Bosonic Hofstadter butterflies in the presence of phonon modes

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Abstract. We have investigated the influence of lattice sites vibrations on bosonic Hofstadter’s butterfly (HB) spectrum for the case of conventional square lattice. Only the pair of specific phonon modes with opposite quasimomenta has been taken into account. The study has shown that HB-type spectra can be substantially modified by the presence of phonons, depending on the ratios of such parameters of the system as site-to-site transition amplitudes, particle-phonon interaction constant, and characteristic vibration frequency.

1. Introduction
Since the invention in 1976 [1], the renowned Hofstadter’s butterflies have been thoroughly studied for various lattice geometries [2–5] and in different implementations [6–11]. From this point of view, the behaviour of both fermionic and bosonic particles in two-dimensional systems subject to the magnetic or other gauge field seems to be scrupulously investigated.

On the other hand, the lattice vibrations within the second quantization formalism and tight binding approach has been recently attracted attention [12, 13]. Unfortunately, the exploration of behaviour of bosonic particles affected by both gauge field and lattice vibrations within the scope of Hofstadter butterflies can be hardly found.

In the present work, we research bosonic Hofstadter butterflies altered by the presence of lattice phonons. Tight binding approximation and the second quantization formalism are utilized throughout the paper.

2. Theory
We start with the conventional tight-binding Hofstadter Hamiltonian yielding the butterfly spectrum:

\[ \hat{H}_0 = t \sum_{n_1, n_2} \left( \hat{a}_{n_1+1, n_2} \hat{a}_{n_1, n_2} + \hat{a}_{n_1, n_2+1} \hat{a}_{n_1, n_2} e^{-2\pi i \xi n_1} + \text{h.c.} \right). \]  \( (1) \)

The lattice considered is square, only the nearest neighbour hoppings are taken into account. Operators \( \hat{a}_{n_1, n_2}^{(\dagger)} \) are the bosonic annihilation (creation) operators at the site \( (n_1, n_2) \) (the indices 1 and 2 correspond to x and y axes, respectively). The tunneling amplitude equals \( t \), \( \xi \) is the ratio of the magnetic field flux through the unit cell to the quantum of magnetic field flux. In the present paper, we scrutinize rational magnetic fields implying \( \xi = p/q \), where \( p \) and \( q \) are coprime integers. Hereinafter, the magnetic field is treated within Landau gauge, i.e. \( \vec{A} = (0, Bx, 0) \).
Within the assumption of rational fields, Hamiltonian (1) can be transformed into the reciprocal space. In that case, the unit cell should be extended in the x-direction so as to possess q sites. Axis y remains, in the sense, unchanged. Redefining \( n_1 \) to enumerate the supercell, and setting \( s \) to itemize the sites within each supercell, we arrive at

\[
\hat{H}_0 = \sum_{k_1,k_2} \sum_{s=0}^{q-2} \left\{ \hat{a}_{k_1,k_2,s+1}^\dagger \hat{a}_{k_1,k_2,s} + \hat{a}_{k_1,k_2,s+1} \hat{a}_{k_1,k_2,s-1} e^{-ik_1} + \sum_{s=0}^{q-1} \hat{a}_{k_1,k_2,s} \hat{a}_{k_1,k_2,s} e^{-2\pi i q s} e^{-ik_2} + \text{h.c.} \right\}
\]

\[
= \sum_{k_1,k_2} \hat{a}_{k_1,k_2} \left\{ \hat{p}_q^+ \hat{p}_q e^{-ik_1} + \hat{e}_q e^{-ik_2} + \text{h.c.} \right\} \hat{a}_{k_1,k_2},
\]

where \( \hat{a}_{k_1,k_2} = (a_{k_1,k_2,1}, a_{k_1,k_2,2}, \ldots a_{k_1,k_2,q-1})^T \), and the rest matrices are

\[
\hat{p}_q = \begin{pmatrix}
0 & 1 & \cdots & 0 \\
1 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 1 & 0
\end{pmatrix}, \quad \hat{p}_q'' = \begin{pmatrix}
0 & \cdots & 0 \\
0 & 1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & 1
\end{pmatrix}, \quad \hat{e}_q = \text{diag} \left( e^{-2\pi i q s} \right)_{s=0,1,\ldots,(q-1)}
\]

(All the empty positions are set to zero, the index \( q \) explicitly shows the dimension of the matrices.)

The influence of the gauge field reveals in the phase factor \( e^{-2\pi i q n_1} \) in (1) that transforms into \( e^{-2\pi i q s} \) in (3) and (4). This factor is calculated as linear integral of \( \varphi \) (with the corresponding premultipliers) along the straight path between the sites. For Landau gauge, the following expression can be derived:

\[
\varphi_{1\to2} = \frac{\pi \xi}{L^2} \left( Y_2 - Y_1 \right) (X_2 + X_1) + \xi \left( Y_2 - Y_1 \right) (x_2 + x_1)
\]

\[
\approx \frac{\pi \xi}{L^2} \left( Y_2 - Y_1 \right) (X_2 + X_1) + \varphi_{1\to2}^0 + \frac{\pi \xi}{L^2} \left( Y_2 - Y_1 \right) (x_2 + x_1)
\]

Here, the capital characters \( X \) and \( Y \) with 0 superscript stand for the equilibrium positions of the lattice sites, the lowercase characters are the corresponding displacements. The subscripts 1 and 2 respectively indicate initial and final states of tunneling. The zero-model phase factor \( \varphi_{1\to2}^0 \) is that calculated for the frozen vibrations. In (6), only the terms up to the first order in \( x \) and \( y \) are kept (the vibrations are believed to be small compared to the intersite distance, \( L \)). One of the major assumptions made here is that we consider only the vibrations in y-direction. (If we assume the vibrations along one of the axes to be frozen, then the choice of the exact direction is arbitrary.) Therefore,

\[
\varphi_{1\to2} \approx \varphi_{1\to2}^0 + \frac{\pi \xi}{L^2} \left( X_2 + X_1 \right) (y_2 - y_1).
\]

Another way the vibrations can manage the tunnelings and phases is the particle-phonon interaction that can be included via the effective interaction constant, \( \lambda \), and alters the tunneling amplitudes. Then, the Hamiltonian of the system can be put down as

\[
\hat{H} = \sum_{n_1,n_2} \left\{ \hat{a}_{n_1,n_2}^\dagger \hat{a}_{n_1,n_2} e^{-\frac{2\pi i n_1}{L} (2n_1+1)(y_{n_1,n_2} - y_{n_1,n_2})} + \hat{a}_{n_1,n_2}^\dagger \hat{a}_{n_1,n_2} e^{-2\pi i n_1} e^{-\frac{2\pi i n_1}{L} (2n_1+1)(y_{n_1,n_2} - y_{n_1,n_2})} \left[ 1 - \lambda (y_{n_1,n_2+1} - y_{n_1,n_2}) \right] + \text{h.c.} \right\} + \hat{H}_{\text{vib}}
\]

\[
\approx \hat{H}_0 + \hat{H}_{\text{vib}}
\]

\[
- t \sum_{n_1,n_2} \left\{ \hat{a}_{n_1,n_2}^\dagger \hat{a}_{n_1,n_2} (y_{n_1,n_2+1} - y_{n_1,n_2}) e^{-2\pi i n_1} \left( \lambda + \frac{2\pi i n_1}{L} \right) + \text{h.c.} \right\} = \hat{H}_0 + \hat{H}_{\text{vib}} + \hat{H}'.
\]
The vibrations Hamiltonian \( \hat{H}_{\text{vib}} \) can be written in the form of second quantization as well (\( \hbar = 1 \)):

\[
\hat{H}_{\text{vib}} = \sum_{x, \sigma} \omega_{x, \sigma} \hat{b}_{x, \sigma}^\dagger \hat{b}_{x, \sigma}.
\]  

(10)

If only the nearest neighbours interact, the spectrum of phonons can be obtained in analytic form:

\[
\omega_{x, \sigma} = 4k_\text{B} \sin^2 \left( \frac{\pi x}{2} \right),
\]

(11)

where \( x \) is the quasimomentum (one-dimensional), and \( \sigma \) denotes the phononic branch that is actually the only one, acoustic. The spectrum of phonons is \( q \)-fold degenerate, the matrix to be diagonalized is proportional to the identity matrix of shape \( q \times q \). Our goal here is to consider the influence of one specific phonon mode, that is distinguished by the motion of the entire supercell as a whole. The normalized eigenvector for the mode is \( (1, 1, \ldots, 1)/\sqrt{q} \). Afterwards, the displacements can be expressed in terms of creation and annihilation operators as

\[
y_{n_1, n_2} = \sum_x \sqrt{\frac{1}{2\omega_{x, q}}} (\hat{b}_{x, n_2}^\dagger e^{-i\omega_{x, n_2}} + \text{h.c.}) = \sum_x \mathcal{A}(x) (\hat{b}_{x, n_2}^\dagger e^{-i\omega_{x, n_2}} + \text{h.c.}) .
\]

(12)

This representation eliminates line (9). In line (8), we suppose that the particle-phonon interaction constant is much greater compared to the reciprocal \( L, \lambda \gg 1/L \).

The next step consists in expressing operators \( \hat{a}_{k_1, k_2, \sigma}^{\dagger} \) in terms of operators \( \hat{a}_{k_1, k_2, \sigma}^\dagger \) diagonalizing \( \hat{H}_0 \), in order to write the interaction Hamiltonian (8) and (9):

\[
\hat{d}_{k_1, k_2} = \mathcal{U}(k) \hat{a}_{k_1, k_2}, \quad \hat{H}_0 = \sum_{k_1, k_2, \sigma} \varepsilon_{k_1, k_2, \sigma} \hat{a}_{k_1, k_2, \sigma}^\dagger \hat{d}_{k_1, k_2, \sigma}^\dagger,
\]

(13)

where \( \mathcal{U} \) is \( q \)-dimensional tranisition matrix. After straightforward but lengthy algebra, we can obtain the following expression for the interaction Hamiltonian:

\[
\hat{H}' = -i \sum_{k, \sigma, \tau, \tau'} \sum_{s=0}^{q-1} \sum_{s'=0}^{q-1} A(x, k, \tau, \tau') \mathcal{U}_{\sigma, \tau'}^\dagger(k) \mathcal{U}_{\sigma, \tau}^\dagger(k + x) \hat{d}_{k, \tau, \tau'}^\dagger \hat{d}_{k + x, \tau', \tau} \left( \hat{b}_{-x, \tau} \delta_{n_1} + \hat{b}_{x, \tau}^\dagger \delta_{n_2} \right) \times \left[ e^{-2\pi i \xi_{s} - ik_k} \left( e^{-i\pi \tau} - 1 \right) - \text{h.c.} \right] \mathcal{A}_\tau(\xi, k, \tau).
\]

(14)

The symbol \( \delta_{n_1,j} \) is put here to respect the energy conservation law during the process of absorption or emission of a phonon. Finally, we restrict the analysis to the minimal set of two phonon modes within the chosen acoustic branch, namely with quasimomenta \( +\beta \) and \( -\beta \), which leads to the simplification in (14) where \( \lambda \) no longer span the whole Brillouin zone but can take only these two values. Denote the occupation of these phononic states by \( m_+ \) and \( m_- \). The eigenstate of the total Hamiltonian can be searched in the form

\[
|\mu\rangle = \sum_{k, \tau, m_+, m_-} \alpha_{k, \tau, m_+, m_-} |l_{k, \tau}; m_+, m_-\rangle.
\]

(15)

(The total Hamiltonian \( \hat{H} \) commutes with the operator of total number of bosons, \( \sum_{k, \tau} \hat{a}_{k, \tau}^\dagger \hat{a}_{k, \tau} \), and we study the states with one boson and arbitrary number of phonons in the two states described above.) The equation

\[
\hat{H}|\mu\rangle = \mu|\mu\rangle
\]

formulated in terms of coefficients \( \alpha_{k, \tau, m_+, m_-} \) can be treated as an eigenvalue problem, which may be more convenient for numeric calculations.
3. Numeric results
We have numerically investigated the case of $k = 0$ (Gamma-point in the first Brillouin zone). That, as can be inferred from (14), demanded diagonalization of the Hofstadter Hamiltonian in the Gamma-point and at $k_2 = \pm \beta$ (to get $\hat{\mathcal{U}}(k=0)$ and $\hat{\mathcal{U}}(k_2=\pm \beta)$). In the end, the eigenvalue problem for coefficients $\alpha_{k,\tau,m_+,m_-}$ has been numerically solved. Hopping amplitude $t$ has been taken as a unit of energy scale.

In the calculations, we studied the case when the populations of the phonon modes can be equal to either 0 or 1: $m_\pm \in \{0,1\}$.

Figure 1 demonstrates the HB spectra. Figure 1(A) shows the pristine HB without the lattice vibrations. Figure 1(B) shows the spectrum for moderate parameters ($\lambda = 1$, $\omega_0 = 1$). The spectrum may be roughly understood as the three replicas of the pristine one shifted with respect to each other, the influence of $\hat{H}'$ in this case is present but almost negligible within the computing accuracy accepted. Figure 1(C) presents the spectrum for a huge value of vibrations frequency, $\omega_0 = 10$. No particle-phonon interaction takes place (in (14), all the $\delta_{m_1,2}$ symbols equal zero). Figure 1(D) demonstrates the spectrum for small $\omega_0 = 0.01$. Such a small value of the characteristic frequency results in overall lower shifts and separation of the butterflies. On the other hand, the influence of $\hat{H}'$ becomes more notable, a much greater amount of non-zero summands in (14) occur, which gives rise to notable alterations that smear the original spectrum.

4. Conclusion
We have investigated the behaviour of bosonic Hofstadter butterflies subject to the influence of lattice phonons. We have developed the theoretical model taking into account both phase acquisition due to the presence of magnetic (or another gauge) field and lattice vibrations. Within the second quantization formalism, the Hamiltonian of the system has been derived. Finally, we scrutinized the reduced system with only two specific phonon modes and numerically calculated the spectra.

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Figure 1. Hofstadter butterflies, the hopping amplitude $t = 1$ everywhere. (A) without vibrations, $\lambda = 0$; (B) $\lambda = 1$, $\omega_0 = 1$, $\beta = \pi/4$; (B) $\lambda = 0.5$, $\omega_0 = 10$, $\beta = \pi/2$; (D) $\lambda = 1$, $\omega_0 = 0.01$, $\beta = \pi/8$. 