$p$ band in a rotating optical lattice

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We investigate the effects of rotation on the excited bands of a tight-binding lattice, focusing particularly on the first excited ($p$) band. Both the on-site energies and the hopping between lattice sites are modified by the effective magnetic field created by rotation, causing a nontrivial splitting and magnetic fine structure of the $p$ band. We show that Peierls substitution can be modified to describe $p$ band under rotation, and use this method to derive an effective Hamiltonian. We compare the spectrum of the effective Hamiltonian with a first-principles calculation of the magnetic band structure and find excellent agreement, confirming the validity of our approach. We also discuss the on-site interaction terms for bosons and argue that many-particle phenomena in a rotating $p$ band can be investigated starting from this effective Hamiltonian.

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I. INTRODUCTION

Ultracold atom experiments display amazing versatility and promise to improve our understanding of many-particle physics. There is now hope for direct experimental realization of many models which were constructed as effective models of condensed matter systems, such as the Hubbard model [1]. However, the extent of the ultracold atom experiments are not limited to previously discussed models; novel systems such as dipolar [2] and spinor gases [3] are created as well. Through the interplay of these experiments and theories aimed at explaining or stimulating them, a better understanding of quantum many-particle physics emerges.

One of the problems that has been discussed extensively in the condensed matter literature, but never experimentally realized is the effect of a periodic potential under high magnetic fields [4]. When the magnetic flux through the unit cell of the periodic potential is of the order of one flux quantum, the energy spectrum displays complex magnetic fine structure within the Bloch bands. Conventional condensed matter systems with lattice constants in the order of nanometers require thousands of tesla magnetic fields to be able to see these effects, which is very far from being experimentally feasible.

Recently a number of authors have argued that this model can be realized in a cold atom setup within current experimental capability [5–11]. As the atoms are neutral the magnetic field is expected to be created either by rotating the optical lattice, or by optically induced potentials. A weak rotating optical lattice has already been realized in vortex pinning experiments [12], and there is ongoing work about creating effective magnetic fields via light induced coupling [13]. Theoretical studies of these systems promise interesting phenomena such as lattice quantum Hall effects [14–17] or the observation of topological conductance quantization [18].

Most of the recent theory, as well as the previous investigations in the condensed matter literature are focused on the lowest ($s$) band of the lattice. An important reason for this focus is that the magnetic fine structure of this lowest band is very well described by the Peierls substitution [19]. The resulting band structure for the split $s$ band is easily obtained from a difference equation and is a self-similar fractal, known as the Hofstadter butterfly [4]. The original tight-binding Hamiltonian is modified only by the addition of phases to hopping amplitudes and serves as a starting point for the investigation of many-body physics in this system.

An exciting development in cold atom physics has been the realization that higher bands in an optical lattice are also experimentally accessible [20,21]. The physics of the first excited band, the $p$ band, contains surprises such as Bose condensation at nonzero momentum [22], or orbitally ordered Mott insulators [23–26]. For a system of fermions $p$-band physics can be accessed trivially by filling the $s$ band completely; surprisingly the relaxation time for bosons in the $p$ band is long enough to allow experimental access to pure $p$-band physics.

A natural question to ask about the $p$-band physics is how the particles in the $p$ band respond to the effective magnetic field created by rotation. Experimentally, if a strong rotating optical lattice is realized, the $p$ band should be as accessible as the $s$ band. One can imagine the already rich physics of the $p$ band [27–30] to be strongly affected by the magnetic field, as both the orbital order within each lattice site and the hopping between different lattice sites will be modified. Beyond the single particle physics, it is not clear how the various many-particle phases, such as orbitally ordered Mott insulators, will be affected by rotation.

The theoretical investigation of such effects requires a consistent method of incorporating the phases generated by the magnetic field into the lattice Hamiltonian. For the $s$ band, Peierls substitution, in which one builds an effective Hamiltonian by replacing $k$ with $(p - eA/c)/\hbar$ in the energy band function gives a satisfactory description of the one particle physics [4]. Starting from this effective Hamiltonian interaction effects can be investigated. The accuracy of Peierls substitution for the $s$ band has been checked by numerical solutions of the Schrödinger equation [19]. However, as for degenerate bands (of which the $p$ band is the simplest example) the conjecture was that “wherever the unperturbed Bloch bands touch or overlap, it is not possible to obtain the

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magnetic substructure by semiclassical methods, even
approximately, by means of a universal rule for the whole Bril-
loiuin zone“ [19].

In this paper, we generalize the Peierls substitution proce-
dure to the \( p \) band, and obtain an effective Hamiltonian for the \( p \) band of the rotating optical lattice. We show that after an appropriate diagonalization in \( k \) space, which assumes temporarily that only the on-site energies are affected by the
degeneracy lifting field, Peierls substitution is still a good option to obtain the detailed magnetic fine structure. We
check the spectrum obtained from the effective Hamiltonian
with an accurate numerical solution of the two-dimensional
Schrödinger equation and obtain excellent agreement. This
method should in principle be applicable to other degenerate
bands and it provides us with a means to examine inter par-
ticle interactions.

The paper is organized as follows: In the next section, we
introduce the Hamiltonian for a rotating optical lattice, and
discuss the tight-binding limit. Section III contains a dis-
sussion of the Peierls substitution scheme, the resulting mag-
netic fine structure, and its comparison with direct numerical
solutions. In Sec. IV, we give the effective Hamiltonian in-
cluding interactions and conclude in Sec. V.

II. MODEL

We start with the Hamiltonian for a particle in the rotating
frame of a two-dimensional square lattice

\[
H = \frac{1}{2m} \mathbf{p}^2 + \frac{1}{2} \hbar \omega^2 \mathbf{r}^2 - \Omega \mathbf{z} \cdot \mathbf{r} \times \mathbf{p}_z + V_0[\sin^2(kx) + \sin^2(ky)] ,
\]

(1)

where \( \mathbf{p}_z = (p_x, p_y) \) and \( \mathbf{r} = (x, y) \). \( m \) is the mass of the par-
ticle, \( \omega_z \) is the transverse harmonic trapping frequency, \( \Omega \) is the rotation frequency, and \( V_0 \) is the depth of the optical
potential created by a laser beam with wave number \( k = 2\pi/\lambda \) (for counterpropagating laser beams lattice constant
\( a \) is equal to \( \lambda/2 \)). In what follows, we use photon recoil energy \( E_R = \hbar^2 k^2/(2m) \) as the energy unit. This Hamiltonian
can be rearranged as

\[
H = \frac{(\mathbf{p}_z - m\Omega \mathbf{z} \times \mathbf{r})^2}{2m} + V_0[\sin^2(kx) + \sin^2(ky)] + \frac{1}{2} m(\omega_z^2 - \Omega^2) r^2.
\]

(2)

We neglect the last term assuming that \( \Omega \) is very close to \( \omega_z \),
so essentially we deal with a particle under an effective mag-
netic field \( B = 2mc\Omega/e \) in a lattice potential. We assume that
\( V_0 \) is deep enough for a tight-binding description to apply to
the system and furthermore concentrate on the dynamics of the
particles in the first excited (\( p \) ) band of the lattice. Our
approach is to first cast this Hamiltonian into a second quan-
tized form which includes the anisotropic hopping between
nearest neighbor sites, the on-site zero point energies, and
also the shift caused by rotation. Not only do we expect the
hopping between lattice sites to be affected, as it was for the
\( s \) band, but also the on-site energies to be modified. How-
ever, since the hopping and on-site Hamiltonians do not
commute, a common transformation that accounts for both
modifications cannot be found.

To overcome this difficulty, we temporarily assume that
the hopping amplitudes are not affected by the effective mag-
netic field and the only change is in the on-site energies. Our
expectation is that in this way we will obtain two nondegen-
erate bands to which we can apply Peierls substitution. This
procedure is rather ad hoc the validity of which is later
checked through a comparison with the first-principles re-
sults presented previously [19] and reproduced here partially.

We proceed with considering the following \( p \)-band tight-
binding Hamiltonian (the energy spectrum of which is mea-
sured relative to the center of the tight-binding \( s \) band) for
noninteracting particles including the on-site zero-point ener-
gies and the rotation term \((-\Omega L_z) \) [22,33]

\[
H = \sum_{\mathbf{R}, \mu, \nu} t_{\mu \nu}(b_{\mu \mathbf{R}}b_{\nu \mathbf{R}}^\dagger + H.c.) + \hbar \omega \sum_{\mathbf{R}, \mu} b_{\mu \mathbf{R}}^\dagger b_{\mu \mathbf{R}} + i\hbar \Omega \sum_{\mathbf{R}} (b_{\mu \mathbf{R}}^\dagger b_{\mu \mathbf{R}}^\dagger - b_{\mu \mathbf{R}} b_{\mu \mathbf{R}}^\dagger),
\]

(3)

where the summation is over all lattice sites \( \mathbf{R} \) and band
indices \( \mu = x, y \) (since the problem is two-dimensional, the \( p_z \)
orbital will not be considered). As usual, \( b_{\mu \mathbf{R}}^\dagger \) (\( b_{\mu \mathbf{R}} \)) is the
creation (annihilation) operator for a particle in the \( p_{\mu} \) band
at lattice site \( \mathbf{R}, \mathbf{e}_\nu \) is the unit vector along the \( \nu \) direction, \( \omega \)
is the frequency of the isotropic harmonic oscillator potential
which models the lattice potential around its minima, and \( t_{\mu \nu} \)
is the anisotropic hopping amplitude. The explicit expression
for \( t_{\mu \nu} \) (in the absence of rotation) is

\[
t_{\mu \nu} = \int \frac{\phi_{\mu}^{*}(\mathbf{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \phi_{\nu}(\mathbf{r} + a\mathbf{e}_\nu) d\mathbf{r}}{t_0} - (1 - \delta_{\mu \nu}) \Omega \mathbf{z} \mathbf{r}.
\]

(4)

where \( V(\mathbf{r}) \) is the periodic lattice potential and \( \phi_{\mu}(\mathbf{r}) \) is the
localized Wannier function corresponding to the \( p_{\mu} \) band.
When we approximate the lattice potential by a harmonic
oscillator around a minimum, these can be expressed as a
product of harmonic oscillator eigenfunctions, i.e.,

\[
\phi_{\mu}(\mathbf{r}) = u_\mu(x)u_\mu(y)
\]

and

\[
\phi_{\nu}(\mathbf{r}) = u_\nu(x)u_\nu(y),
\]

\( u_n(x) \) being the \( n \)th harmonic oscillator eigenfunction. \( t_0 \)
is the hopping amplitude between two neighboring \( p \) orbitals aligned along the orbital orientation and \( t_\perp \) is the amplitude when the orbitals are
oriented transversely with respect to the line connecting
them. Both amplitudes are defined to be positive and \( t_\parallel > t_\perp \)
due to larger overlap. Since the lattice potential is separable
in \( x \) and \( y \) coordinates, \( t_\parallel \) and \( t_\perp \) indeed have simple expres-
sions in reference to the one-dimensional problem. \( t_\parallel \) and \( t_\perp \)
are one quarter of the widths of the lowest and next lowest
bands for \( V = V_0 \sin^2(kx) \), respectively. By solving the
Schrödinger equation numerically, we find \( t_\parallel = 0.0025E_R \) and
\( t_\perp = 0.0603E_R \) for \( V_0 = 20E_R \). The on-site zero-point energy \( \hbar \omega \)
exto also has the simple interpretation of being the energy differ-
ence between \( s \) and \( p \) levels (bearing in mind the harmonic
description, see Fig. 1).
The diagonal Hamiltonian has the form 

\[ H = \sum_{\mathbf{k}} [E_\alpha(\mathbf{k})a_\mathbf{k}^\dagger a_\mathbf{k} + E_\beta(\mathbf{k})b^\dagger_\mathbf{k}b_\mathbf{k}], \]

with

\[ E_{\alpha,\beta}(\mathbf{k}) = \frac{f_{1\mathbf{k}} + f_{2\mathbf{k}}}{2} \pm \hbar \Omega \sqrt{1 + \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^2}, \]

where upper (lower) sign refers to \( \alpha (\beta) \). From this point on, we can apply Peierls substitution to the dispersion relation [Eq. (7)] to obtain an operator out of it, i.e., we change \( \mathbf{k} \) to \((\mathbf{p} - e\mathbf{A} / c) / \hbar \) using the Landau gauge \( \mathbf{A} = Bx\hat{y} \). The resulting Hamiltonian is transparent only when expressed in terms of a power series

\[ E_{\alpha,\beta}(\mathbf{k}) = \frac{f_{1\mathbf{k}} + f_{2\mathbf{k}}}{2} \pm \hbar \Omega \left[ 1 + \frac{1}{2} \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^2 \right. \]

\[ \left. - \frac{1}{8} \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^4 + \cdots \right], \]

with the assumption that \( |f_{1\mathbf{k}} - f_{2\mathbf{k}}| / 2\hbar \Omega = |\cos(k_x) - \cos(k_x)|(t_x + t_y) / \hbar \Omega \) is smaller than one. If \((t_x + t_y) / \hbar \Omega \) is much smaller than one, terms of lower order in \((f_{1\mathbf{k}} - f_{2\mathbf{k}}) / 2\hbar \Omega \) will be more dominant and one needs to consider only a few terms for a desired accuracy, instead of summing the whole series. Increasing accuracy is achieved by adding higher order terms. In a typical experimental condition, for instance, with \( V_0 = 20E_R \) and \( \hbar \Omega \sim E_R \), the ratio \((t_x + t_y) / \hbar \Omega \) is \(-0.063\), so a first order approximation may be sufficient for the desired accuracy. Here, we give the results to second order in \((f_{1\mathbf{k}} - f_{2\mathbf{k}}) / 2\hbar \Omega \), for completeness. The approximate energy band functions, where we retain terms up to second order, are then

\[ E_{\alpha,\beta}(\mathbf{k}) = \frac{f_{1\mathbf{k}} + f_{2\mathbf{k}}}{2} \pm \hbar \Omega \left[ 1 + \frac{1}{2} \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^2 \right. \]

\[ \left. - \frac{1}{8} \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^4 + \cdots \right], \]

where \( c_0^\pm = \hbar(\omega \pm \Omega) \), \( c_1 = t_x - t_y \), and \( c_2^\pm = \pm (t_x + t_y)^2 / 2\hbar \Omega \).

After converting cosines into sums of exponentials and making the Peierls substitution we obtain discrete translation operators, which allow us to express the eigenvalue problem as a difference equation. Since translations along \( y \) are multiplied by phases depending on \( x \) in the Landau gauge, one should be careful in creating an operator from cross terms such as \( \exp(ik_x) \exp(ik_y) \). The correct way of transforming should yield Hermitian operators and is obtained by symmetric combinations such as

FIG. 1. Lowest three bands for the two-dimensional sinusoidal lattice potential. The energy difference between the lowest two bands (\( s \) and degenerate \( p \) levels) (measured from the band centers) is \( \hbar \omega \) within the harmonic oscillator approximation for the potential minima, \( \omega \) being the oscillator frequency. For \( V_0 = 20E_R \), \( \hbar \omega = 7.7739E_R \).

III. PEIERLS SUBSTITUTION AND MAGNETIC FINE STRUCTURE

We perform a Fourier transformation on the Hamiltonian [Eq. (3)] as a preliminary for diagonalization in momentum space. The transformed Hamiltonian is

\[ H = \sum_{\mathbf{k}} \left[ (\epsilon_{\mathbf{k}} + \hbar \omega)b^\dagger_{\mathbf{k}}b_{\mathbf{k}} + (\epsilon_{\mathbf{k}} + \hbar \omega)b^\dagger_{\mathbf{k}}b_{\mathbf{k}} \right. \]

\[ + i \hbar \Omega (b^\dagger_{\mathbf{k}}b_{\mathbf{k}} - b^\dagger_{\mathbf{k}}b_{\mathbf{k}})], \]

where \( \epsilon_{\mathbf{k}} = 2\Sigma_{\mu} j_{\mu} \cos(k_{\mu}) \). Since the Hamiltonian is bilinear in creation and annihilation operators, it is diagonalizable by a Bogoliubov transformation. Defining \( f_{1\mathbf{k}} = \epsilon_{\mathbf{k}} + \hbar \omega \) and \( f_{2\mathbf{k}} = \epsilon_{\mathbf{k}} + \hbar \omega \), we observe that the Hamiltonian is diagonalized in \( \mathbf{k} \) space by the following transformation:

\[ \epsilon_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left[ \epsilon_{\mathbf{k}} + \sin \theta_{\mathbf{k}} \right] b_{\mathbf{k}} + i (\cos \theta_{\mathbf{k}} - \sin \theta_{\mathbf{k}}) b_{\mathbf{k}}^\dagger, \]

\[ \epsilon_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left[ \epsilon_{\mathbf{k}} - \sin \theta_{\mathbf{k}} \right] b_{\mathbf{k}} - i (\cos \theta_{\mathbf{k}} + \sin \theta_{\mathbf{k}}) b_{\mathbf{k}}^\dagger, \]

with

\[ \cos 2\theta_{\mathbf{k}} = \frac{1}{\sqrt{1 + \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^2}}, \]

\[ \sin 2\theta_{\mathbf{k}} = \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \frac{1}{\sqrt{1 + \left( \frac{f_{1\mathbf{k}} - f_{2\mathbf{k}}}{2\hbar \Omega} \right)^2}}. \]

The diagonal Hamiltonian has the form

\[ H = \sum_{\mathbf{k}} [E_\alpha(\mathbf{k})a_\mathbf{k}^\dagger a_\mathbf{k} + E_\beta(\mathbf{k})b^\dagger_\mathbf{k}b_\mathbf{k}], \]
Due to the translational invariance of the problem along the y direction, the y dependent part of the wave function is a plane wave [4]

\[ e^{ik_y a} \phi_{k_y a} = \frac{e^{ip_y a/h} e^{i(p_y - eBx)/a} + e^{i(p_y - eBx)/a} e^{ip_y a/h}}{2}. \]  

(10)

Making the substitutions \( x = na \) and \( y = la \), \( n \) and \( l \) being integers, and acting the effective Hamiltonian \( E_{a,b} \mathbf{p} - eB \mathbf{y}/c + \hbar \) on the wave function [Eq. (11)], we get the following difference equation:

\[
\begin{align*}
\frac{c_0^2}{4} & \{g(n+2) + g(n-2)\} + \left( \frac{c_1}{2} - \frac{c_2^*}{2} \right) \{\cos(2\pi n \phi - k_y a) + \cos[2\pi(n+1) \phi - k_y a]\} g(n+1) \\
+ \left( \frac{c_1}{2} - \frac{c_2^*}{2} \right) \{\cos(2\pi n \phi - k_y a) + \cos[2\pi(n-1) \phi - k_y a]\} g(n-1) \\
+ \left[ \frac{c_2^*}{2} \cos(4\pi n \phi - 2k_y a) + c_1 \cos(2\pi n \phi - k_y a) + c_1^* + c_2^* \right] g(n) = Eg(n),
\end{align*}
\]

(12)

where \( c_0^* \), \( c_1 \), and \( c_2^* \) were introduced following Eq. (9) and \( \phi = aB/(hc/\epsilon) \) is the magnetic flux quantum per unit cell. \( \phi \) can be expressed in terms of the rotation frequency \( \Omega \) as \( \phi = 2m\pi^2/\Omega \).

When \( \phi = p/q \), \( p \) and \( q \) being relatively prime integers, the difference equation [Eq. (12)] yields \( q \) equations together with the Bloch condition \( g(n+q) = e^{i\omega \alpha} g(n) \) due to the \( q \)-site translational invariance in the \( x \) direction. By diagonalizing the resulting \( q \times q \) coefficient matrix for several \( k \), and \( k_y \) pairs, we obtain the energy eigenvalues, which are plotted in Fig. 2, as a function of \( \phi \). We observe that each split band further divides into \( q \) subbands forming a pattern which has close resemblance to the Hofstadter butterfly. This result is in fact anticipated since \( c_2^* = \pm(t_1 + t_2)^2/2\hbar \Omega \) is much smaller than \( c_1 = t_1 - t_2 \) and if we simply neglect it as a first approximation, the energy band function [Eq. (9)] will just be that of the tight-binding \( s \) band, except that we have \( \hbar \Omega \) which gives rise to increasing separation between the split \( p \) bands with increasing \( \phi \). Our approximation becomes poorer as \( \phi \) (or \( \Omega \)) becomes smaller since we require that \( (t_1 + t_2)/\hbar \Omega \) be small. This is apparent in Fig. 2 in which we highlight the region where two bands overlap. However, if we increase the lattice depth, which decreases the hopping amplitudes, we can increase the region of validity. Equivalently, we can say that our results should improve as \( \phi \) increases. Another improvement option would be to consider a higher order expansion in translation operators, which models long-range hopping with yet smaller amplitudes.

To be able to judge the accuracy of the magnetic fine structure obtained by our method we compare it with a direct numerical solution of the Schrödinger equation, starting from the Hamiltonian [Eq. (2)]. One method of numerical solution is to reduce the problem to a magnetic unit cell using magnetic translation symmetry and solve the two-dimensional Schrödinger equation within this unit cell using finite difference methods. Unfortunately, the magnetic unit cell size increases with \( q \), the denominator of the flux \( \phi = p/q \), and the nontrivial boundary conditions required by magnetic translation symmetry makes this direct solution method computationally inefficient. Another, more efficient method, which was first developed by Zak [34], and then expanded on by Obermaier et al. [19], is to use magnetic translation symmetry to reduce the two-dimensional Schrödinger equation to a set of \( p \) one-dimensional equations with nonlocal couplings. This equation can be handled with relative ease using a truncated basis of harmonic oscillator wave functions. Still, a numerical calculation is efficient only for pure cases with \( \phi = 1/q \) and for small \( q \) values.

In Figs. 3 and 4, we compare our results with those obtained by a direct numerical calculation along the lines of Ref. [19]. Calculations with the effective Hamiltonian are

FIG. 2. Magnetic fine structure of the \( p \) band for \( V_0 = 20E_a \). Two-fold degenerate zero-field \( p \) band is split into two as \( \phi = p/q \) grows. Each split band further has \( q \) subbands. Our approximation fails in the shaded region, corresponding to \( \phi \approx 1/6 \) (the nearest \( \phi = 1/q \) to 1/5, for which the spectrum is displayed in Fig. 3), where two bands overlap. This region can be made narrower if the lattice depth \( V_0 \) is increased.
much faster and the results are as good as the direct numerical solution. For instance, in the case of $\phi = 1/5$ (Fig. 3) the agreement is already good, but if we increase $\phi$ to 1/3 (Fig. 4), apart from a slight overall shift, we see that band gaps are also more faithfully reproduced. The computational efficiency of the effective Hamiltonian method for the single particle problem is striking, but its real utility is that it can be used as a starting point to include interactions in the system.

IV. EFFECTIVE HAMILTONIAN

Until now, we have essentially been dealing with the single particle spectrum. The results we obtained can be utilized to examine the case of many particles, if we first write the effective Hamiltonian in real space

$$H_{\text{eff}} = \frac{1}{4} \sum_{\langle (r,r') \rangle} A_{(r,r')} (c_r^\dagger \alpha_r c_{r'} + c_{r'}^\dagger \beta_r^\dagger \beta_{r'})$$

$$- \frac{1}{4} \sum_{\langle (r,r') \rangle} B_{(r,r')} (c_r^\dagger \alpha_r c_{r'} + c_{r'}^\dagger \beta_r^\dagger \beta_{r'})$$

$$+ \frac{c_1}{2} \sum_r C_{(r,r')} (\alpha_r^\dagger \alpha_r + \beta_r^\dagger \beta_r)$$

$$+ \sum_r [(c_0^2 + c_2^2) \alpha_r^\dagger \alpha_r + (c_0^2 + c_2^2) \beta_r^\dagger \beta_r],$$

$$A_{(r,r')} = \begin{cases} e^{\pm i 4 \pi \phi}, & r \text{ and } r' \text{ have } x = na \\ 1, & \text{otherwise.} \end{cases}$$

$$B_{(r,r')} = \begin{cases} e^{i 2 \pi (n+1) \phi} + e^{i 2 \pi n \phi}, & r \text{ and } r' \text{ on } y = -x \\ e^{i 2 \pi (n-1) \phi} + e^{i 2 \pi n \phi}, & r \text{ and } r' \text{ on } y = x \\ 1, & (r \text{ or } r' \text{ has } x = na). \end{cases}$$

$$C_{(r,r')} = e^{i 2 \pi n \phi},$$

where $\langle (r,r') \rangle$ denotes summation over nearest neighbors in the square lattice (with separation $a$, $\langle (r,r') \rangle$) over next-nearest neighbors (with separation $\sqrt{2}a$, and $\langle \langle (r,r') \rangle \rangle$) over next-next-nearest neighbors (with separation $2a$); $\pm$ sign refers to the hopping direction. We note that the next-nearest and next-next-nearest coupling amplitudes turn out to be the same in our approximation. This effective Hamiltonian represents noninteracting particles moving in the $p$ band of a square lattice under a particular magnetic flux $\phi$. The connection between the new and old operators is made through the following definition:

$$\alpha_k = \cos \theta_k b_k^x + \sin \theta_k b_k^y,$$

$$\beta_k = \cos \theta_k b_k^x - \sin \theta_k b_k^y,$$

with $b_k^x = (b_{k\uparrow} \pm ib_{k\downarrow})/\sqrt{2}$. The operator $b_k^x$ ($b_k^y$) annihilates a particle with momentum $h \mathbf{k}$ whose $z$ component of angular momentum is $-h$ ($h$). To first order in $(\hbar^2 I_0)/\hbar \Omega$, $\alpha_k$ and $\beta_k$ are of the following form:

$$(\alpha, \beta_k) = b_k^x \pm \frac{\hbar^2 I_0}{2 \hbar \Omega} \cos k \cdot a - \cos k \cdot a),$$

where the upper (lower) sign refers to $\alpha$ ($\beta$). After expressing cosines as exponentials, we make the Peierls substitution, i.e., we change $k$ to $k - eB \mathbf{r} \mathbf{\hat{y}}/\hbar$ in the coefficients of $b_k^x$ and interpret the resulting factors $\exp(\pm i 2 \pi \mathbf{a} \cdot k)$ as momentum translation operators whose action on a function of $k$ is given by $\exp(\pm i 2 \pi \mathbf{a} \cdot k)/\hbar$ ($f(k) \mapsto \pi \mathbf{a} \cdot k$). Fourier transformation of these modified operators yields the real space operators as

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\begin{equation}
(\alpha, \beta)_{n_l} = b_{n_l}^\dagger \pm \frac{t_l + t_{l-1}}{4\hbar \Omega} \times (b_{n+1,l}^\dagger + b_{n-1,l}^\dagger - e^{i2\pi \delta_l} b_{n+1,l-1}^\dagger - e^{-i2\pi \delta_l} b_{n-1,l-1}^\dagger),
\end{equation}

where the indices \((n, l)\) specify the \(x (=na)\) and \(y (=la)\) coordinates.

For bosons, the short-range repulsive interactions between particles can be incorporated into our model as an on-site interaction energy which can be written, up to terms renormalizing the chemical potential, as [22]

\begin{equation}
H_{\text{int}} = \frac{U}{2} \sum_r \left( n^2_r - \frac{L^2_r}{3\hbar^2} \right),
\end{equation}

\begin{equation}
U = g \int |\phi_{\mu, \nu}(r)|^4 dr,
\end{equation}

where \(n_r := \sum \nu b_{\mu, \nu}^\dagger b_{\mu, \nu}^\dagger\) is the boson number operator, \(L_r := -i\hbar (b_{\mu, \nu}^\dagger b_{\mu, \nu}^\dagger - b_{\mu, \nu} b_{\mu, \nu}^\dagger)\) is the \(z\) component of the angular momentum of a boson at site \(r\), and \(g > 0\) is the short-range repulsive interaction strength. The interaction Hamiltonian can be written in a microscopically more revealing way using \(n^\pm_r := (b_{\mu, \nu}^\dagger)^\pm b_{\mu, \nu}^\pm\). In this notation \(n_r = n^+_r + n^-_r\) and \(L_r := -\hbar (n^+_r - n^-_r)\). So the interaction becomes

\begin{equation}
H_{\text{int}} = \frac{2U}{3} \sum_r \left( (n^+_r)^2 + (n^-_r)^2 + 4n^+_r n^-_r \right).
\end{equation}

By adding \(H_{\text{int}}\) [Eq. (17)] to \(H_{\text{eff}}\) [Eq. (13)], we obtain the Hamiltonian for interacting bosons in the \(p\) band of a rotating optical lattice.

V. CONCLUSION

We considered how the degenerate excited bands of a tight-binding optical lattice are affected by the effective magnetic field created by rotation. Specifically considering the first excited \((p)\) band of a two-dimensional lattice, we pointed out that the magnetic field causes not only the hopping between different lattice sites to be modified, but also changes the on-site energies. We showed that once the modification of the on-site energies are explicitly taken into account, the Peierls substitution scheme can be used to obtain an effective Hamiltonian and the energy spectrum of the system.

The energy spectrum contains not only the splitting of the two bands under the effective magnetic field, but also the fine structure forming a pattern similar to the Hofstadter butterfly. We compare the energies obtained from the Peierls substitution procedure with a direct numerical solution of the Schrödinger equation, and observe that our procedure matches the numerical solution to a very good accuracy.

The effective Hamiltonian is obtained by using a series expansion in the ratio of the hopping parameter \(t_l (\gg t_{l-1})\) to \(\hbar \Omega\), which is a small parameter for tight-binding lattices except in the limit of very slow rotation. We carry out this expansion to second order and the resulting effective Hamiltonian contains hopping between all lattice sites that can be connected by traversing two links [Eq. (13)].

While we performed a second order expansion, it is instructive to display the effective Hamiltonian to first order in \((t_l + t_{l-1})/\hbar \Omega\) in terms of the original operators \(b_{\mu, \nu}\)

\begin{equation}
H_{\text{eff}} = \frac{t_l + t_{l-1}}{2} \sum_{\langle x, x' \rangle} \left[ C_{x, x'}(b_{x, \nu}^\dagger)^\dagger b_{x', \nu}^\dagger (1 - 2 \delta_{\langle x, x' \rangle}) + \text{H.c.} \right]
\end{equation}

\begin{equation}
+ \frac{t_l - t_{l-1}}{2} \sum_{\langle x, x' \rangle} C_{x, x'}(b_{x, \nu}^\dagger b_{x', \nu}^\dagger + (b_{x', \nu}^\dagger)^\dagger b_{x, \nu}^\dagger)
\end{equation}

\begin{equation}
+ \sum_r [\hbar (\omega + \Omega) n^+_r + \hbar (\omega - \Omega) n^-_r]
\end{equation}

\begin{equation}
= \sum_{\langle x, x' \rangle} \sum_{\mu, \nu} f_{\mu, \nu, \lambda}^r \left( b_{\mu, \nu}^\dagger b_{\mu, \nu}^\dagger + C_{x, x'} \exp \left\{ \frac{i e}{\hbar c} \int_{r}^{r' \rightarrow x} \mathbf{A} \cdot \mathbf{dr}' \right\} \right) + \text{H.c.}
\end{equation}

\begin{equation}
+ i \hbar \omega \sum_{\mu, \nu} b_{\mu, \nu}^\dagger b_{\mu, \nu}^\dagger + i \hbar \Omega \sum_r (b_{\mu, \nu}^\dagger b_{\mu, \nu}^\dagger - b_{\mu, \nu}^\dagger b_{\mu, \nu}^\dagger)
\end{equation}

\begin{equation}
C_{x, x'} = \begin{cases} e^{i2\pi \phi_x}, & (r) = (r')\ , \ n = na \\ 1, & (r) \neq (r') \ . \end{cases}
\end{equation}

This Hamiltonian incorporates the first nonvanishing effects of rotation and can be used as an effective Hamiltonian if \((t_l + t_{l-1})/\hbar \Omega\) is not large. Indeed a recent preprint which appeared while this paper was in preparation uses this form as a starting point [33]. However, to investigate corrections for slower rotation one has to go to higher orders as in Eq. (13). In Eq. (18), we display the vector potential \(\mathbf{A}\) explicitly to express the gauge invariance of the effective Hamiltonian. Our numerical work was carried out using a higher order approximation [Eq. (15)] which is also gauge invariant.

In conclusion, we showed how Peierls substitution can be used for degenerate bands and checked its accuracy with direct numerical solutions. By investigating how operator transformations are modified through Peierls substitution [Eq. (15)] we derived a first order effective Hamiltonian in real space [Eq. (18)].

Going to the next order, we obtain a more accurate, but more complicated effective Hamiltonian, which displays how higher order hopping is modified by the effective magnetic field. Finally, we also give the expression for on-site interaction for bosons in terms of the angular momentum “up” and “down” operators. We hope that our results stimulate further theoretical and experimental investigations of the \(p\)-band physics under an effective magnetic field.

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