates and low energy excitation. As a result, the effects of the Dirac points are very weak for a $k = 0$ condensate to be detected. This is the reason why no signatures of Dirac points is observed in experiments.[16, 17]. To observe the effects of the Dirac points, we have to drive the bosons to condense at $k = K$. However, when the bosons are driven to condense at $k = K$, there is modulational instability, this can be confirmed by the discrete nonlinear Schrödinger equation (DNLS)[22],

\[
\begin{align*}
\hbar \frac{\partial \tilde{\psi}_A}{\partial t} &= \sum_s s \tilde{\psi}_{Bs} + U |\tilde{\psi}_A|^2 \tilde{\psi}_A, \\
\hbar \frac{\partial \tilde{\psi}_B}{\partial t} &= \sum_s s \tilde{\psi}_{A\bar{s}} + U |\tilde{\psi}_B|^2 \tilde{\psi}_B,
\end{align*}
\]

where $s(\bar{s})$ denotes the nearest-neighbor vectors from $A(B)$ to $B(A)$. The stationary solutions of Eq.(10) are plane waves $\tilde{\psi}^{A,B}_0 \exp[i(k \cdot A(B) - \nu t)]$, of frequency $\nu = \pm |\phi(k)| + U$ (here we assume $n_0^A = |\psi_0^A|^2 = n_0^B = |\psi_0^B|^2 = n_0 = 1$). To check the stability of these states, we perturb the carrier wave with small amplitude phonons: $\psi_{A,B} = (\psi_0^{A,B} + u_{A,B} e^{i\phi k \cdot A(B)} + v_{A,B} e^{i\phi k \cdot A(B)} ) e^{i(k \cdot A(B) - \nu t)}$, The DNLS excitation spectrum is determined by

\[
\begin{align*}
\lambda^2 - |\Delta_{k}^2 + 4U \xi_k + |\phi(k + q)|^2 + |\phi(k - q)|^2| \lambda^2
-2(U + \xi_k) [ |\phi(k + q)|^2 - |\phi(k - q)|^2] \lambda + (\xi_k^2 + 2U \xi_k)^2
-U^2 [ |\phi(k + q)|^2 + |\phi(k - q)|^2] \lambda + |\phi(k + q)|^2 |\phi(k - q)|^2
-(\xi_k^2 + 2U \xi_k)[|\phi(k + q)|^2 + |\phi(k - q)|^2] = 0,
\end{align*}
\]

where $\xi_k = |\phi(k)|$. When $k = 0$, the spectrum is given as $\lambda_\pm = \sqrt{\xi_0^2 + 2U \xi_0 + |\phi(k)|^2} \pm 2(\xi_0 + U)|\phi(k)|$, the same as Eq.(6) and therefore it is just the Bogoliubov spectrum. When $k = K$, imaginary will naturally appear in the excitation spectrum, and as a result, the condensate is modulationally unstable.

In fact, when the bosons are condensed at $k = K$, we can even see that the Dirac points are destroyed by the interaction within the Bogoliubov theory. Based on the Bogoliubov theory, the Hamiltonian is given as $H_{BG} = \frac{1}{2} \sum_q B^d_q H^*_q B_q$, where $B^d_q = (a^d_{q}, a^d_{-q}, b^d_{q}, b^d_{-q})$ and

\[
H_q = \begin{pmatrix}
U & U & \phi(q + K) & 0 \\
U & U & 0 & \phi(q + K) \\
\phi^*(q + K) & 0 & U & U \\
0 & \phi^*(q + K) & U & U
\end{pmatrix}.
\]

The energy spectrum is given as

\[
\varepsilon_k(q) = \sqrt{|\phi(q + K)| \pm 2U)|\phi(q + K)|. (12)
\]

We see no matter how weak the interaction is, imaginary always appears in the long-wavelength limit, i.e. $q \rightarrow 0$. As a result, the topology of the Dirac points will be altered by the long-wavelength excitations, which agrees with the result obtained in Refs.[6, 18]. All these results indicate that to observe the Dirac point structure in Bose condensates is a challenge. Recently, a way to handle this problem of stability was introduced[20] and the vortex patterns suggested there can be used as a probe of the Dirac point structure in experiments.

The study above is based on the tight-binding model. We know the tight-binding model is based on the assumption that the lattice is deep enough to guarantee that the Wannier wave function is well-localized. However, for a lattice that is not sufficiently deep, the tight-binding model with just the NN hopping is much less accurate than the one with both NN hopping and the NNN hopping[23], and therefore, the NNN hopping should be taken into account for such not sufficiently deep lattice. In the following, we will consider the NNN hopping to see what effects the NNN hopping has to the condensate.

After we introduce the NNN hopping into Eq.(1), the excitation spectrum takes the form

\[
\tilde{\varepsilon}_\pm(k) = -\mu - h(k) \pm |\phi(k)|, \tag{13}
\]

FIG. 2: (Color online) (a) 1, 2, 3 stand for three different kind of hopping. (b) The common parameters for both the solid line (black) and the dashed line (red) are $\beta = \lambda = 1$, $U = 0.5$ and $k_x = 0$, while $\gamma = 0$ for the solid line and $\gamma = 0.1$ for the dashed line.
where
\[ \tilde{\mu} = -2\gamma(1 + 2\lambda) - \beta - 2, \]
\[ h(k) = 2\gamma(\cos k_y + 2\lambda\cos \frac{\sqrt{3}k_x}{2}\cos \frac{k_y}{2}), \]
where \( \gamma \) is the NNN hopping constant in unit of \( t \) and \( \lambda \) is the anisotropic of the NNN hopping. Based on the anisotropy of the lattice and the anisotropy of the NN hopping, the hopping amplitudes along the path labelled by 2 and 3 in Fig.2(a) are equal but different to the one along the path labelled by 1. From Eq.(13), it is direct to see that the two bands still touch. However, when we expand the dispersion relation around the Dirac points and keep only the terms related to the lowest order of momentum, we find
\[ \tilde{\varepsilon}_\pm(q) = -2\gamma(\beta - \lambda)\sqrt{1 - \frac{\beta^2}{4}q_y^2} \pm \sqrt{\tilde{v}_x^2q_x^2 + \tilde{v}_y^2q_y^2}, \]
(14)
this indicates that if the anisotropy of the NNN hopping is different from the NN hopping, the Dirac point structure is no longer well defined even though the two bands still touch with each other (as shown in Fig.3). In the harmonic approximation, we calculate the NN hopping and the NNN hopping and find when \( \beta \neq 1, \lambda \) is not equal to \( \beta \) (if we further consider the next-next-nearest-neighbor (NNNN) hopping, the NNNN hopping will induce a small gap for the case of \( \beta \neq 1 \)). Therefore, to observe the Dirac point structure, it’s better to choose the system to be isotropic, i.e. \( \beta = \lambda = 1 \). In the following, we set \( \beta = \lambda = 1 \).

When the interaction is tuned on, the dispersion relations change into
\[ \tilde{\varepsilon}_\pm(k) = \sqrt{\epsilon_k^2 + 2U\epsilon_k + |\phi(k)|^2 \pm 2(\epsilon_k + U)|\phi(k)|}, \]
(15)
where \( \epsilon_k = -\tilde{\mu} - h(k) \). By expanding the dispersion relation around \( k = 0 \), we obtain
\[ \tilde{\varepsilon}_-(k) = \sqrt{\tilde{v}_x^2k_x^2 + \tilde{v}_y^2k_y^2}, \]
(16)
where the modified velocity \( \tilde{v}_x = \tilde{v}_y = \sqrt{\frac{U}{2}(1 + 6\gamma)} \).

Compared to \( v_x = v_y = \sqrt{U/2} \) in Eq.(7) with \( \beta = 1 \), we see the sound velocity is effectively increased due to the NNN hopping (as illustrated in Fig.2(b)). By expanding the dispersion relation around the Dirac points, we obtain,
\[ \tilde{\varepsilon}_\pm(q) = A(\gamma, U) \pm \frac{B(\gamma, U)}{A(\gamma, U)} \sqrt{\tilde{v}_x^2q_x^2 + \tilde{v}_y^2q_y^2}, \]
(17)
where \( A(\gamma, U) = 9(1 + \gamma)^2 + 6U(1 + \gamma) \) and \( B(\gamma, U) = 3(1 + \gamma) + U \). By a direct calculation with concrete parameters, we find that unlike the case around \( k = 0 \), the NNN hopping nearly does not affect the velocity around the Dirac points (also shown in Fig.2(b)). Based on these results, we obtain the conclusion that for an isotropic lattice, the NNN hopping mainly affects the dynamics of the modes around the \( k = 0 \), it nearly does not affect the dynamics of the modes around the Dirac points; However, for an anisotropic lattice, the NNN hopping not only affects the dynamics of the modes around the \( k = 0 \), but also alters the topology of the Dirac points and makes the Dirac points no longer well defined.

From the above analysis, we see that to guarantee that the tight-binding model gives an accurate description to the condensates, the lattice indeed has to be sufficiently deep to guarantee that the NNN hopping is far smaller than the NN hopping, i.e. \( \gamma \ll 1 \).

In summary, we have studied the Bose-Einstein condensates in a honeycomb lattice and found that for a \( k = 0 \) condensate, the Dirac points appear in the Bogoliubov excitation spectrum when \( 0 < \beta < 2 \), and when the bosons are condensed at \( k = K \), the topology of the Dirac points will be altered by arbitrary weak interaction. Furthermore, we find that the NNN hopping of not small strength has obvious effects to the dynamics of the condensates, and therefore it should be taken into account when the lattice is not sufficiently deep.

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**FIG. 3:** (Color online) (Right) The isotropic case, i.e. \( \beta = \lambda = 1 \); (Left) The anisotropic case, i.e. \( \beta \neq \lambda \).
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