Quantized Hall effect in three dimensions

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When the Fermi level lies in a gap, the Hall conductivity of three-dimensional (3D) electrons in a periodic potential can be expressed in a topologically invariant form with a set of three integers. These integers are explicitly found as a solution of a Diophantine equation, the structure of which relies on the flux of the magnetic field through three areas of the periodic lattice. In a simple geometry, we detail a tight-binding model which is found to be reduced to a generalized 1D Harper equation. The existence of a complex gap structure is explicitly shown. The spectrum depends on the field orientation.

The quantized Hall effect (QHE) in two dimensions has been extensively studied since the experimental work of von Klitzing *et al.*[1] Laughlin[2] argued from a general gauge principle that the Hall conductivity should be integrally quantized $\sigma_{xy}=ne^2/h, n\in Z$, when the Fermi level lies in a gap of extended states. Then, from the Kubo formula, Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) (Ref. 3) derived an explicit formula for the Hall conductance of noninteracting electrons in periodic systems. This expression is independent of the detailed structure of the periodic potential.[4] The integer is a topological invariant—the first Chern class of a $U(1)$ principal fiber bundle of a torus.[5] It relates to the structure of the magnetic subbands and thus to the flux ϕ of the magnetic field through a unit area of the periodic lattice.

Up to now, very little work has been devoted to the quantized Hall effect in a three-dimensional (3D) electronic system. As a generalization of the integer QHE in two dimensions and following the lines of TKNN, Halperin[6] showed that, for electrons in a periodic potential, when the Fermi level lies in a gap, the general form of the Hall conductivity is given by

$$\sigma_{xy}=\frac{e^2}{2\pi h}G_z \,, \tag{1}$$

where G_z is the z component of a reciprocal lattice vector of the periodic potential. The value of it, however, has not been given explicitly. On the other hand, Avron *et al.*[7] found that every quantized invariant on a d-dimensional torus T^d is a function of the $d(d-1)/2$ sets of TKNN integers obtained by slicing T^d by the $d(d-1)/2$ distinct T^2. In 3D, the three TKNN integers are precisely related to the three components of the vector $\mathbf{G}$.

More recently, Montambaux and Littlewood[8] presented a physical situation in which the Fermi level is pinned in a gap, in the absence of any disorder. This is the magnetic-field-induced spin-density-wave (SDW) subphase of a 3D quasi-one-dimensional conductor. Their description neglected the lattice periodicity along the direction of highest conductivity.

In this paper, we study 3D electrons in a periodic potential without additional SDW ordering. Our purpose is twofold: First we describe the gap structure and then we derive explicitly the Hall conductivity. We have found that the three integers t_i, which define the reciprocal lattice vector $\mathbf{G}=\sum_{i=1}^{3} t_i\mathbf{a}_i^*$ ($\mathbf{a}_i^*$, are the primitive vectors in the reciprocal lattice) in (1) are the solutions of a diophantine equation that we are going to give explicitly.

Our starting point is the 3D tight-binding Hamiltonian

$$H=-t_a\sum_{\langle ij\rangle_a} c_j^\dagger c_i e^{i\theta_{ij}}-t_b\sum_{\langle ij\rangle_b} c_j^\dagger c_i e^{i\theta_{ij}}-t_c\sum_{\langle ij\rangle_c} c_j^\dagger c_i e^{i\theta_{ij}} \,, \tag{2}$$

where c_i is the usual fermion operator on the lattice. The 3D Bravais lattice is spanned by primitive vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. The summations are taken over nearest-neighbor sites, respectively, along the $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ directions. The phase factor $\theta_{ij}=-\theta_{ji}$ defines the magnetic field. One can introduce *three fluxes* ϕ_a,ϕ_b,ϕ_c (instead of one ϕ in two dimensions) through the three elementary plaquettes of the periodic lattice. The areas $\mathbf{S}_\alpha$ of these plaquettes are given by $\mathbf{S}_\alpha=\mathbf{a}_\beta\times\mathbf{a}_\gamma$. The fluxes are written, in units of the quantum h/e, as

$$\phi_\alpha=\frac{1}{2\pi}\sum_{\text{plaquette}}\theta_{lm}=\frac{e}{h}\int_{S_\alpha}\mathbf{B}\cdot d\mathbf{s} \tag{3}$$

so that the uniform field $\mathbf{B}$ is totally characterized by these three quantities.

When t_c vanishes, the problem reduces to a 2D crystal in a magnetic field.[9] The spectrum has an extremely rich structure as shown by Hofstadter.[9] In fact, if ϕ is irrational, it is a Cantor set that consists of infinitely many "bands" with scaling properties.[10] For a rational $\phi=p/q$, we have q magnetic subbands and each subband carries an integer Hall conductivity. If the Fermi energy is in the rth gap from the bottom, one has a relation $r=ps_r+qt_r$, where s_r and $-q/2\le t_r\le q/2$ are integers. The Hall conductivity is given by $t_r e^2/h$.[3,10]

It is interesting to see whether the quantization takes place in three dimensions. Since the motion of electrons parallel to the field is not affected by the field, one could expect some 2D character in 3D system. In fact, if the magnetic field is parallel to **c** in three dimensions, i.e., $t_c\neq 0$, the third term in (2) decouples and simply gives an additional term—$2t_c\cos\mathbf{k}\cdot\mathbf{c}$ in the energy dispersion. So, if a gap for $t_c=0$ is not closed, the Hall conductivity per plane is given by the 2D formula *but more and more gaps disappear when t_c increases.*

In Ref. 7, it has been stressed that an interesting situation could take place as soon as the field **B** is not aligned along one of the cristallographic axes. This is essentially due to the fact that we have three parameters ϕ_a,ϕ_b,ϕ_c (instead of one ϕ in two dimensions). In such a case, the t_c term does no longer decouple and a more complex structure occurs in the energy spectrum with *many more bands* (see Fig. 1). Let us first, for simplicity, restrict ourselves to a simple geometry. Vectors **a**, **b**, **B** form a rectangular triad and **c** axis is tilted with an angle θ in the **B**-**b** plane. The flux through a plaquette in the **a**-**b** plane is $\phi_c=eBab/h$ and the flux through a plaquette in the **a**-**c** plane is $\phi_b=eBac\sin\theta/h$. Note that there is no flux through the **b**-**c** plane in this geometry.

A site on the square lattice i has coordinates (n,m,l) where n, m, and l are integers. A gauge is chosen in which $\theta_{ij}=0$ for the links along the x direction, $\theta_{ij}=2\pi n\phi_c$ for the link between $i=(n,m,l)$ and $j=(n,m+1,l)$ along the b direction and $\theta_{ij}=2\pi n\phi_b$ for the link between $i=(n,m,l)$ and $j=(n,m,l+1)$ along the c direction. This corresponds to the Landau gauge in the continuum case. A rather straightforward calculation transforms (2) to

$$H=\frac{1}{(2\pi)^3}\int d^3k H(\mathbf{k})$$

with

$$\mathbf{H}(\mathbf{k})=-2t_a\cos k_a c^\dagger(\mathbf{k})c(\mathbf{k})-t_b[e^{-ik_b}c^\dagger(k_a+2\pi\phi_c,k_b,k_c)c(\mathbf{k})+e^{ik_b}c^\dagger(k_a-2\pi\phi_c,k_b,k_c)c(\mathbf{k})]$$
$$-t_c[e^{-ik_c}c^\dagger(k_a+2\pi\phi_b,k_b,k_c)c(\mathbf{k})+e^{ik_c}c^\dagger(k_a-2\pi\phi_b,k_b,k_c)c(\mathbf{k})]\ , \tag{4}$$

where $c(\mathbf{k})$ is a fermion operator defined by $c_{nml}=1/(2\pi)^3\int d^3k\exp[i(nk_a+mk_b+lk_c)]\ c(\mathbf{k})$. We have defined $k_a=\mathbf{k}\cdot\mathbf{a}, k_b=\mathbf{k}\cdot\mathbf{b}, k_c=\mathbf{k}\cdot\mathbf{c}$. There is no coupling between different k_b's and k_c's, and k_a couples to $k_a+2\pi\phi_c, k_a-2\pi\phi_c, k_a+2\pi\phi_b, k_a-2\pi\phi_b$. We choose the magnetic field **B** so that the fluxes have rational values $\phi_c=p/q$ and $\phi_b=p'/q'$. Therefore, the Schrödinger equation $H|\Psi\rangle=E|\Psi\rangle$ is reduced to

$$-2t_a\cos(k_a^0+2\pi j/Q)\psi_j-t_b[e^{-ik_b}\psi_{j-pq'}+e^{ik_b}\psi_{j+pq'}]-t_c[e^{-ik_c}\psi_{j-p'q}+e^{ik_c}\psi_{j+p'q}]=E(k_a^0,k_b,k_c)\psi_j\ , \tag{5}$$

where $Q=qq'$, k_a is written as $k_a^0+2\pi j/Q$ and $\psi_{j+Q}=\psi_j$. A state is given by

$$|\Psi\rangle=\sum_{j=1}^{Q}\psi_j c^\dagger\left[k_a^0+2\pi\frac{j}{Q},k_b,k_c\right]|0\rangle\ , \tag{6}$$

where $|0\rangle$ represents the vacuum state. This equation has Q eigenvalues for fixed values of k_a^0, k_b, and k_c. *Therefore the original single band for the tight-binding model has Q bands due to the application of the magnetic field* and each band has a reduced Brillouin zone: $-\pi/Q\le k_a^0\le\pi/Q, -\pi\le k_b\le\pi, -\pi\le k_c\le\pi$. The overlapping of these Q bands depend on the couplings t_a, t_b, and t_c. The largest number of gaps available is $Q-1$ and this is certainly realized when $t_b,t_c\ll t_a$. Figures 1(b) and 1(c) show the structure of these bands for a choice of parameters. *There are more gaps in the spectrum.*

By a transform $\psi_j=\sum_{j=1}^{Q}e^{i2\pi jl/Q}f_l$, Eq. (5) becomes

$$-t_a[e^{ik_a^0}f_{l-1}+e^{-ik_a^0}f_{l+1}]-[2t_b\cos(k_b+2\pi l\phi_b)+2t_c\cos(k_c+2\pi l\phi_c)]f_l=E(k_a^0,k_b,k_c)f_l\ . \tag{7}$$

This generalized Harper equation describes a 1D tight-binding model with two commensurabilities ϕ_c and ϕ_b, and has interesting localization phenomenon in incommensurate limits.[11]

In a different approach, one starts with the energy dispersion *without* magnetic field, $E(\mathbf{k})=-2t_a\cos\mathbf{k}\cdot\mathbf{a}$, $-2t_b\cos\mathbf{k}\cdot\mathbf{b}$, $-2t_c\cos\mathbf{k}\cdot\mathbf{c}$ and makes the Peierls-Onsager substitution $\mathbf{k}\to(\mathbf{p}+e/c\,\mathbf{A})/\hbar$. Here **p** is the quantum-mechanical momentum operator and **A** is a vector potential. The two approaches give the same energy spectrum and states.

When $t_b,t_c\ll t_a$ one can calculate the Hall conductance explicitly. The unperturbed energy dispersion (i.e., for $t_b=t_c=0$) is simply the first term of (5): $E_0(k_a)=-2t_a\cos(k_a)$. The second and third terms give coupling between different k_a's

$$k_a'=k_a+2\pi\left[\frac{p}{q}t+\frac{p'}{q'}t'\right]\ . \tag{8}$$

The unperturbed spectrum is doubly degenerate. The gaps open when $E_0(k_a)=E_0(k_a')$ (namely, $k_a'=-k_a+2\pi s$ for an integer s). So k_a and k_a' couple by $|t|$th order in t_b and $|t'|$th order in t_c, and the size of the gap is of order of $t_b^{|t|}t_c^{|t'|}$. If s is chosen appropriately, k_a is put between 0 and π and is written as $k_a=(r/Q)\pi$ with $0\le r\le Q$. Thus we obtain

$$\frac{r}{Q}=s+\frac{p}{q}t+\frac{p'}{q'}t' , \qquad (9)$$

where $|t|\le q/2$, $|t'|\le q'/2$, and $0\le r\le Q$. A gap is labeled by an integer r from the bottom of the spectrum.

A convenient way to obtain the Hall conductance when the Fermi energy is in the rth gap is to use the Streda formula:[12] $\sigma_{xy}=e\partial N/\partial B$, where N is the total density of states below the gap. It is simply given by $N=r/QV$, $V=abc\cos\theta$ being the volume of the unit cell. Since $p/q=\phi_c$ and $p'/q'=\phi_b$, one gets, from (9)

$$\sigma_{xy}=\frac{e}{V}\frac{\partial}{\partial B}[s+t\phi_c+t'\phi_b]=\frac{e^2}{hc\cos\theta}(t+Rt') , \qquad (10)$$

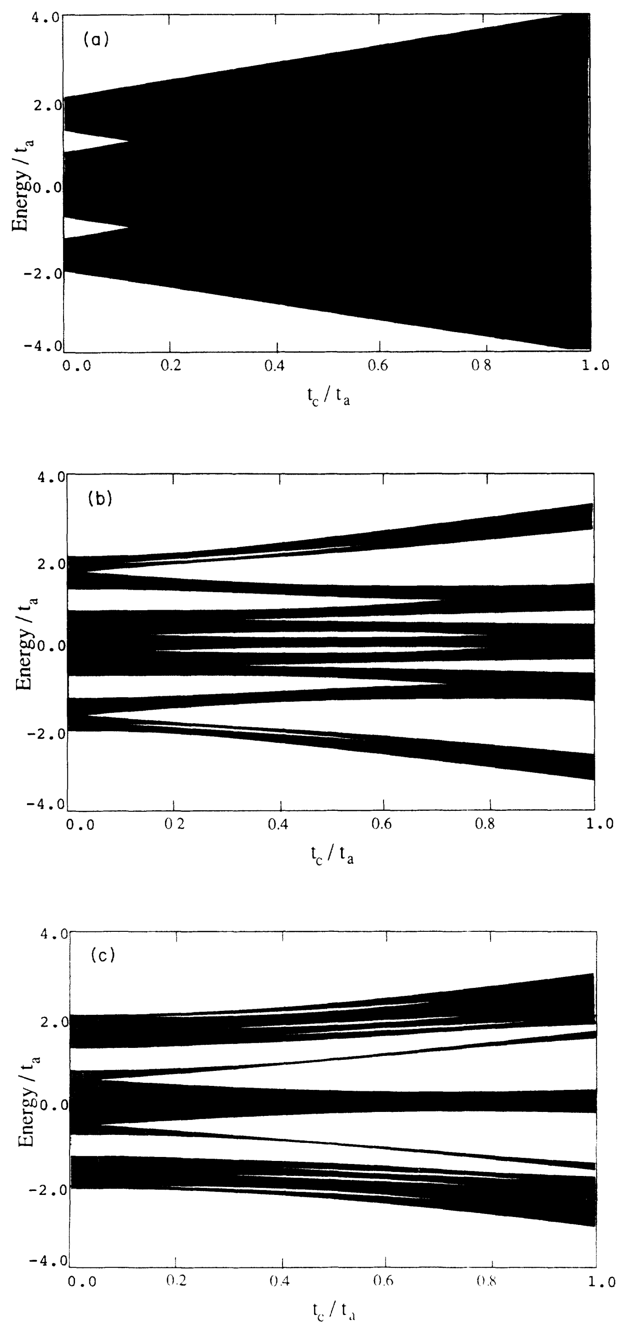

FIG. 1. Evolution of the spectrum with increasing t_c, (a) when the field is aligned along the c direction ($p/q=\frac{1}{3}$); (b) when the c axis is tilted with the angle θ given so that $p'/q'=\frac{1}{5}$; (c) with θ so that $p'/q'=\frac{2}{5}$. Here, $t_a=1$, $t_b=0.3$.

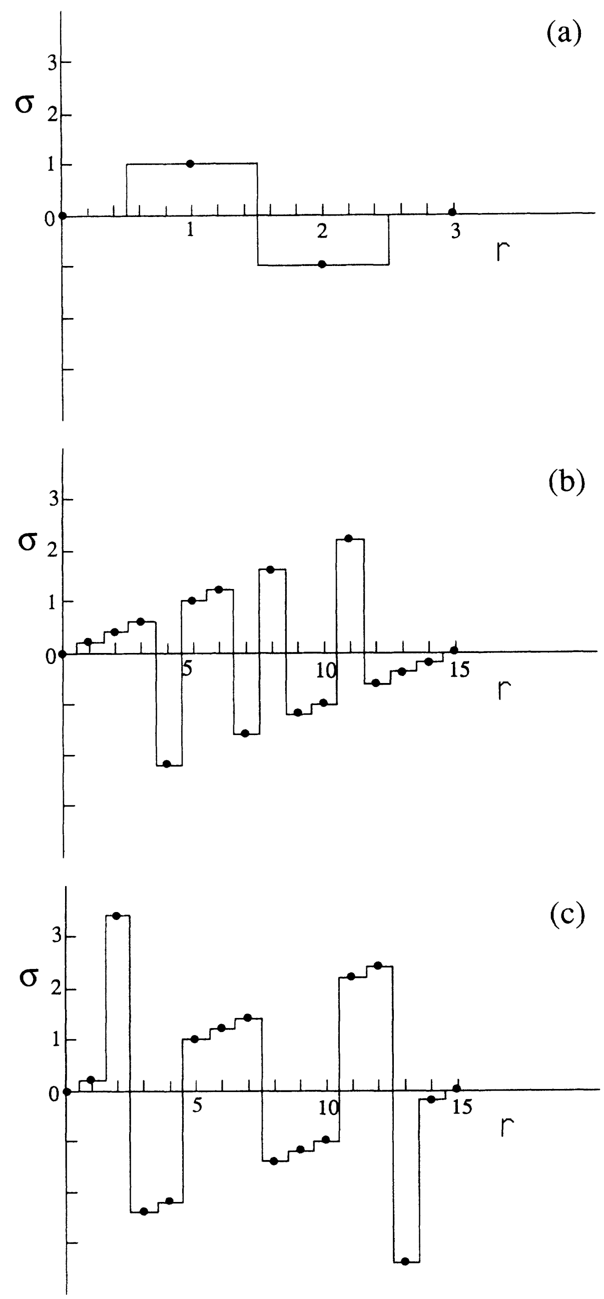

FIG. 2. Hall conductivity σ in a plane (a) when the field and the c direction are colinear; (b) when the direction c is tilted ($p'/q'=\frac{1}{5}$); (c) when $p'/q'=\frac{2}{5}$. The lines are guides for the eyes: The Hall conductivity is only computed in the gaps. The conductivity is expressed in units of e^2/h.

where $R = p'q/pq'$ is the ratio of the two fluxes ϕ_c and ϕ_b. Then the Hall conductance per a plane is

$$\sigma_{xy}^{\text{plane}} = \frac{e^2}{h}(t + Rt') . \quad (11)$$

Note that we assumed s, t, and t' do not depend on B. This can be understood for t_b, $t_c \ll t_a$ where t and t' are number of steps to connect the two degenerate points in k_a space and s is the winding number. Note that k_a space is topologically a circle. So those integers do not change when the magnetic field is changed infinitesimally.[13]

In another approach, one writes the contribution to the Hall conductivity as

$$\frac{h}{e^2}\sigma_{xy} = \frac{1}{(2\pi)^2 i}\int_{\text{RBZ}} d^3k \sum_{j=1}^{Q} \left[\frac{\partial\psi_j^*}{\partial k_a^0}\frac{\partial\psi_j}{\partial k_b} - \frac{\partial\psi_j^*}{\partial k_b}\frac{\partial\psi_j}{\partial k_a^0} \right] . \quad (12)$$

This is a generalization of the 2D result.[3,10] The integral is performed on the reduced Brillouin zone. This is a topological expression[5] since the integrand is related to the phase of the wave function. The determination of the phase in k space is a delicate procedure that can be achieved explicitly in the weak-coupling limit. The energy dispersion is doubly degenerate. The wave function changes character across the boundaries of the Brillouin zone. For the rth band, it gets a phase $\theta_r = t_r k_b + t_r' k_c$ on one side and θ_{r-1} on the other side. We apply Stokes theorem and get

$$\frac{h}{e^2}\sigma_{xy} = \frac{1}{c\cos\theta}\int_0^{2\pi} dk_y \sum_{j=1}^{Q} \frac{\partial}{\partial k_y}(\theta_r - \theta_{r-1}) , \quad (13)$$

which also leads to the result (10).

In the following, we show an example, in the simple geometry we have discussed. We choose the field **B** so that its flux through the **a**-**b** plane is given by $\phi_c = eBab/h = \frac{1}{3}$. We first assume $\theta = 0$ so that $\phi_a = \phi_b = 0$. The spectrum has three bands. The **c** direction decouples and the Hall conductivity has the structure of the 2D result (c is the distance between **a**-**b** planes) $\sigma_{xy} = n\, e^2/hc$. There are three bands in the spectrum and the gaps tend to disappear if t_c is too large [Fig. 1(a)]. Now, assume that the **c** axis is tilted with an angle θ given by $c\sin\theta/b = \frac{3}{5}$ (or $\frac{6}{5}$) so that the flux through the **a**-**c** plaquette is now $\phi_b = eBac\sin\theta/h = \frac{1}{5}$ (or $\frac{2}{5}$). *We now have 15 bands in the spectrum.* Figures 1(b) and 1(c) show the evolution of these bands when t_c increases, for fixed t_b. The Hall conductivity is shown in Fig. 2.

We have chosen a special geometry in which only two fluxes are nonzero. One can easily generalize this result to the most general form if the three fluxes are rational $\phi_i = p_i/q_i$

$$\sigma_{xy} = \frac{e^2}{hV}\sum_{i=1}^{3} t_i \frac{\partial\phi_i}{\partial B} = \frac{e^2}{2\pi h}\sum_{i=1}^{3} t_i \mathbf{a}_i^* \cdot \mathbf{k} , \quad (14)$$

where the t_i are solutions of the diophantine equation ($Q = \prod q_i$)

$$\frac{r}{Q} = s + \sum_i \frac{p_i}{q_i} t_i . \quad (15)$$

In order to study a simple example, we concentrated on the tight-binding approach. As in two dimensions, our results could be very easily generalized beyond this approach and in particular to the weak lattice potential limit.[3,4]

In conclusion, it is worth again stressing that our result cannot be reduced to a 3D picture, since the reciprocal lattice vector **G** of Eq. (1) belongs to a 3D space. Its orientation changes for the different Hall plateaux. This means that, for a given field, the conductivities carried by each subband are characterized by noncolinear vectors.

As in two dimensions, the observation of the lattice effects described in this paper requires enormous fields for a lattice of atomic units. These effects will be probably observable with the evolution of new microelectronics. However, this may already be a useful framework for the study of the SDW 3D systems in which additional periodicities may conspire with the lattice periodicity to give interesting effects.[14]

Finally, let us emphasize that such effects do not necessarily require a special geometry but can be found even in an orthorhombic symmetry if the field is tilted and that *the spectrum varies dramatically with the field orientation.* When the field is not perpendicular to the x-y plane where σ_{xy} is measured, calculation of σ_{xy} has to be done carefully and ρ_{xy} is different from $1/\sigma_{xy}$.[8]

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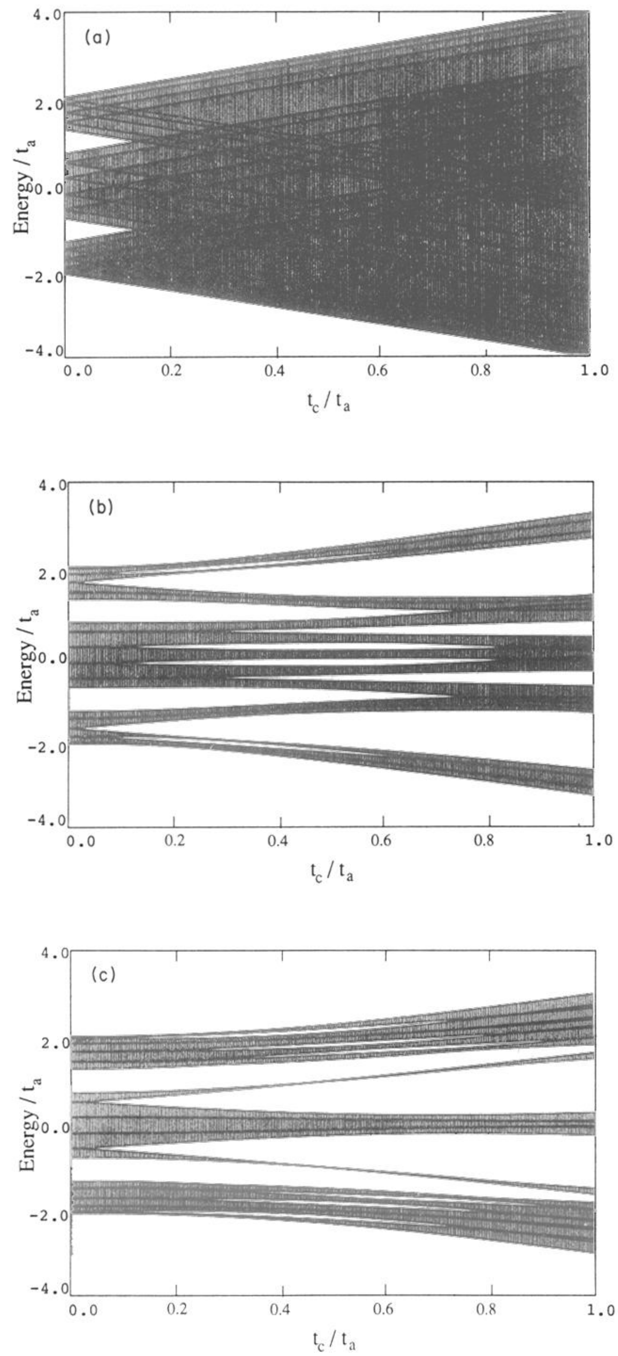

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