IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Peierls substitution in the energy dispersion of a hexagonal lattice

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2000 J. Phys.: Condens. Matter 12 1539

(http://iopscience.iop.org/0953-8984/12/7/334)

View the table of contents for this issue, or go to the journal homepage for more

Download details:

IP Address: 132.174.255.116
This content was downloaded on 10/07/2014 at 12:32

Please note that terms and conditions apply.

J. Phys.: Condens. Matter **12** (2000) 1539–1543. Printed in the UK PII: S0953-8984(00)06839-9

COMMENT

Peierls substitution in the energy dispersion of a hexagonal lattice

Gi-Yeong Oh

Department of Basic Science, Hankyong National University, Kyonggi-do 456-749, Korea

E-mail: ogy@hnu.hankyong.ac.kr

Received 11 August 1999

Abstract. The method of Peierls substitution in studying the magnetic subband structure of a hexagonal lattice is re-examined. Several errors in the formalism of a couple of recent papers are pointed out and rectified so as to describe the effect of the magnetic field correctly.

Recently, Fekete and Gumbs [1] reported on the study of the energy spectrum of two-dimensional (2D) Bloch electrons subject to a perpendicular sine-modulated magnetic field:

$$B_z(x, y) = B_0 + B_1(x) = B_0 + B_1 \sin(2\pi x/T_x) \tag{1}$$

by making the Peierls substitution $\vec{k} \rightarrow (\vec{p} + e\vec{A})/\hbar$ in the first-order energy dispersion $\varepsilon(\vec{k})$ obtained by the tight-binding method. The content of [1] consists of two parts. The first part deals with the formalism that describes the effect of magnetic modulation (i.e., $B_1 \neq 0$) on the energy spectrum of a *square lattice*, where a correction of some errors in a paper [2] was given. (Concerning this problem, it may be worth consulting [3].) The second part deals with the energy spectrum of a *hexagonal lattice* in the presence of magnetic modulation, where the authors attempted to generalize the formalism presented in another paper [4] which deals with the problem of the energy spectrum of the hexagonal lattice under a uniform magnetic field. Through the studies, the authors of [1,2,4] calculated energy eigenvalues, in the absence and/or presence of magnetic modulation, by diagonalizing the effective Hamiltonian obtained by the Peierls substitution. However, *for the hexagonal lattice*, the formalism and the numerical data presented in [1, 4] are flawed in several ways, whose origin lies in a simple but fundamental mistake made at an early stage of the Peierls substitution. In this comment, we shall point out the mistake and the relevant errors of [1, 4], and derive an *exact* formalism that enables one to correctly describe the effect of the magnetic field given by (1) on the energy spectrum of the hexagonal lattice. For illustration purposes, we will present numerical data for the energy eigenvalues obtained by diagonalizing the corrected matrix with and without magnetic modulation.

To derive the Hamiltonian matrix that describes the effect of the magnetic field given by equation (1), we consider the energy dispersion of a 2D hexagonal lattice given by

$$\varepsilon(\vec{k}) = 2\left\{t_0 \cos(k_x a) + t_+ \cos(k_x b + k_y c) + t_- \cos(k_x b - k_y c)\right\} \tag{2}$$

where a is the lattice constant, $b = a/2$, and $c = \sqrt{3}a/2$. Making the Peierls substitution in equation (2) yields the effective Hamiltonian

$$\mathcal{H} = t_0 \mathrm{e}^{\mathrm{i}p_x a/\hbar} + t_+ \mathrm{e}^{\mathrm{i}[p_x b + p_y c + eA_y(x)c]/\hbar} + t_- \mathrm{e}^{\mathrm{i}[p_x b - p_y c - eA_y(x)c]/\hbar} + \text{c.c.} \tag{3}$$

0953-8984/00/071539+05$30.00 © 2000 IOP Publishing Ltd

where

$$A_y(x) = B_0 x - (B_1 T_x/2\pi)\cos(2\pi x/T_x) \tag{4}$$

is the y-component of the vector potential under the Landau gauge.

The four exponents of the form $\mathrm{e}^{Ap_x+Bp_y+f(x)}$ in (3) contain the operators p_x and x simultaneously in their arguments—unlike in the case of the square lattice—and thus we should be very careful in manipulating them. Since p_y commutes with p_x and x, we can easily decouple $\mathrm{e}^{Ap_x+Bp_y+f(x)}$ as

$$\mathrm{e}^{Ap_x+Bp_y+f(x)} = \mathrm{e}^{Bp_y}\mathrm{e}^{Ap_x+f(x)} = \mathrm{e}^{Ap_x+f(x)}\mathrm{e}^{Bp_y}. \tag{5}$$

However, since p_x does not commute with x, we cannot simply decouple $\mathrm{e}^{Ap_x+f(x)}$ as

$$\mathrm{e}^{Ap_x+f(x)} = \mathrm{e}^{Ap_x}\mathrm{e}^{f(x)} \qquad \text{or} \qquad \mathrm{e}^{f(x)}\mathrm{e}^{Ap_x}. \tag{6}$$

Instead, it should be written as

$$\mathrm{e}^{Ap_x+f(x)} = \mathrm{e}^{Ap_x}\exp\left(\int_0^1 f(x+\mathrm{i}\hbar A\lambda)\,\mathrm{d}\lambda\right) \tag{7}$$

which is a generalization of Weyl's formula and can be derived by using the Baker–Hausdorff lemma [5]. In particular, for $f(x) = Cx + D\cos(Kx)$, equation (7) becomes

$$\mathrm{e}^{Ap_x+Cx+D\cos(Kx)} = \mathrm{e}^{Ap_x}\mathrm{e}^{C(x+\mathrm{i}\hbar A/2)-\mathrm{i}D\xi(x)/\hbar AK} \tag{8}$$

where

$$\xi(x) = \sin[K(x+\mathrm{i}\hbar A)] - \sin(Kx). \tag{9}$$

Combining (5) and (8) with (3), we can write

$$\begin{aligned}\mathcal{H} = {} & t_0(\mathrm{e}^{\mathrm{i}p_x a/\hbar} + \mathrm{e}^{-\mathrm{i}p_x a/\hbar}) + t_+\mathrm{e}^{-\mathrm{i}\pi\alpha/2}(\mathrm{e}^{\mathrm{i}p_y c/\hbar}\mathrm{e}^{\mathrm{i}p_x b/\hbar}\mathrm{e}^{\mathrm{i}(\pi\alpha x'+\nu_-)} + \mathrm{e}^{-\mathrm{i}p_y c/\hbar}\mathrm{e}^{-\mathrm{i}p_x b/\hbar}\mathrm{e}^{-\mathrm{i}(\pi\alpha x-\nu_+)}) \\ & + t_-\mathrm{e}^{\mathrm{i}\pi\alpha/2}(\mathrm{e}^{-\mathrm{i}p_y c/\hbar}\mathrm{e}^{\mathrm{i}p_x b/\hbar}\mathrm{e}^{-\mathrm{i}(\pi\alpha x'+\nu_-)} + \mathrm{e}^{\mathrm{i}p_y c/\hbar}\mathrm{e}^{-\mathrm{i}p_x b/\hbar}\mathrm{e}^{\mathrm{i}(\pi\alpha x'-\nu_+)})\end{aligned} \tag{10}$$

where

$$\nu_\pm(x') = \frac{\alpha\gamma}{\pi\beta^2}\left\{\sin[\pi\beta(x'\pm 1)] - \sin(\pi\beta x')\right\} \qquad x' \equiv \frac{x}{b} \tag{11}$$

and

$$\alpha = eB_0 ac/2\pi\hbar \qquad \beta = a/T_x \qquad \gamma = B_1/B_0. \tag{12}$$

Denoting the lattice points as $(m, n) = (x/b, y/c)$ and using the translational property $\mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}}|\vec{r}\rangle = |\vec{r}+\vec{\xi}\rangle$, we can write the Schrödinger equation $\langle\vec{r}|\mathcal{H}|\psi\rangle = E\psi(\vec{r})$ as

$$\begin{aligned}E\psi_{m,n} = {} & t_0(\psi_{m-2,n} + \psi_{m+2,n}) + t_+(\mathrm{e}^{-\mathrm{i}\theta_{m-1}}\psi_{m-1,n-1} + \mathrm{e}^{\mathrm{i}\theta_m}\psi_{m+1,n+1}) \\ & + t_-(\mathrm{e}^{\mathrm{i}\theta_{m-1}}\psi_{m-1,n+1} + \mathrm{e}^{-\mathrm{i}\theta_m}\psi_{m+1,n-1})\end{aligned} \tag{13}$$

where

$$\theta_m \equiv \theta_m^{(0)} + \theta_m^{(1)} = \pi\alpha\left(m+\frac{1}{2}\right) - \frac{\alpha\gamma}{\pi\beta^2}\{\sin[(m+1)\pi\beta] - \sin(m\pi\beta)\} \tag{14}$$

is the magnetic phase factor. Note that θ_m plays a key role in studying the magnetic subband structure within the tight-binding approximation since all the effects of the applied magnetic field are held in it; $\theta_m^{(0)}$ reflects the effect of B_0 while $\theta_m^{(1)}$ reflects the effect of $B_1(x)$. Since the variable y is cyclic under the Landau gauge, we can write the wave function as $\psi(x, y) = \mathrm{e}^{\mathrm{i}k_y y}\psi(x)$, which in turn enables us to write (13) as

$$E\psi_m = t_0\psi_{m-2} + \delta_{m-1}^*\psi_{m-1} + \delta_m\psi_{m+1} + t_0\psi_{m+2} \tag{15}$$

where

$$\delta_m = t_+ \mathrm{e}^{\mathrm{i}\mu_m} + t_- \mathrm{e}^{-\mathrm{i}\mu_m} \tag{16}$$

with

$$\mu_m = \theta_m + k_y c. \tag{17}$$

Let us assume that $\alpha = p/q$ where p and q are coprime integers and that T_x ($\geqslant 2$) is an integer. Then, the period of $\theta_m^{(0)}$ is q ($2q$) for even (odd) p and that of $\theta_m^{(1)}$ is $2T_x$ if we set $a \equiv 1$. Thus, the period of θ_m is given by

$$T = \begin{cases} \text{L.C.M.}(q, 2T_x) & \text{for even } p \\ \text{L.C.M.}(2q, 2T_x) & \text{for odd } p \end{cases} \tag{18}$$

which leads to the relations $\mu_{m+T} = \mu_m$ and $\delta_{m+T} = \delta_m$. Therefore, the Bloch condition along the x-direction can be expressed as $\psi_{m+T} = \mathrm{e}^{\mathrm{i}k_x Tb}\psi_m$, and the characteristic matrix that gives rise to energy eigenvalues in the presence of magnetic modulation can be written as

$$\mathbf{A} = \begin{pmatrix} 0 & \delta_1 & t_0 & 0 & \cdots & 0 & t_0\mathrm{e}^{-\mathrm{i}\eta} & \delta_T^*\mathrm{e}^{-\mathrm{i}\eta} \\ \delta_1^* & 0 & \delta_2 & t_0 & \cdots & 0 & 0 & t_0\mathrm{e}^{-\mathrm{i}\eta} \\ t_0 & \delta_2^* & 0 & \delta_3 & \cdots & 0 & 0 & 0 \\ 0 & t_0 & \delta_3^* & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \delta_{T-2} & t_0 \\ t_0\mathrm{e}^{\mathrm{i}\eta} & 0 & 0 & 0 & \cdots & \delta_{T-2}^* & 0 & \delta_{T-1} \\ \delta_T\mathrm{e}^{\mathrm{i}\eta} & t_0\mathrm{e}^{\mathrm{i}\eta} & 0 & 0 & \cdots & t_0 & \delta_{T-1}^* & 0 \end{pmatrix} \tag{19}$$

where $\eta = k_x Tb$. Note that, when $\gamma = 0$, the period of θ_m, and thus the order of $\mathbf{A}$, is given by T_0 which equals q ($2q$) for even (odd) p.

We are now in position to discuss the formalism of [1, 4]. To this end, we refer to (14) and (16) of [1] as $\mathbf{A}^{\mathrm{F}}$ and μ_m^{F}, and (6) of [4] as $\mathbf{A}^{\mathrm{G}}$. The most fundamental mistake made by the authors of [1, 4] lies in the fact that they employed (6) instead of (7) for developing the formalism. Since (6) is meaningful only in the $\hbar \to 0$ limit, it is evident that the formalism in [1, 4] is not suitable for describing the quantum-mechanical behaviour of Bloch electrons in the presence of the magnetic field. To put this concretely, μ_m^{F} is an erroneous expression as a result of the mistake; $\theta_m^{(0;\mathrm{F},\mathrm{G})}$ ($\equiv 2\pi m\alpha$) and $\theta_m^{(1;\mathrm{F})}$ ($\equiv -(\alpha\gamma/\beta)\cos(2\pi m\beta)$) should be replaced by $\theta_m^{(0)}$ and $\theta_m^{(1)}$, respectively, in order to describe correctly the effect of the magnetic field given by (1). Note that μ_m^{F} in turn has a crucial influence on the order of the characteristic matrix. Since the period of $\theta_m^{(0;\mathrm{F},\mathrm{G})}$ is q and that of $\theta_m^{(1;\mathrm{F})}$ is T_x, the period of μ_m^{F} becomes $T' = qT_x$, resulting in $\psi_{m+T'} = \mathrm{e}^{\mathrm{i}k_x T'b}\psi_m$. Thus, the order of $\mathbf{A}^{\mathrm{F}}$ is T' for generic values of q and T_x. However, as shown above, the order of the corrected matrix $\mathbf{A}$ is not T' but T. Besides which, the order of $\mathbf{A}$ for $\gamma = 0$ is not q but T_0, in contrast to the assertion of [4]. Another indication that the formalism of [1, 4] is incorrect can be found in the fact that $\mathbf{A}^{\mathrm{F}}$ and $\mathbf{A}^{\mathrm{G}}$ are non-Hermitian, contrary to the general rule that a matrix which gives rise to real eigenvalues should be Hermitian. All of these arguments in this paragraph indicate that the relevant numerical data, i.e., figures 3 and 4 in [1] and all the figures in [4], obtained by diagonalizing $\mathbf{A}^{\mathrm{F}}$ and/or $\mathbf{A}^{\mathrm{G}}$ are not in fact the solutions of the problem that the authors of [1, 4] attempted to solve.

Figures 1(a) and 1(b) show plots of the energy eigenvalues versus α in the absence of magnetic modulation (i.e., $\gamma = 0$). We can see that figure 1(a) is the same as figure 3 of [6] while it is quite different from figure 1 of [4], which shows how greatly the energy spectrum is changed when $\theta_m^{(0;F,G)}$ instead of $\theta_m^{(0)}$ is employed in the calculation. Indeed, even though the

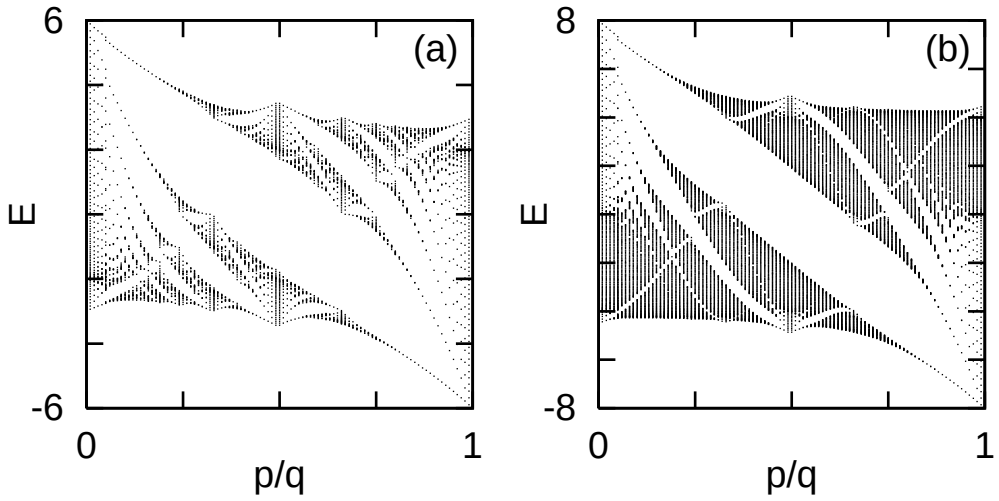

Figure 1. Energy eigenvalues versus α for $\gamma = 0$ with (a) $(t_0, t_+, t_-) = (1, 1, 1)$ and (b) $(t_0, t_+, t_-) = (2, 1, 1)$. Calculations are performed for $\alpha = p/101$ $(1 \leqslant p \leqslant 100)$ and $(k_x, k_y) = (0, 0)$.

authors of [4] were aware that their result differs from that of [6], they might not have realized that the two works [4, 6] deal with exactly the same problem. Comparison of figure 1(b) with figure 3 of [4] also shows how sensitively the energy spectrum depends on $\theta_m^{(0)}$ in the presence of the hopping anisotropy. Figures 2(a) and 2(b) show plots of the energy eigenvalues versus α in the presence of the magnetic modulation, where the same parameters as in [1] are chosen for comparison. The plots show that introducing magnetic modulation leads to very complicated subband structure; gap closing and subband broadening observed in the case of a square lattice [3, 7] can also be seen. Comparison of figures 2(a) and 2(b) with figures 3 and 4 of [1] also shows the importance of the correct choice of $\theta_m^{(1)}$. For instance, the straight lines

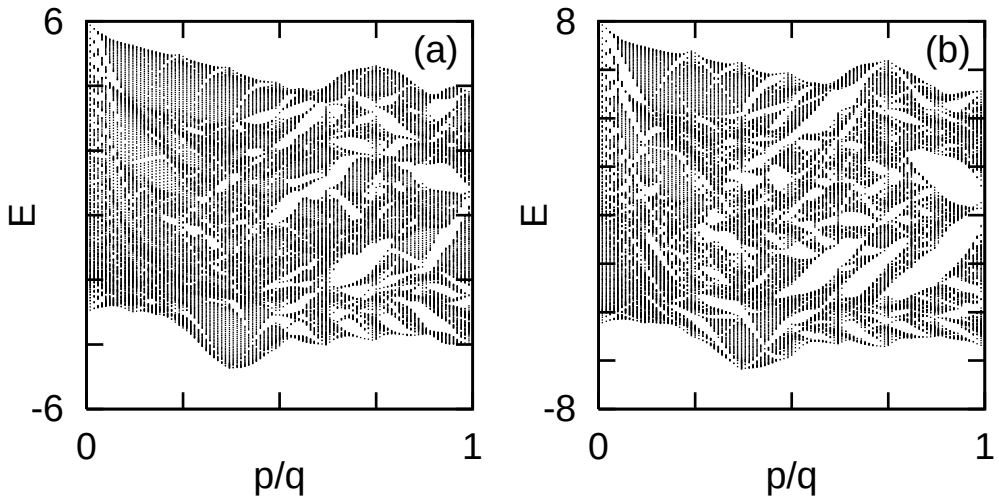

Figure 2. As figure 1, except that $\gamma = 2$ and $T_x = 4$.

of $E = -2$ and/or $E = -4$ along the α-axis in some plots of [1, 4] do not appear if we use the correct form of the magnetic phase factor (i.e., equation (14)) in the calculation.

Before finishing this comment, we would like to make two remarks. One is that, since we focused our attention in this comment on the formalism of [1, 4], detailed description of the effect of magnetic modulation on the energy spectrum of the hexagonal lattice is still lacking and thus further study on this problem is required for better understanding. The other is that (13) and thus (19) can also be obtained without difficulty if we start directly from the tight-binding Hamiltonian given by

$$\mathcal{H} = \sum_{ij} t_{ij} \mathrm{e}^{\mathrm{i}\theta_{ij}} |i\rangle\langle j| \tag{20}$$

where

$$\theta_{ij} = (e/\hbar) \int_i^j \vec{A} \cdot \mathrm{d}\vec{l}.$$

Indeed, it can be easily checked that

$$\theta_{m,n;m\pm2,n} = 0 \qquad \theta_{m,n;m+1,n\pm1} = \pm\theta_m \qquad \theta_{m,n;m-1,n\pm1} = \pm\theta_{m-1} \tag{21}$$

and that combining (21) with (20) leads to (13), which confirms the correctness of the formalism derived in this comment.

References

[1] Fekete P and Gumbs G 1999 *J. Phys.: Condens. Matter* **11** 5475
[2] Gumbs G, Miessein D and Huang D 1995 *Phys. Rev.* B **52** 14 755
[3] Oh G Y 1999 *Phys. Rev.* B **60** 1939
[4] Gumbs G and Fekete P 1997 *Phys. Rev.* B **56** 3787
[5] Baym G 1969 *Lectures on Quantum Mechanics* (New York: Benjamin/Cummings) ch 5
[6] Claro F H and Wannier G H 1979 *Phys. Rev.* B **19** 6068
[7] Oh G Y and Lee M H 1996 *Phys. Rev.* B **53** 1225