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Bloch Electrons of a Carbon Nanotube in a Perpendicular Magnetic Field

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Abstract

The Peierls substitution in the energy functions of carbon nanotube's sub-bands is carried out for a carbon nanotube of arbitrary chiral indices subjected to a perpendicular uniform magnetic field. The Peierls substitution represents a zero-order term of the asymptotically convergent power series in the magnetic field. It provides a very good approximation for electron energy spectrum of a carbon nanotube subjected to a perpendicular uniform magnetic field, for magnetic fields currently accessible in laboratories.

I. INTRODUCTION

There is hardly another single-electron problem in quantum mechanics that has attracted as much attention as the behavior of Bloch electrons in a magnetic field. Since the pioneering work of Peierls[1] it has been customary to treat the motion of Bloch electrons in a magnetic field using two different approaches, both of which are often referred to as the "Peierls substitution". The first one amounts to multiplication of the zero-field matrix elements of the nearest-neighbor tight-binding Hamiltonian by the phase factors, $\exp\left[-\frac{ie}{\hbar}\int \mathbf{A}d\mathbf{r}\right]$, containing the line integral of the vector potential, $\mathbf{A}$, along the straight-line path connecting the nearest neighbors. The second one involves substituting $-i\hbar\nabla - \frac{e}{c}\mathbf{A}$ for $\hbar\mathbf{k}$ in the energy function for a band. In the simplest case of the one-dimensional tight-binding Hamiltonian, the equivalence of the two approaches can be readily established[2]. A discussion of higher dimensions entails ambiguity of the path connecting neighboring atoms[3–6], but the straight-line choice can be justified by requiring gauge invariance of the tight-binding Hamiltonian[5,6]. It can then be shown that the two approaches are exactly equivalent for a two-dimensional tight-binding Hamiltonian on a square lattice, immersed in a uniform magnetic field perpendicular to it[4,7–9].

The nearest-neighbor tight-binding model on a honeycomb lattice leads to the electron energy spectrum where the conduction and valence bands touch at the K and K' points of the two-dimensional Brillouin zone. One can make the Peierls substitution in the matrix elements of the tight-binding Hamiltonian and expand resulting equations near the K and K' points to lowest orders in the wave vector and the vector potential. This procedure is equivalent to using the effective massless Dirac Hamiltonian with the Peierls substitution made for the momentum operator[10–14]. This Hamiltonian can be used to analyze the low-energy part of the electron spectrum in carbon nanotubes in applied magnetic fields[11–14].

Beyond the limitations of the tight-binding approximation, numerous attempts have been made to justify the Peierls substitution in the energy function for a band[15,16]. These attempts culminated in the work of Blount[17], who formulated the problem in the framework of the crystal momentum representation[17,18]. In this representation the electron Hamiltonian comprises a matrix diagonal in the band indices, s, and crystal momenta, $\mathbf{k}$, with the elements $\varepsilon_s(\mathbf{k})$. The difficulty in treating the problem of a Bloch electron in a uniform magnetic field is that the vector potential is a linearly growing function of the coordinates that

can be very large. Lifshitz and Pitaevskii argued that, in the limiting case of a constant vector potential (which corresponds to a zero magnetic field), the legitimacy of the Peierls substitution in $\varepsilon_s(\mathbf{k})$ follows from the gauge invariance[18]. Then $\varepsilon_s(\mathbf{q} - \frac{e}{\hbar c}\hat{\mathbf{A}})$, where $\mathbf{q}$ is the generalized crystal momentum[18], corresponds to the Hamiltonian describing the motion of a Bloch electron from the s-th band in a weakly changing vector potential, or in the "zeroth order" in the magnetic field, $\mathbf{B}$. Blount devised a procedure yielding corrections to this Hamiltonian of higher orders in the magnetic field[17]. This procedure is based on the formalism of the pseudoclassical representation developed for treating perturbations which may be large but vary slowly from cell to cell in a crystal lattice. Blount also showed that this procedure converges asymptotically[17].

In this work we will study the energy spectrum of a single-walled carbon nanotube with the chiral indices (n, m)[4] in a uniform magnetic field directed perpendicular to the nanotube axis. For definiteness, we will choose the z axis along the nanotube and the y axis along the magnetic field. Neglecting the atomic bond curvature and assuming nearest-neighbor tight-binding approximation, one can obtain the electron energy spectrum of a carbon nanotube in zero magnetic field in two different ways. On one hand, one can consider a unit cell of a carbon nanotube containing $\mathcal{N} = 2\left(n^2 + m^2 + nm\right)/d_R$ hexagons, or $2\mathcal{N}$ atoms, where d_R is the greatest common divisor of $2n + m$ and $2m + n$[4], and write down the tight-binding Hamiltonian as a $2\mathcal{N} \times 2\mathcal{N}$ matrix for each value of the one-dimensional crystal wave vector $k \equiv k_z$ along z. We will refer to this Hamiltonian as the Hamiltonian in the tight-binding representation. This Hamiltonian yields energy dispersion for $\mathcal{N}$ subbands in the conduction band and $\mathcal{N}$ subbands in the valence band. On the other hand, one can consider a unit cell of graphene containing just two atoms and the energy dispersion $\varepsilon_c(k_x, k_z) = -\varepsilon_v(k_x, k_z)$ of a graphene sheet oriented in such a way that rolling it up along the x direction (to become the nanotube circumference) would produce a nanotube with given chirality indices. Then $\varepsilon_s(\mu/R, k)$, where R is the nanotube radius and $\mu = 0, 1, ..., \mathcal{N} - 1$ will yield energy spectra for the $\mathcal{N}$ subbands of the band $s = c, v$. This way of getting the nanotube electron energy spectrum is known as "zone folding"[4]. The resulting $2\mathcal{N} \times 2\mathcal{N}$ diagonal matrix, with $\varepsilon_s(\mu/R, k)$ on the diagonal, comprises the electron Hamiltonian in the crystal momentum representation.

Thus, carbon nanotubes provide a perfect proving ground to test the two kinds of the Peierls substitution. Indeed, both ways of getting electron energy spectrum of a carbon

nanotube can be modified to account for the applied uniform magnetic field directed perpendicular to the nanotube axis. Saito *et al.*[19] modified the Hamiltonian in the tight-binding representation using the Peierls substitution for its matrix elements resulting in the phase factors induced by the magnetic field. Numerical calculations in Ref.[19] were done for a $(10, 0)$ zigzag carbon nanotube for different values of the ratio R/a_B, where $a_B = \sqrt{\hbar\, c/|e|\, B}$ is the magnetic length. Their numerical results were reproduced in numerous textbooks and review articles[4,20–22]. Similar approach was used in[12,23,24]. Most of these studies refer to achiral (zigzag and armchair) carbon nanotubes[12,19,24].

The aim of the present work is to account for the uniform perpendicular magnetic field, applied to a carbon nanotube, by modifying the electron Hamiltonian in the crystal momentum representation. We have demonstrated[25,26] that, in the framework of this representation, it is often possible to obtain straightforward derivations of analytical results having a "universal" form in the sense that they can be applied to nanotubes with arbitrary chiral indices, not limited to achiral nanotubes.

For a nanotube in a uniform perpendicular magnetic field, one has a freedom to choose the gauge condition. One possibility is $\mathbf{A} = B\, z\, \mathbf{e}_x$. In this gauge, the vector potential is a linearly growing function of the coordinate along the nanotube axis. Therefore, the argument due to Lifshitz and Pitaevskii applies to nanotubes, and one can expect that the "zeroth order" term in the electron Hamiltonian, corresponding to the Peierls substitution, prevails at weak magnetic fields. Because of the gauge invariance, this should be true for any gauge. Another possible gauge choice is $\mathbf{A} = -B\, x\, \mathbf{e}_z$. This choice will be made in the present study. Since, for a nanotube, $|x| < R$, the vector potential in this gauge is a bounded function of the coordinates on the nanotube surface. Therefore, there is no need to invoke the pseudoclassical approximation, and we can perform our analysis entirely in the framework of the crystal momentum representation. Yet, the present treatment is based, to a large extent, on the work of Blount[17].

II. CRYSTAL MOMENTUM REPRESENTATION FOR BLOCH ELECTRONS OF A CARBON NANOTUBE WITHOUT MAGNETIC FIELD

The wave function of a Bloch electron in a carbon nanotube belonging to the band $s = c, v$ and having the subband index μ and one-dimensional wave-vector k can be written as

$$\langle z, \varphi | s, \mu, k \rangle = u_{s,\mu,k}(z, \varphi)\, e^{ikz}\,, \tag{1}$$

where the periodic Bloch amplitude, $u_{s,\mu,k}$ within the zone-folding scheme is related to the atomic orbital, $\Phi_b(\mathbf{r} - \mathbf{R}_b)$ by

$$u_{s,\mu,k}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{b=A,B} C_b(s, \mu, k) \sum_{\mathbf{R}_b} e^{i\mu\varphi_b}\, e^{ik(z_b - z)}\, \Phi_b(\mathbf{r} - \mathbf{R}_b)\,.$$

Here the first sum is over the two atoms in the unit cell of graphene and N is the number of graphene unit cells in a sample. Within the zone-folding scheme the coefficients $C_A(s, \mu, q)$ and $C_B(s, \mu, k)$ are found to be[4,26]

$$\begin{pmatrix} C_A(c, \mu, k) \\ C_B(c, \mu, k) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi} \\ 1 \end{pmatrix}, \qquad \begin{pmatrix} C_A(v, \mu, k) \\ C_B(v, \mu, k) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{i\phi} \\ 1 \end{pmatrix}, \tag{2}$$

where

$$\phi = \begin{cases} \arctan \frac{\mathcal{B}}{\mathcal{A}}, & \mathcal{A} > 0 \\ \\ \arctan \frac{\mathcal{B}}{\mathcal{A}} + \pi, & \mathcal{A} < 0 \end{cases}, \tag{3}$$

$$\mathcal{A} = 2\, \cos\left(K_x a/2\sqrt{3}\right)\, \cos\left(K_y a/2\right) + \cos\left(K_x a/\sqrt{3}\right),$$

$$\mathcal{B} = 2\, \sin\left(K_x a/2\sqrt{3}\right)\, \cos\left(K_y a/2\right) - \sin\left(K_x a/\sqrt{3}\right),$$

$K_x = \mu/R\, \cos\alpha - k\, \sin\alpha$, $K_y = \mu/R\, \sin\alpha + k\, \cos\alpha$, a is the lattice constant of graphene, R is the nanotube radius, and the angle α is related to the nanotube chiral angle θ by $\alpha = \pi/6 - \theta$. The band energy is given by

$$\varepsilon_{c(v)}(\mathbf{k}) \equiv \varepsilon_{c(v)}(\mu, k) = \pm\gamma_0 \sqrt{1 + 4\, \cos\frac{\sqrt{3}\, K_x\, a}{2}\, \cos\frac{K_y\, a}{2} + 4\, \cos^2\frac{K_y\, a}{2}}\,, \tag{4}$$

where γ_0 is the transfer integral of the tight-binding method and $\mathbf{k} = (\mu/R, k)$.

III. PEIERLS SUBSTITUTION IN THE BAND ENERGY DISPERSION

We consider a carbon nanotube parallel to the z-axis subjected to a uniform magnetic field $\mathbf{B}$ directed along the y-axis. Then the vector potential can be chosen in the form $\mathbf{A} = -B\,x\,\mathbf{e}_z$. The essence of the Peierls substitution is[18] (i) to introduce the generalized quasi-momentum

$$\mathbf{q} = \mathbf{k} + \frac{e\,\mathbf{A}}{\hbar\,c} = \mathbf{k} + \frac{2\,\pi\,R\,B\,\cos\varphi}{\Phi_0}\,\mathbf{e}_z\,, \tag{5}$$

where φ is the polar angle, $\mathbf{k} = (\mu/R, k)$ is the quasi-momentum in the absence of the magnetic field with the quantized component along the nanotube circumference, $\Phi_0 = hc/|e|$ is the flux quantum, and (ii) to consider

$$\varepsilon_s\left(\mathbf{q} - \frac{2\,\pi\,R\,B\,\cos\varphi}{\Phi_0}\,\mathbf{e}_z\right) \equiv \varepsilon_s\left(\mathbf{q} - \frac{\mathcal{N}\,B\,S_{hex}\,\cos\varphi}{\Phi_0\,|\mathbf{T}|}\,\mathbf{e}_z\right)\,, \tag{6}$$

where $s = c, v$ is the band index, S_{hex} is the area of a hexagon, $\mathbf{T}$ is the translational vector of the nanotube[4], as a Hamiltonian in the $\mathbf{q}$-representation. The difficulty here arises from the fact that, in this representation, the operator $\cos\varphi$ has only inter-subband matrix elements on the electron Bloch states. As a result, the electron Hamiltonian is non-diagonal even in the "zeroth order" in the magnetic field. In order to formally circumvent this difficulty we use the fact that $\varepsilon_s(\mu, k)$ is a periodic function of k:

$$\varepsilon_s\,(\mu, k) = \varepsilon_s\left(\mu, k + \frac{2\,\pi}{|\mathbf{T}|}\right)\,.$$

Therefore, $\varepsilon_s(\mu, k)$ can be expanded into a Fourier series:

$$\varepsilon_s(\mu, k) = \sum_m A_{sm}(\mu)\,e^{i\,k\,m\,|\mathbf{T}|}\,, \tag{7}$$

where

$$A_{sm}(\mu) = \frac{|\mathbf{T}|}{2\,\pi}\int\limits_{-\frac{\pi}{|\mathbf{T}|}}^{\frac{\pi}{|\mathbf{T}|}} dk\,\varepsilon_s(\mu, k)\,e^{-i\,k\,m\,|\mathbf{T}|}\,.$$

Using the generating function for the Bessel functions in the form

$$e^{-i\,t\,\cos\varphi} = \sum_l (-i)^l\,e^{-i\,l\,\varphi}\,J_l(t)\,, \tag{8}$$

we obtain

$$\varepsilon_s\left(\mathbf{q} - \frac{2\,\pi\,R\,B\,\cos\varphi}{\Phi_0}\,\mathbf{e}_z\right) = \sum_m A_{sm}(\mu)\,e^{i\,q\,m\,|\mathbf{T}|}\,\sum_l (-i)^l\,e^{-i\,l\,\varphi}\,J_l\left(\frac{\mathcal{N}\,B\,S_{hex}\,m}{\Phi_0}\right)\,, \tag{9}$$

where we used $2\,\pi\,R\,|\mathbf{T}| = \mathcal{N}\,S_{hex}$, and $\mathcal{N}$ is the number of hexagons within a unit cell of the nanotube. Eq. (9) represents an operator acting on the states in the crystal momentum representation. However, we can interpret

$$\langle s,\mu,q|H|s',\mu',q\rangle = \sum_m e^{i\,q\,m\,|\mathbf{T}|}\,\frac{A_{sm}(\mu)+A_{s'm}(\mu')}{2} \tag{10}$$

$$\times\sum_l (-i)^l\,\langle s,\mu,q|e^{-i\,l\,\varphi}|s',\mu',q\rangle\,J_l\left(\frac{\mathcal{N}\,B\,S_{hex}\,m}{\Phi_0}\right)$$

as the matrix element of the Hamiltonian in the **q**-representation (cf. the limit at $B=0$).

The next step is then to calculate the matrix element $\langle s,\mu,q|e^{-i\,l\,\varphi}|s',\mu',q\rangle$. We first neglect the effect of the magnetic field on the electron wave function. Then, using the wave function (1), we obtain

$$\langle s,\mu,q|e^{-i\,l\,\varphi}|s',\mu',q\rangle = \sum_n \delta_{\mu'-\mu-l,n\mathcal{N}}\,\sum_b C_b^*(s,\mu,q)\,C_b(s',\mu',q)\,. \tag{11}$$

Here we used

$$\frac{1}{N}\sum_{\mathbf{R}_b} e^{i\,m\,\varphi_b} = \sum_n \delta_{m,n\mathcal{N}}\,. \tag{12}$$

Eq. (10) can be rewritten as

$$\langle s,\mu,q|H|s',\mu',q\rangle = \sum_l (-i)^l\,\langle s,\mu,q|e^{-i\,l\,\varphi}|s',\mu',q\rangle\,\frac{|\mathbf{T}|}{2\,\pi}\int\limits_{-\frac{\pi}{|\mathbf{T}|}}^{\frac{\pi}{|\mathbf{T}|}} dk\,\frac{\varepsilon_s(\mu,k)+\varepsilon_{s'}(\mu',k)}{2} \tag{13}$$

$$\times\sum_m e^{i\,(q-k)\,m\,|\mathbf{T}|}\,J_l\left(\frac{\mathcal{N}\,B\,S_{hex}\,m}{\Phi_0}\right)\,.$$

Summation over m in Eq. (13) can be performed using the identity

$$\sum_{m=-\infty}^{\infty}\delta(x-m) = \sum_{n=-\infty}^{\infty} e^{2\,\pi\,i\,n\,x}\,. \tag{14}$$

We obtain

$$\sum_m e^{i\,(q-k)\,m\,|\mathbf{T}|}\,J_l\left(\frac{\mathcal{N}\,B\,S_{hex}\,m}{\Phi_0}\right) = \sum_n \int\limits_{-\infty}^{\infty} dx\,J_l\left(\frac{\mathcal{N}\,B\,S_{hex}\,x}{\Phi_0}\right)\,e^{i\,[(q-k)\,|\mathbf{T}|+2\,\pi\,n]\,x}$$

$$= 2\,i^l\,\frac{\Phi_0}{\mathcal{N}\,B\,S_{hex}}\,\sum_{n=-\infty}^{\infty}\frac{T_l(y_n)}{\sqrt{1-y_n^2}}\,\theta(1-|y_n|)\,,$$

where

$$y_n = \frac{(q-k)\,|\mathbf{T}| + 2\,\pi\,n}{\mathcal{N}\,B\,S_{hex}}\,\Phi_0\,,$$

$T_m(y) = \cos\left(m\,\arccos y\right)$ is the Chebyshev polynomial, and we used the following integral[27]

$$\int\limits_{-\infty}^{\infty} dz\,J_l(c\,z)\,e^{i\,p\,z} = 2\,i^l\,\frac{T_l\left(\frac{p}{c}\right)}{\sqrt{c^2-p^2}}\,\theta\left(1-\left|\frac{p}{c}\right|\right)\,. \tag{15}$$

We have two restrictions on the variable y_n:

$$-1 < y_n < 1$$

and

$$-\frac{\pi}{|\mathbf{T}|} < k = q - \frac{y_n\,\mathcal{N}\,B\,S_{hex}}{\Phi_0\,|\mathbf{T}|} + \frac{2\,\pi\,n}{|\mathbf{T}|} < \frac{\pi}{|\mathbf{T}|}\,.$$

Because $\varepsilon_s(\mu,k)$ is a periodic function in k with the period $2\,\pi/|\mathbf{T}|$, Eq. (13) reduces to

$$\langle s,\mu,q|H|s',\mu',q\rangle = \sum_l \langle s,\mu,q|e^{-i\,l\,\varphi}|s',\mu',q\rangle \tag{16}$$

$$\times\frac{1}{\pi}\int\limits_0^{\pi} d\theta\,\frac{\varepsilon_s\left(\mu,q-\frac{\mathcal{N}BS_{hex}\cos\theta}{\Phi_0\,|\mathbf{T}|}\right)+\varepsilon_{s'}\left(\mu',q-\frac{\mathcal{N}BS_{hex}\cos\theta}{\Phi_0\,|\mathbf{T}|}\right)}{2}\,\cos l\theta\,.$$

This allows one to combine Eqs. (11) and (16) to yield

$$\langle s,\mu,q|H|s',\mu',q\rangle = \frac{1}{\pi}\int\limits_0^{\pi} d\theta\,\frac{\varepsilon_s\left(\mu,q-\frac{\mathcal{N}BS_{hex}\cos\theta}{\Phi_0\,|\mathbf{T}|}\right)+\varepsilon_{s'}\left(\mu',q-\frac{\mathcal{N}\,B\,S_{hex}\cos\theta}{\Phi_0\,|\mathbf{T}|}\right)}{2} \tag{17}$$

$$\times\sum_b C_b^*(s,\mu,q)\,C_b(s',\mu',q)\,\sum_n \cos\left(\mu'-\mu+n\mathcal{N}\right)\theta\,.$$

Now we can use

$$\sum_n \cos\left(\mu'-\mu+n\mathcal{N}\right)\theta = \frac{2\,\pi}{\mathcal{N}}\,\cos\left(\mu'-\mu\right)\theta\,\sum_m \delta\left(\theta-\frac{2\pi m}{\mathcal{N}}\right)\,. \tag{18}$$

Therefore, we obtain

$$\langle s,\mu,q|H|s',\mu',q\rangle = \sum_b C_b^*(s,\mu,q)\,C_b(s',\mu',q) \tag{19}$$

$$\times\frac{1}{\mathcal{N}}\sum_{m=0}^{\mathcal{N}/2}\frac{2-\delta_{m,0}-\delta_{m,\mathcal{N}/2}}{2}\,\left[\varepsilon_s\left(\mu,q-q_m\right)+\varepsilon_{s'}\left(\mu',q-q_m\right)\right]\,\cos\left(\mu'-\mu\right)\frac{2\pi m}{\mathcal{N}}\,,$$

where we have introduced the following notation:

$$q_m = \frac{\mathcal{N}BS_{hex}}{\Phi_0\,|\mathbf{T}|}\,\cos\frac{2\pi m}{\mathcal{N}}\,. \tag{20}$$

IV. BASIS TRANSFORMATION INDUCED BY A MAGNETIC FIELD

The wave function $\langle z, \varphi | s, \mu, q \rangle$ is also affected by the magnetic field[18]:

$$\langle z, \varphi | s, \mu, q \rangle \to \left\langle z, \varphi \left| s, \mu, q - \frac{2\pi RB \cos\varphi}{\Phi_0} \right\rangle \right. = u_{s,\mu,q-\frac{2\pi RB\cos\varphi}{\Phi_0}}(z, \varphi)\, e^{iqz} \,.$$

We will follow Blount[17] and introduce the following transformation matrix

$$S^{(0)}_{s,\mu;s',\mu'}\left(q - \frac{2\pi RB\cos\varphi}{\Phi_0}; q\right) \equiv \left\langle s, \mu, q - \frac{2\pi RB\cos\varphi}{\Phi_0} \right| \left. s', \mu', q \right\rangle \,. \tag{21}$$

Using Eq. (1) we obtain

$$S^{(0)}_{s,\mu;s',\mu'}\left(q - \frac{2\pi RB\cos\varphi}{\Phi_0}; q\right) = \sum_b \sum_{\mathbf{R}_b} e^{i(\mu'-\mu)\,\varphi_b} C^*_b \left(s, \mu, q - \frac{2\pi RB\cos\varphi_b}{\Phi_0}\right) C_b(s', \mu', q) \,. \tag{22}$$

Using the direct and the inverse Fourier tranforms, one can write

$$C^*_b \left(s, \mu, q - \frac{2\pi RB\cos\varphi_b}{\Phi_0}\right) = \frac{1}{\pi} \int_{-1}^{1} dy\, C^*_b \left(s, \mu, q - \frac{\mathcal{N}\, B\, S_{hex}\, y}{\Phi_0\, |\mathbf{T}|}\right) \sum_m \frac{e^{im\varphi_b} T_m(y)}{\sqrt{1-y^2}} \,, \tag{23}$$

where $y = \frac{(q-k)\,|\mathbf{T}|}{\mathcal{N}\, B\, S_{hex}}\, \Phi_0$ and we used Eqs. (8) and (15). Then, using Eqs. (12), (18), and (23), Eq. (22) can be easily transformed into

$$S^{(0)}_{s,\mu;s',\mu'}\left(q - \frac{2\pi RB\cos\varphi}{\Phi_0}; q\right) = \frac{2}{\mathcal{N}} \sum_{m=0}^{\mathcal{N}/2} \frac{2 - \delta_{m,0} - \delta_{m,\mathcal{N}/2}}{2} \cos(\mu' - \mu) \frac{2\pi m}{\mathcal{N}} \tag{24}$$

$$\times \sum_b C^*_b\,(s, \mu, q - q_m)\; C_b(s', \mu', q) \,.$$

V. ZEROTH ORDER HAMILTONIAN

In this section we give an explicit expression for the Hamiltonian describing Bloch electrons of a carbon nanotube in a perpendicular magnetic field valid in the zeroth order in the field (but not in the vector potential, cf. Refs.[17,18]).

Applying transformation (21) to the Hamiltonian (19) we obtain

$$\langle s, \mu | S^{(0)} H S^{(0)\,\dagger} | s', \mu' \rangle = \sum_{s_1, s_2, \mu_1, \mu_2} \left\langle s, \mu, q - \frac{2\pi RB\cos\varphi}{\Phi_0} \right| \left. s_1, \mu_1, q \right\rangle \tag{25}$$

$$\times \langle s_1, \mu_1, q | H | s_2, \mu_2, q \rangle \left\langle s_2, \mu_2, q \left| s', \mu', q - \frac{2\pi RB\cos\varphi}{\Phi_0} \right\rangle \right. \,.$$

A straightforward derivation leads to the following result:

$$\langle s,\mu|S^{(0)}HS^{(0)\,\dagger}|s',\mu'\rangle = \langle s,\mu|S^{(0)}H_1S^{(0)\,\dagger}|s',\mu'\rangle + \langle s,\mu|S^{(0)}H_2S^{(0)\,\dagger}|s',\mu'\rangle\,, \tag{26}$$

where

$$\langle c,\mu|S^{(0)}H_1S^{(0)\,\dagger}|c(v),\mu'\rangle = \frac{1}{2\mathcal{N}}\sum_{m=0}^{\mathcal{N}/2}\frac{2-\delta_{m,0}-\delta_{m,\mathcal{N}/2}}{2}\cos(\mu'-\mu)\frac{2\pi m}{\mathcal{N}} \tag{27}$$

$$\times\left[e^{i\,\phi(\mu',q)-i\,\phi(\mu,q-q_m)}\,\varepsilon_c(\mu',q-q_m)\pm e^{i\,\phi(\mu',q-q_m)-i\,\phi(\mu,q)}\,\varepsilon_c(\mu,q-q_m)\right],$$

$$\langle c,\mu|S^{(0)}H_2S^{(0)\,\dagger}|c(v),\mu'\rangle = \frac{1}{\mathcal{N}^2}\sum_{\mu''=0}^{\mathcal{N}-1}\sum_{m=0}^{\mathcal{N}/2}\frac{2-\delta_{m,0}-\delta_{m,\mathcal{N}/2}}{2}\sum_{m'=0}^{\mathcal{N}/2}\frac{2-\delta_{m',0}-\delta_{m',\mathcal{N}/2}}{2} \tag{28}$$

$$\times\left[e^{i\,\phi(\mu'',q)-i\,\phi(\mu,q-q_m)}\,\varepsilon_c(\mu'',q-q_{m'})\pm e^{i\,\phi(\mu',q-q_{m'})-i\,\phi(\mu'',q)}\,\varepsilon_c(\mu'',q-q_m)\right]$$

$$\times\cos(\mu-\mu'')\frac{2\pi m}{\mathcal{N}}\,\cos(\mu''-\mu')\frac{2\pi m'}{\mathcal{N}}\,,$$

and q_m is given by Eq. (20). We note, however, that, for numerical calculations, it is more efficient to directly use Eq. (25) and perform matrix multiplication numerically.

In Fig. 1 by black dotted line is shown the energy spectrum of an electron in a $(10,0)$ zigzag carbon nanotube without magnetic field. By blue dashed line is shown the electron spectrum of the same nanotube in the perpendicular magnetic field for $R/a_B = 1$ calculated using the tight-binding Hamiltonian[19]. By red solid line is shown the same spectrum calculated using Eq. (25). The results of the two calculations agree rather well, although the magnetic field corresponding to $R/a_B = 1$ is quite strong ($B \approx 4.3\times10^3$ T.)

We also note that, as can be demonstrated by numerical calculations, the eigen energies of the two terms in Eq. (26), $S^{(0)}H_1S^{(0)\,\dagger}$ and $S^{(0)}H_2S^{(0)\,\dagger}$, are very close to one another.

VI. BLOUNT'S PERTURBATIVE PROCEDURE

One can check that the transformation matrix $S^{(0)}_{s,\mu;s',\mu'}\left(q-\frac{2\pi RB\cos\varphi}{\Phi_0};q\right)$ is not unitary. To be more precise, it is unitary only in the zeroth order in the magnetic field. Therefore, one can calculate corrections to the unitarity condition up to a certain order in the magnetic field and modify the transformation matrix as a means to eliminate these corrections in that order. This is the essence of the perturbation procedure proposed by Blount[17].

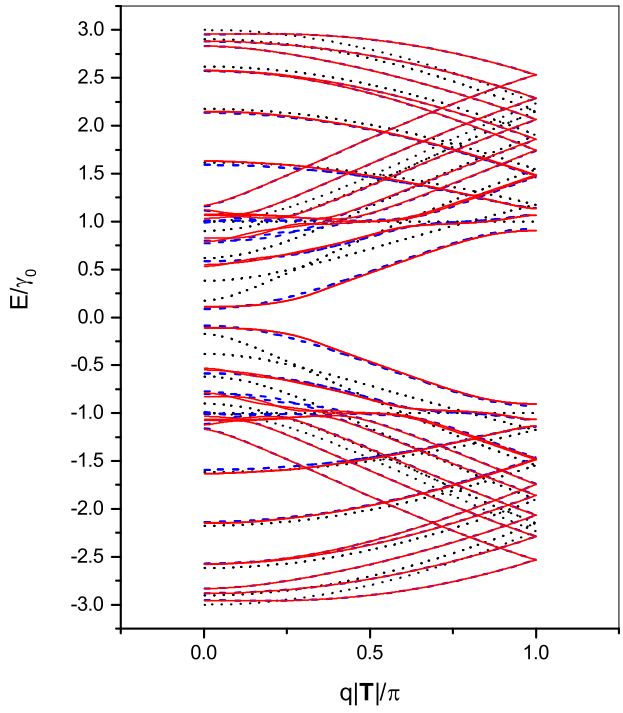

FIG. 1. Electron energy spectrum for a $(10, 0)$ zigzag nanotube in a perpendicular magnetic field corresponding to $R/a_B = 1$ calculated using tight-binding Hamiltonian (blue dashed lines) and Eq. (25) (red solid lines). By black dotted lines is shown electron energy spectrum of the same nanotube without magnetic field.

For example, up to the first order

$$\langle s,\mu|S^{(0)}\,S^{(0)\,\dagger}|s',\mu'\rangle = \delta_{s,s'}\,\delta_{\mu,\mu'} + \frac{i}{2}\,\frac{\mathcal{N}BS_{hex}}{\Phi_0\,|\mathbf{T}|}\,C_A^*(s,\mu,q)\,C_A(s',\mu',q)\,\left(\frac{d\phi(\mu,q)}{dq} - \frac{d\phi(\mu',q)}{dq}\right)$$
$$\times\,(\delta_{\mu',\mu+1} + \delta_{\mu',\mu-1}) \equiv \delta_{s,s'}\,\delta_{\mu,\mu'} + \langle s,\mu|g^{(1)}|s',\mu'\rangle\,.$$

Therefore, one can define

$$S^{(1)} = S^{(0)} - \frac{1}{2}\,g^{(1)}\,S^{(0)}\,.$$

which will be unitary to the first order in the magnetic field.

However, this procedure has only asymptotic convergence[17,28]. For this reason, we will not go beyond zeroth order in numerical calculations.

VII. CONCLUSIONS

We have shown how the perpendicular uniform magnetic field acting on a carbon nanotube can be introduced into the electron's Hamiltonian in the crystal momentum represen-

tation and discussed legitimacy of the so-called Peierls substitution in the energy function for a band. This substitution is not exact but, for magnetic fields currently accessible in laboratories, it provides a very good approximation. Generally speaking, the Peierls substitution represents a zero-order term of the asymptotically convergent power series in the magnetic field. Due to a non-trivial geometry of a carbon nanotube, carrying out Peierls substitution in the energy functions of its numerous sub-bands turned out to be a not so easy task. We have shown how this task can be accomplished and derived analytical expressions for the electron Hamiltonian in the crystal momentum representation in the "zeroth" order in the magnetic field, valid for nanotubes of arbitrary chiralities.

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