Comment on ''Hofstadter butterfly for the hexagonal lattice''

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The magnetic subband structure of a hexagonal lattice is reexamined and the flaws made in the formalism of an existing literature [Phys. Rev. B **56**, 3787 (1997)] are corrected. Dependence of the energy spectrum on the strength of the hopping integral is also illustrated.

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In a recent paper, Gumbs and Fekete[1] studied the energy spectrum of a two-dimensional hexagonal lattice under a uniform perpendicular magnetic field $\vec{B}=B\hat{z}$. By applying the Peierls substitution $\vec{k}\rightarrow(\vec{p}+e\vec{A})/\hbar$ for the energy dispersion $\varepsilon(\vec{k})$ given by Eq. (1) of Ref. 1, the authors constructed an effective Hamiltonian and calculated the energy eigenvalues by diagonalizing the Hamiltonian matrix. From this, the authors illustrated the dependence of the magnetic subband structure on the strength of the hopping integral. However, unfortunately, the authors made a simple but serious mistake in formulating the problem, and thus presented totally wrong results. In this comment, we reexamine the problem to put a correct formalism. Dependence of the subband structure on the strength of the hopping integral is also illustrated.

To our end, let us consider the tight-binding Hamiltonian given by

$$H=\sum_{ij} t_{ij}e^{i\theta_{ij}}|i\rangle\langle j|, \tag{1}$$

where t_{ij} is the hopping integral between the nearest sites i and j, $|i\rangle$ is a state of an atomiclike orbital centered at the site i, and $\theta_{ij}=(2\pi/\phi_0)\int_i^j\vec{A}\cdot d\vec{l}$ is the magnetic phase factor in units of the magnetic flux quantum $\phi_0=h/e$. Under the Landau gauge, $\vec{A}=(0,Bx,0)$. Let us denote the lattice point as (m,n), i.e., $(x,y)=(mb,nc)$, where $b=a/2$ and $c=\sqrt{3}a/2$, a being the lattice constant. Then θ_{ij} can be written as

$$\theta_{ij}=\begin{cases} 0, & j=(m\pm 2,n),\\ \pm\pi\phi(m+1/2), & j=(m+1,n\pm 1),\\ \pm\pi\phi(m-1/2), & j=(m-1,n\pm 1),\end{cases} \tag{2}$$

where $i=(m,n)$ and $\phi=2\sqrt{3}Bb^2/\phi_0$ is the magnetic flux through the unit cell. By means of Eq. (2), the tight-binding equation $H\Psi_{m,n}=E\Psi_{m,n}$, can be written as

$$\begin{aligned} E\Psi_{m,n}=&t_a(\Psi_{m-2,n}+\Psi_{m+2,n})+t_b\{\exp[i\pi\phi(m-1/2)]\\ &\times\Psi_{m-1,n-1}+\exp[-i\pi\phi(m+1/2)]\Psi_{m+1,n+1}\}\\ &+t_c\{\exp[i\pi\phi(m+1/2)]\Psi_{m+1,n-1}\\ &+\exp[-i\pi\phi(m-1/2)]\Psi_{m-1,n+1}\}, \end{aligned} \tag{3}$$

where t_a is the hopping integral along the x direction and $t_{b(c)}$ is the hopping integral along the direction, which makes $\pi/3$ $(2\pi/3)$ with the x direction. Since y is cyclic under the Landau gauge, $\Psi_{m,n}$ can be written as $\Psi_{m,n}=e^{ik_yy}\psi_m$, and thus Eq. (3) can be simplified as

$$E\psi_m=t_a\psi_{m-2}+\xi^*_{m-1}\psi_{m-1}+\xi_m\psi_{m+1}+t_a\psi_{m+2}, \tag{4}$$

where

$$\begin{aligned}\xi_m=&t_c\exp\{i[\pi\phi(m+1/2)-k_yc]\}\\ &+t_b\exp\{-i[\pi\phi(m+1/2)-k_yc]\}.\end{aligned} \tag{5}$$

Denoting $\phi=p/q$ with relative primes p and q, it can be easily checked that $\xi_{m+M}=\xi_m$, where $M=q$ $(2q)$ for an even (odd) p. Thus, m in Eq. (4) satisfies the condition $1\leqslant m\leqslant q$ $(1\leqslant m\leqslant 2q)$ for an even (odd) p, and the Bloch condition along the x direction can be written as

$$\psi_{m+M}=\exp(ik_xMb)\psi_m. \tag{6}$$

By means of Eqs. (4) and (6), the characteristic matrix that yields the energy eigenvalues can be written as

$$\begin{pmatrix} 0 & \xi_1 & t_a & 0 & \cdots & 0 & t_ae^{-i\delta} & \xi^*_Me^{-i\delta}\\ \xi^*_1 & 0 & \xi_2 & t_a & \cdots & 0 & 0 & t_ae^{-i\delta}\\ t_a & \xi^*_2 & 0 & \xi_3 & \cdots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & \cdots & 0 & \xi_{M-2} & t_a\\ t_ae^{i\delta} & 0 & 0 & 0 & \cdots & \xi^*_{M-2} & 0 & \xi_{M-1}\\ \xi_Me^{i\delta} & t_ae^{i\delta} & 0 & 0 & \cdots & t_a & \xi^*_{M-1} & 0 \end{pmatrix}, \tag{7}$$

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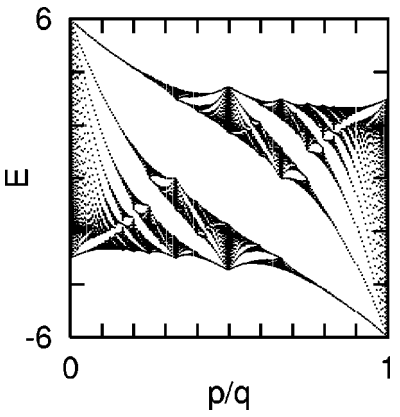

FIG. 1. Energy eigenvalues vs ϕ for $(t_a,t_b,t_c)=(1,1,1)$. Calculations are performed for $\phi=p/199$ with $1\leqslant p\leqslant 198$, and the central value of $\vec{k}$ in the MBZ is taken into account.

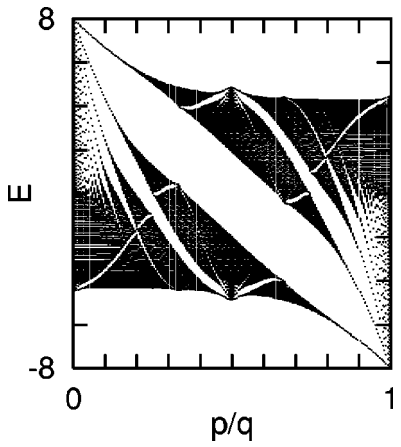

FIG. 2. Energy eigenvalues vs ϕ for $(t_a,t_b,t_c)=(2,1,1)$. Other parameters are the same as Fig. 1.

where $\delta=k_xqa/2$ (k_xqa) for an even (odd) p.

Now let us point out the mistake made in Ref. 1: The fundamental mistake in deriving the effective Hamiltonian [i.e., Eq. (2) of Ref. 1] lies in operating $\exp[\pm i(p_x \pm\sqrt{3}eBx)a/2\hbar]$ to $\Psi_{m,n}$. According to Ref. 1, the results of the operations are given by

$$\begin{aligned}\exp[\pm i(p_x+\sqrt{3}eBx)b/\hbar]\Psi_{m,n}&=\exp\pm 2(i\pi\phi m)\Psi_{m\mp 1,n},\\ \exp[\pm i(p_x-\sqrt{3}eBx)b/\hbar]\Psi_{m,n}&=\exp(\mp 2i\pi\phi m)\Psi_{m\mp 1,n}.\end{aligned}\tag{8}$$

However, these are erroneous ones that result from ignoring the commutation relation $[x,p_x]=i\hbar$. The correct expressions should be as follows:[2]

$$\begin{aligned}&\exp[\pm i(p_x+\sqrt{3}eBx)b/\hbar]\Psi_{m,n}\\ &\quad=\exp[\pm i\pi\phi(m\mp 1/2)]\Psi_{m\mp 1,n},\\ &\exp[\pm i(p_x-\sqrt{3}eBx)b/\hbar]\Psi_{m,n}\\ &\quad=\exp[\mp i\pi\phi(m\mp 1/2)]\Psi_{m\mp 1,n}.\end{aligned}\tag{9}$$

One can easily check that the same equation as Eq. (3) can be obtained by the method of the Peierls substitution if Eq. (9) instead of Eq. (8) is adopted. Indeed, one can check that Eq. (6) of Ref. 1, the key equation of the paper, is non-Hermitian, which indicates that the results of Ref. 1 are wrong, since the energy eigenvalues should be ''real'' numbers.

We now present our results for the magnetic subband structure obtained by diagonalizing Eq. (7). Figure 1 shows the $E-\phi$ diagram for $(t_a,t_b,t_c)=(1,1,1)$, $\vec{k}=0$, and $\phi=p/199$ with $1\leqslant p\leqslant 198$; it clearly shows that the energy spectrum is *not* ''symmetric about $\phi=1/2$'' and there is *no* ''distinct array of energy eigenvalues parallel to the energy axis in the two largest energy gaps,'' contrary to the result of Ref. 1 [see Fig. 1 of Ref. 1]. Note that Fig. 1 of this comment is exactly the same as Fig. 3 of Ref. 3 presented by Claro and Wannier if E is replaced by $-(E-\epsilon_0)/2\epsilon_1$, which is quite natural since both works deal with exactly the same problem.

Figure 2 is the plot for $(t_a,t_b,t_c)=(2,1,1)$. The increase of total bandwidths and the occurrence of gap closing except for a few large ones are clearly seen. We argue that these phenomena may be the generic effects of the hopping anisotropy, since the same phenomena were also observed in the square lattice.[4] Note that, from Fig. 3 of Ref. 1, which is plotted for the same parameters as in Fig. 2 of this comment, Gumbs and Fekete argued that ''the bottom of the energy band is very flat near $E=-4$'' and that ''the spectrum is symmetric about $\phi=1/2$.'' However, Fig. 2 of this comment clearly shows that these arguments are incorrect. Besides, in regard to Figs. 2–4 of Ref. 1, we would like to point out that the $E-\phi$ diagrams for the parameters $(t_a,t_b,t_c)=(1,2,1)$, $(2,1,1)$, and $(1,1,2)$ should be identical when all the values of $\vec{k}$ in the magnetic Brillouin zone (MBZ; $|k_x|\leqslant 2\pi/Ma$ and $|k_y|\leqslant\pi/\sqrt{3}a$) are taken into account, since there is no preferable direction in the lattice plane under a uniform perpendicular magnetic field.

Figure 3 shows the t_a dependence of the band structure for $\phi=1/5$, where $t_b=t_c=1$ and all the values of $\vec{k}$ in the MBZ are taken into account. Note that we introduce the rescaled energy defined by $E_{re}=3E/(t_a+t_b+t_c)$, which is always in the range of $[-6,6]$ regardless of the strength of the hopping anisotropy, as in the isotropic case. The figure

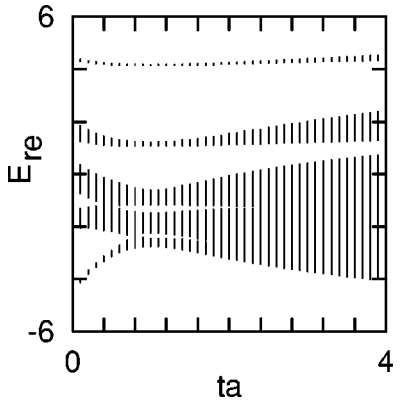

FIG. 3. Rescaled energy eigenvalues as a function of t_a for $\phi=1/5$ with $t_b=t_c=1$. All the values of $\vec{k}$ in the MBZ are taken into account.

shows that introducing the hopping anisotropy changes the band structure considerably. Particularly, for $t_a > 1$, one can see that widths of the subgaps (subbands) decrease (increase) with increasing t_a such that the subgaps will close in the limit of $t_a \to \infty$. Meanwhile, for $t_a < 1$, one can see the closing and reopening of some subgaps with decreasing t_a, resulting in a symmetric band structure about $E = 0$ in the limit of $t_a \to 0$, which is quite a natural result since the lattice with $(t_a, t_b, t_c) = (0,1,1)$ is topologically equivalent to the square lattice with isotropic hopping integrals.

In summary, the mistakes made in Ref. 1 were properly corrected, and the dependence of the magnetic subband structure on the strength of the hopping integral was illustrated.

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