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Magnetic oscillations, disorder and the Hofstadter butterfly in finite systems

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Abstract

We present numerical calculations of a tight-binding model applied to a finite square lattice in the presence of a perpendicular magnetic field. The persistent current associated with each eigenstate is calculated, the chirality of which is determined by whether the eigenstate exists within the bulk or localised to the edges of the lattice. This treatment allows us to extract oscillations in the magnetization, which are analogous to de Haas-van Alphen oscillations. We consider the influence of short range disorder and long range potential modulations on these systems.

Keywords: Computer simulations, molecular dynamics, lattice dynamics, electron density, excitation spectra calculations

1. Introduction

If a two-dimensional (2D) electron system is subjected to a perpendicular magnetic field B, the energy dispersion is quantised into Landau levels. In a tight-binding model, these Landau levels become self-similar patterns of magnetic subbands and the resulting spectrum is the celebrated Hofstadter butterfly [1]. The increasing interest in nanotechnology and quantum dots has meant simulations of finite systems are of considerable interest [2-4] particularly in order to illustrate the importance of edge states. In addition the advantage of a finite system is that it is characterised by a finite basis of energy eigenfunctions, which can be used to elucidate properties particular to those eigenfunctions. The method is flexible in that it is straightforward to introduce anisotropy and adjust the geometry of the systems. In this work we present the results of numerical simulations of finite sections of a simple square lattice, of lattice constant a, modeled using a tight-binding model.

2. Model

The approach is described in detail elsewhere [3,4,5]. Taking the vector potential $\boldsymbol{A}$ to be given by $\boldsymbol{A}=(0,Bx,0)$ the matrix components of our Hamiltonian at T=0 become

$$\langle\psi_{n,m}|H|\psi_{n,m}\rangle=E_0 \quad (1)$$

$$\langle\psi_{n,m}|H|\psi_{n\pm1,m}\rangle=te^{\pm2\pi im\alpha} \quad (2)$$

$$\langle\psi_{n,m}|H|\psi_{n,m\pm1}\rangle=t \quad (3)$$

where $\alpha=Ba^2/\Phi_0$, the number of flux quanta passing through each plaquette of the square lattice, Φ_0 is the flux quantum, and E_0 is the atomic energy. Each plaquette of the lattice therefore contributes an Aharanov-Bohm phase factor $e^{2\pi i\alpha}$. A routine diagonalisation procedure allows us to calculate the spectra for finite lattice with increasing numbers of plaquettes. The energy eigenvalues for this Hamiltonian can therefore be calculated numerically as a function of magnetic field. The result for an isotropic lattice with 20×20 sites, is an energy spectrum which resembles the Hofstadter butterfly, shown in Figure 1(a). The procedure can in principle be extended to a $T\neq0$ system by including Fermi-Dirac statistics in the calculation of thermodynamic properties.

Next we consider the properties of the eigenfunctions themselves. The probability current is given by

$$\boldsymbol{J}=\sum_{n,m}\frac{\hbar}{2im^*}[\psi_{n,m}^*(\psi_{n,m+1}-\psi_{n,m-1})\boldsymbol{i} + \psi_{n,m}^*(\psi_{n+1,m}e^{+2\pi im\alpha}-\psi_{n-1,m}e^{-2\pi im\alpha})\boldsymbol{j}] \quad (4)$$

where n and m are integers denoting a lattice site located at $\boldsymbol{r}_{n,m}=na\boldsymbol{i}+ma\boldsymbol{j}$. This approach has been useful in quantum dot and antidot studies [3,4]. The persistent current paths are comparable to semiclassical cyclotron orbits, where the cyclotron radius, r_c, shrinks as the magnetic field increases.

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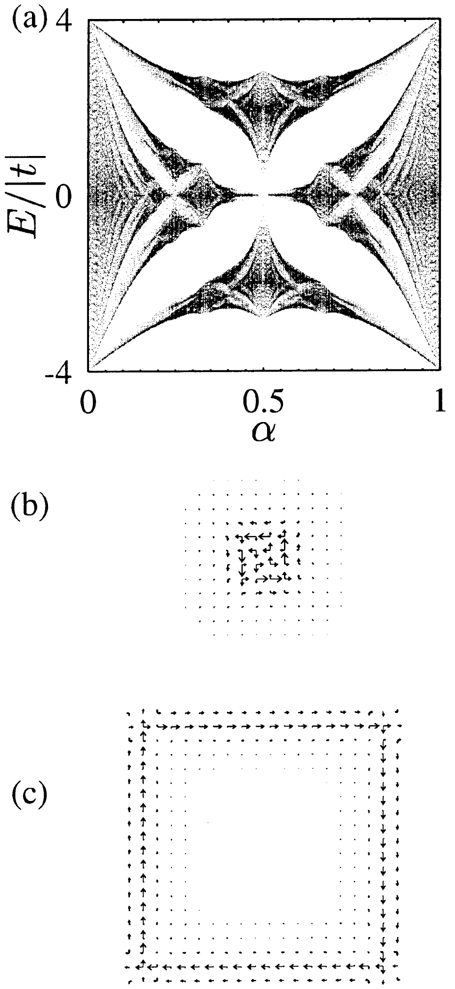

Fig. 1. (a) Is the energy spectrum for an isotropic tight-binding square lattice with 20×20 sites. (b) shows a bulk state at α=0.1 with energy $E/|t|\approx$-3.4. (c) shows an edge state at α=0.1 with energy $E/|t|\approx$-2.7. The arrows show the direction of persistent currents carried by the eigenstate. The bulk state and the edge state have opposite chirality.

In the regions of Figure 1(a) where this cyclotron radius is comparable to the size of the finite lattice (i.e. at small magnetic fields and close to the band centre) many states are edge states ("skipping orbits" in a finite semiclassical picture) and in these regions, the Landau level structure is indistinct. In the opposite limit, these semiclassical skipping orbits carry a current in the opposite direction to the bulk cyclotron orbits; correspondingly, the eigenfunctions in our model carry persistent currents whose chirality in high magnetic fields is associated with whether a given state is localised around the edges or in the bulk of the lattice [6]. Figures 1(b) and (c) illustrate persistent currents associated with bulk and edge eigenstates. The magnetic contribution of these eigenstates as the field is increased is opposite: depending on the region of the spectrum considered, the bulk states will provide a diamagnetic contribution to the magnetisation and the edge states a paramagnetic contribution, or vice versa [3,6].

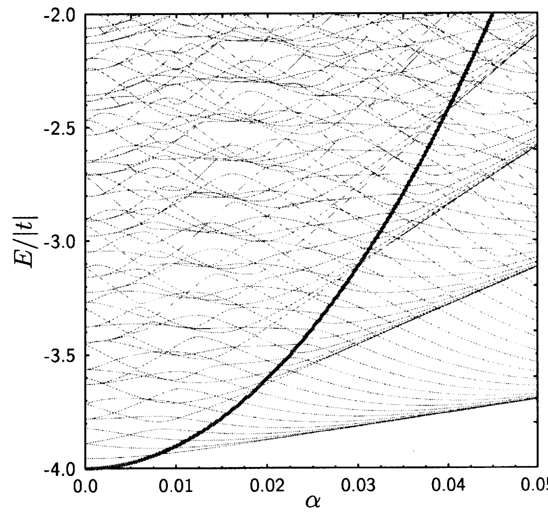

Fig. 2. The low field region of Figure 1(a) The thick solid line represents the energy of a cyclotron orbit with radius r_c=5a. On the high field side of the line edge and bulk levels are well defined. Electric-dipole transitions between these levels have been considered in Reference [9].

Figure 2 shows an enlargement of Figure 1(a) for low magnetic fields. The solid line represents the energy of a state with r_c=5a, one quarter of the length of the edge of our square lattice. On the high-field side of the line, the Landau level structure emerges. In the low-field region, the spectrum is dominated by edge states.

3. Oscillations in the Magnetisation

The magnetisation is related to the internal energy E of the system [8] by

$$M=-\left(\frac{dE}{dB}\right)_N=-\frac{a^2}{\Phi_0}\left(\frac{dE}{d\alpha}\right)_N \qquad (5)$$

where N is the number of electrons and is kept constant as in a canonical ensemble. Oscillations in the magnetisation occur as the Fermi level, which is tied to the energy of the highest occupied energy level, varies with field. In so doing it passes anti-crossings at which states at the Fermi level change from having a paramagnetic response to a diamagnetic response, or vice-versa. Correspondingly, the state at the Fermi level changes from bulk character to edge character. These oscillations dominate the total magnetisation because the corresponding oscillations below the Fermi level tend to compensate each other [4]. Figure 3 illustrates the magnetisation oscillations, resembling de Haas-van Alphen oscillations with fine oscillations superposed due to the numerous anti-crossings traversed by the Fermi level. The frequency F corresponds to the well known semiclassical, saw-tooth

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