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A MATHEMATICAL MODEL FOR THE SPECTRUM OF A TWO-DIMENSIONAL SCHRÖDINGER EQUATION WITH MAGNETIC FIELD UNDER DIRICHLET BOUNDARY CONDITIONS

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A Mathematical Model for the Spectrum of a Two-Dimensional Schrödinger Equation with Magnetic Field under Dirichlet Boundary Conditions

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Resumo

Neste trabalho investigamos o espectro da equação de Schrödinger na presença de campo magnético. Os auto-valores representam as energias dos elétrons em uma nanoestrutura e são calculados para diferentes valores de vetores de onda complexos. Com base nos resultados numéricos e explorando as simetrias do problema propomos um modelo matemático para as curvas espectrais.

Abstract

In this paper we have investigated the spectrum of the Schrödinger equation with magnetic field. The eigenvalues represent the energies of electrons in a nanostructure which are calculated for different values of complex wavevectors. Based on numerical results and exploring the symmetries we propose a mathematical model for the spectral curves.

1 Introduction

In this paper we are concerned with the Schrödinger equation defined in a two-dimensional domain which is unlimited in the x-direction and under Dirichlet boundary conditions in the y-direction. The study is motivated by the analysis of electronic transport in a quantum wire in which a two-dimensional electron gas (2DEG) in the x, y-plane is confined by a symmetric potential $V_c(y)$ and also subject to a magnetic field $\mathbf{B} = B\mathbf{z}$. The potential is supposed to be like *hard-wall*, or

$$V_c(y) = \begin{cases} 0 & \text{if} \quad |y| < w/2 \\ \infty & \text{otherwise.} \end{cases} \tag{1}$$

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The magnetic field is described by a vector potential in the Landau gauge $\mathbf{A} = -By\mathbf{x}$. Thus, the one-electron Schrödinger equation describing electrons in the wire is given by

$$\frac{1}{2m^+}(\mathbf{p} - (-e)\mathbf{A})^2\psi(x,y) + V_c(y)\psi(x,y) = \mathcal{E}\psi(x,y), \tag{2}$$

where m^+ is the electronic effective mass, $(\mathbf{p} - (-e)\mathbf{A})$ is the generalised momentum operator and the total energy $\mathcal{E}$ is defined with respect to the bottom of the occupied 2D subband. We shall also assume the existence of only one 2D subband, which is a good physical approximation in this context.

By writing $\mathbf{p} = -i\hbar\nabla$ the Schrödinger equation (2) is transformed into

$$-\frac{\hbar^2}{2m^+}\Big[(\frac{\partial}{\partial x} - \frac{ieBy}{\hbar})^2 + \frac{\partial^2}{\partial y^2}\Big]\psi(x,y) + V_c(y)\psi(x,y) = \mathcal{E}\psi(x,y). \tag{3}$$

It is convenient to express the Schrödinger equation in admensional units, so we make the following change of variables:

$$y \to y/w, \quad x \to x/w, \quad \mathcal{E} \to \mathcal{E}/\mathcal{E}_0,$$

where

$$\mathcal{E}_0 = \frac{\hbar^2}{2m^+w^2},$$

and w is the width of the confinement region. In the new variables, the partial differential equation is expressed as

$$-(\nabla^2 - 2i\alpha^2 y\frac{\partial}{\partial x} - \alpha^4 y^2)\psi(x,y) = \mathcal{E}\psi(x,y), \tag{4}$$

where $\alpha = w/l_B (l_{B^2} = \hbar/eB)$ and we have omitted the confinement potential which in fact is taken into account via the boundary conditions.

2 Description of the Solutions

The confinement and vector potential do not depend on x, so the electronic motion in the x-direction is decoupled from that in the y-direction. Thus, the modal wavefunction $\psi(x,y)$ can be written as

$$\psi(x,y) = e^{ikx}\phi(y,k), \tag{5}$$

where k is the wavevector. We stress the k-dependence of $\phi(y,k)$. Here we consider not only real values of k, but the more general case when k is complex. One can make it clearer by looking at $|\psi|^2$. In addition, because of the hermicity of the Hamiltonian in (2), $\mathcal{E}$ must be real. Hence, the domain of k is $\mathcal{D} = \{k \in \mathbb{C} \ : \ \mathcal{E} \in \mathbb{R}\}$. Substituting (5) into the Schrödinger equation (4) we find that $\phi(y,k)$ satisfies

$$\frac{d^2}{dy^2}\phi(y,k) + [\mathcal{E} - (\alpha^2 y - k)^2]\phi(y,k) = 0 \tag{6}$$

subject to Dirichlet boundary conditions

$$\phi(1/2,k) = \phi(-1/2,k) = 0. \tag{7}$$

In this paper we are interested in determining the energy curves in the $k, \mathcal{E}$-space. For that, we shall solve (6), although we do not describe the behaviour of $\phi(y,k)$ itself.

It is well known that, for confinement potentials going to infinity when $|y|$ goes to infinity, the value of the energy is associated with a discrete set of complex k. We represent the k's by $k_n = k_{nr} + ik_{ni}$ where k_{nr} and k_{ni} are the real and imaginary parts of k_n respectively. Suppose that we know a solution $\phi(y,k)$ of (6) for a given energy. By inspection on the differential equation we conclude that $\phi(y,k^*)$ is another solution with same energy. Hence, $\phi(y,k)^* = A_1\phi(y,k^*)$, where A_1 is a constant. We calculate $|A_1|$ by normalising the modal wavefunction. Then, A_1 reduces to a phase factor which can be determined by scaling the wavefunctions. Therefore, we can write the complex-conjugate symmetry as

$$\phi(y,k^*) = \phi(y,k)^*. \tag{8}$$

We see that if k is real then so is the wavefunction. Also, the changes of y to $-y$ and k to $-k$ do not alter the differential equation. Hence, $\phi(-y,k) = A_2\phi(y,-k)$, where A_2 is a constant which again can be determined by the normalisation condition and the scaling factor. Thus, we can redefine the modal wavefunctions such that

$$\phi(-y,k) = \phi(y,-k). \tag{9}$$

This symmetry together with (8) generate four different solutions with same energy. Therefore, if we suppose that $\phi(y,k)$ is a modal solution for a fixed energy, then other three solutions associated with $k^*, -k, -k^*$ must appear. Moreover, we can write the following relations

$$\begin{aligned} \phi(y,k) &= \phi(-y,-k), \\ \phi(y,k) &= \phi^*(y,k^*), \\ \phi(y,k) &= \phi^*(-y,-k^*), \end{aligned} \tag{10}$$

which show that $\mathrm{Re}[\phi(y,k)]$ is an even function and $\mathrm{Im}[\phi(y,k)]$ is an odd function when k is purely imaginary. Also, $\mathrm{Im}[\phi(y,k)] = 0$ when k is real.

A number of different calculations, such as perturbation theory [1], WKB [2] and numerical methods [3, 4], have been performed to determine the energy for real values of k. Here, we have to extend the calculation of the energy for complex k's. These energies are of great interest in the study of scattering problems when one uses the wavefunction matching methods.

Two limiting cases [1] are useful and we describe them briefly here. The case of a very low magnetic field ($\alpha \ll 1$) can be treated by perturbation theory [1] giving

$$\mathcal{E}_n(k) = \mathcal{E}_n^0(k) + a_n\alpha + b_n\alpha^2 + c_n\alpha k^2, \tag{11}$$

where $\mathcal{E}_n^0(k)$ is the energy for zero field, a_n and b_n are positive constants and c_n is a positive constant except when $n = 1$. The energy curves are parabolic following the result for the zero field case. The strong magnetic field case must be divided in two cases depending on the values of k. For very small k, the energies are like Landau levels and therefore are flat around $k = 0$. This behaviour is due to the fact that the effect of the confinement potential can be neglected. Thus, in this regime, the parabolic potential is dominant and its curvature is very large. For the case of large k $(k \gg \alpha^2/2)$, the triangular potential approximation can be used. Figure 1 shows schematically the total potential for a hard-wall confinement plus the magnetic potential. In this case, the energies can be expressed as [10]

$$\mathcal{E}_n(k) = (k - \frac{\alpha^2}{2})^2 + a_n(B)(k - \frac{\alpha^2}{2})^{2/3}. \tag{12}$$

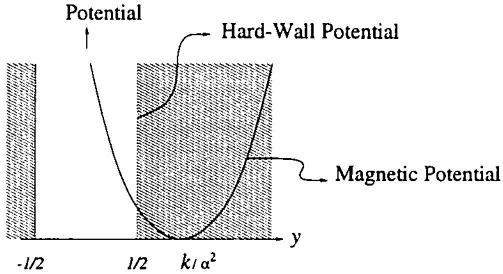

Figure 1: A schematic diagram of the potential acting in the wire. For large values of k the total potential can be approximated by a triangular potential.

Formally, the solution of (6) has an analytic expression [6] which is a combination of two confluent hypergeometric functions

$$\phi(y) = e^{-\eta/2} \quad \Big[\mathcal{A}\ {}_1F_1\ (a;c;\eta) + \mathcal{B}\ \eta^{1-c}\ {}_1F_1\ (a-c+1;2-c;\eta)\Big], \tag{13}$$

with $\eta = \frac{(\alpha^2 y - k)^2}{\alpha^2}$, $a = (1 - \mathcal{E}/\alpha^2)/4$ and $c = 1/2$. The constants $\mathcal{A}$ and $\mathcal{B}$ could be determined by the normalisation of (13), and by imposing the boundary conditions we could also calculate the energy for each value of k. However, instead of solving (13) formally we solve (6) applying numerical methods. The procedure is as follows: we fix a real value of $\mathcal{E}$ to solve (6) and then we determine the corresponding values of k.

In figure 2 we present the energy curves obtained numerically for $\alpha = 4.0$.

We use the fact that the curves are symmetric under reflection about the central axis $k = 0$ to plot a plane diagram. The solid curves on the left-hand side of the picture show the solutions related to imaginary values of k and the dashed curves to the imaginary part of the complex k. The solid curves on the right-hand side are for real k and the dashed ones are related to the real part of k. Therefore, solid curves on the left have $k_r = 0$ and the ones on the right have $k_i = 0$. We label each curve according to the solutions with real k. We know that the first one is the ground state, the second is the first excited state and so on. We draw this conclusion from the number of zeros of the modal wavefunction ϕ for real k. We note from the results on the left-hand side that curves with different modal indices join up (like 1 and 2) and from the minimum of the resulting curve a branch with complex k emerges. For the states on the dashed curves, the number of zeros of the wavefunctions is not well defined: the real part of the wavefunction

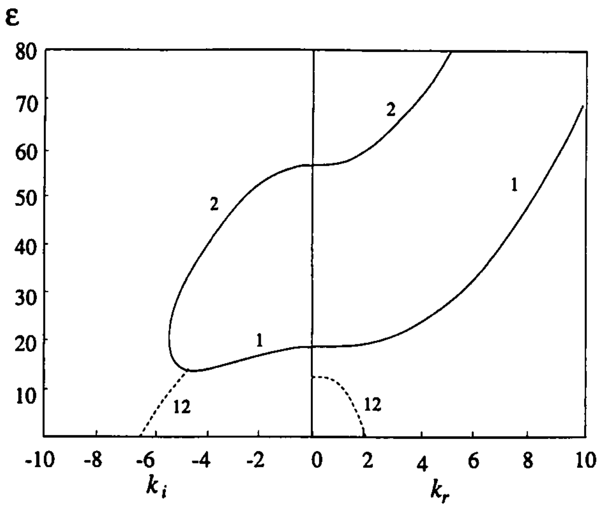

Figure 2: Energy curves when $\alpha = 4.0$.

has a different number of zeros from the imaginary part. If we make a comparison between these results and the case of zero magnetic field we conclude that the solutions related to complex k's are completely different and the solutions related to real k's are similar. The main difference between zero and non-zero magnetic field is that the magnetic field raises the cut-off energies so that curve 1 is flatter than in the zero-field case as suggested by a semi-classical analysis . We note that curve 2 is closer to a parabola than curve 1, and the same conclusion is valid for higher energies. This can be understood by noting that the effect of the magnetic potential is reduced when we go up in the energy scale as indicated by figure 1. The energy curves become more complicated as larger magnetic fields are considered. In figure 3 we present the results when the magnetic field is increased such that $\alpha = 5.0$. We note from curve 1 on the left that not only a local minimum appears,

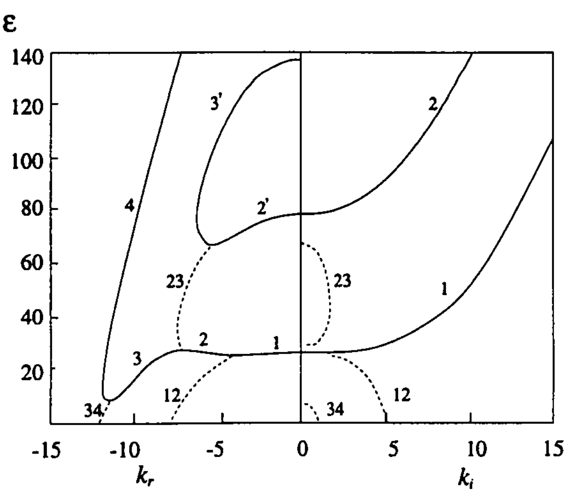

Figure 3: Energy curves for $\alpha = 5.0$.

but also another local minimum and a local maximum. Moreover, at each of these critical points a solution branch with complex k emerges going up in the case of a maximum and down in the case of a minimum. Curves $2'$ and $3'$ are very similar in shape to respectively curves 1 and 2 of figure 2, which present only one critical point. Curve 4 now meets curve 3 which, in turn, meets curve 2. The solid curves on the right are very similar to the results for $\alpha = 4.0$ and again (due to the increased magnetic field) they are flatter near $k_r = 0$. The cut-off energy has increased and become approximately the value os the Landau levels. To illustrate these conclusions we plot in figure 4 the same curve as in figure 3, but on a magnified scale.

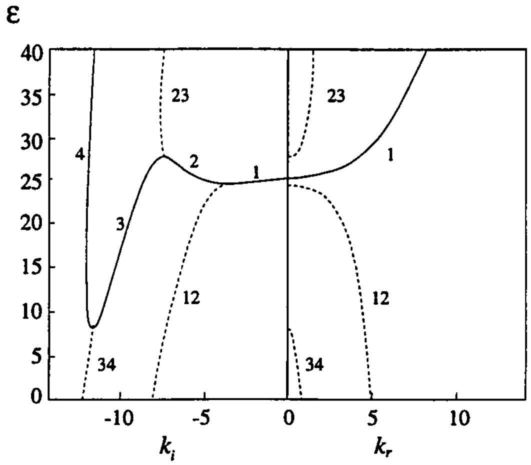

Figure 4: A large-scale plot of the energy curves when $\alpha = 5.0$.

Finally, to illustrate all the conclusions obtained, in figure 5 we present the energy curves for $\alpha = 8.0$. The solid curves on the right are flat near $k = 0$ and the cut-off energies are very close to $(2n + 1)\alpha^2$ which is the value of the Landau levels. We notice that the number of solution branches with complex k has increased to nine for the lower curve on the left, to seven for the next curve, and so on decreasing by 2 when we go up in energy.

2.1 Modeling the Energy Curves

Based on the numerical results presented in the last section we propose a model for the energy. If the magnetic field is zero, then the curves are parabolas centred at $k = 0$ and, therefore, the only possibility for k is to be real or purely imaginary. For non-zero but very small magnetic field ($\alpha \ll 1$) we expect, and verify numerically, that the energy curves are still parabolic but with different curvatures which depend on the magnetic field. This is confirmed by the perturbative calculation (equation (11)). However, as we increase the magnetic field, the curves related to real values of k must be described by a polynomial of even order in k_r due to the symmetries mentioned before. Thus, if k_r is small we model the energy curves by

$$\mathcal{E}_n(k_r) = c_n(\alpha) + b_n(\alpha)k_r^2 + a_n(\alpha)k_r^4 + \mathcal{O}(k_r^6), \tag{14}$$

where higher order in k_r are neglected. In this expression we suppose that a_n, b_n and c_n are real positive constants for a fixed α. With these properties, the polynomial has only

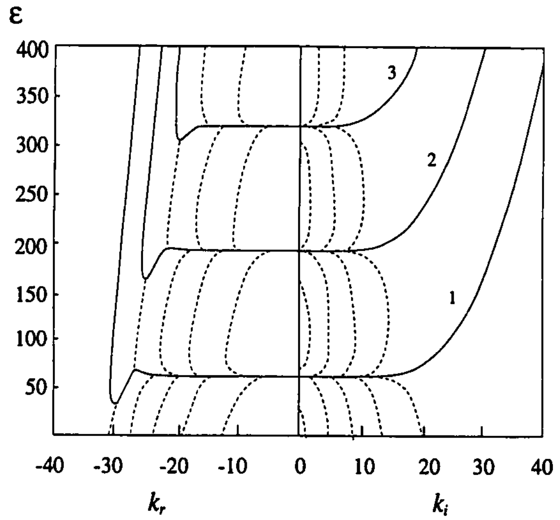

Figure 5: Energy curves for $\alpha = 8.0$.

one zero when $\mathcal{E}_n(k_r) - c_n(\alpha) = 0$, and this zero occurs at $k_r = 0$.

Since the expression for the energy must be an analytical function around $k = 0$, (14) extends for any complex k in a neighbourhood of $k = 0$, so we write

$$\mathcal{E}_n(k) = c_n(\alpha) + b_n(\alpha)k^2 + a_n(\alpha)k^4 + \mathcal{O}(k^6), \tag{15}$$

which reduces to (14) for real values of k. We see from this equation that imaginary values of k (k_i) that satisfies (6) are in the domain $\mathcal{D}$. Moreover, this expression contains all the symmetries of the problem. The substitution of $k = ik_i$ in (15) yields

$$\mathcal{E}_n(k_i) = c_n(\alpha) - b_n(\alpha)k_i^2 + a_n(\alpha)k_i^4 + \mathcal{O}(k_i^6), \tag{16}$$

which shows that the energy curves present critical points in the imaginary plane, that is, the $k_i, \mathcal{E}$-plane. This behaviour is verified by the numerical results discussed before. For higher values of the magnetic field, more elements in the expansion must be taken into account.

Now we consider a value of k in a neighbourhood of an imaginary critical point $k_0 = ik_{0i}$:

$$\mathcal{F}_n(k) = \frac{\mathcal{E}''}{2}(k - k_0)^2, \tag{17}$$

where $\mathcal{E}''$ is the second derivative of $\mathcal{E}$ calculated at k_0 and therefore a real constant. $\mathcal{F}_n(k)$ is real for real values of $k - k_0$ and for purely imaginary values of $k - k_0$. The question raised here is whether there exist other values of k which leave $\mathcal{F}$ real. By using the Cauchy's residue theorem we can write [7, 8]

$$\int_\gamma \frac{1}{\mathcal{F}_n(k)} \frac{d}{dk}\mathcal{F}_n(k)dk = 2\pi i(N - P), \tag{18}$$

where γ is any contour enclosing k_0, N is the number of zeros and P is the number of poles of $\mathcal{F}_n(k)$ inside γ, taking multiplicity into account. The integral in (18) can be solved resulting in $(\ln|\mathcal{F}_n|)_\gamma + i(\theta_n)_\gamma$, where $\ln|\mathcal{F}_n|$ and θ_n are calculated over the contour and $(\ )_\gamma$ denotes the change in a quantity in going round the contour γ. From (17), $\mathcal{F}_n$ has a zero of multiplicity 2 and no poles, so

$$(\ln|\mathcal{F}_n|)_\gamma + i(\theta_n)_\gamma = 4\pi i. \tag{19}$$

Therefore the phase of $\mathcal{F}_n$ increases by 4π in going round the contour. Now, we seek real values of $\mathcal{F}_n$ which occur four times on the contour, for $0, \pi, 2\pi$ and 3π, say. At a critical point which is a maximum, $\mathcal{E}''$ is negative ($\mathcal{F}_n < 0$), and this happens for $\theta = \pi$ and 3π. Analogously, a minimum ($\mathcal{F}_n > 0$) occurs for $\theta = 0$ and 2π. Since these all happen at k_0, we conclude that two new branches of solutions emerge, going down in the direction where k_0 behaviours like a maximum and going up in the direction where k_0 behaviours like a minimum. We then conclude that the point $k = k_0$ is a saddle point in the three-dimensional $k, \mathcal{E}$-space. Again, this behaviour can be verified from the numerical results presented here.

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