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Energy of Electrons in a Nanowire Subject to Spin-orbit Interaction

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Cover Page Footnote
Ryan Brennan, FCRH 2011, is from Long Island, New York. He is a graduating physics major. Ryan conducted research on energy bands in quantum nanowires and is currently studying the properties of graphene. After graduation, Ryan plans to attend graduate school in the hopes of attaining a Ph.D in physics.

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The Physics

The Hamiltonian for a particle subject to spin-orbit interaction is more complicated than that of a free particle, containing terms corresponding to the electric dipole and Thomas precession processes. For a thin quantum wire in the x-y plane, a non-zero electric field perpendicular to the plane of the wire gives rise to yet another process of spin-orbit interaction called the Rashba spin-orbit interaction. The contribution of this Rashba mechanism is dictated by a parameter α which is proportional to the perpendicular electric field. Additionally, a strong potential well within the x-y plane may be associated with an electric field, which is not negligible compared to the field that causes the α-interaction. In this case of planar, as well as perpendicular confinement, there is one more contribution to the Hamiltonian and the spin-orbit interaction, this time corresponding to the parameter β, which is dictated by the width and potential depth of the nanowire. Typical values of β are about one tenth of α.[1] Our goal was to write a program that would compute the eigenenergies of an electron in the nanowire.

The Problem

Electrons are confined to a long, thin nanowire in the x-y plane. They are subject to the Rashba α-coupling due to an electric field in the z-direction. In addition, the particles are confined along the x-direction by the sides of the wire, only able to move between $x=0$ and $x=W$, which gives rise to the β spin-orbit coupling. The total wave function of an electron within the nanowire has the form[1]

$$(1) \qquad \varphi(\mathbf{r}) = \frac{e^{ik_y y}}{\sqrt{L_y}} \begin{bmatrix} \psi_A(x) \\ \psi_B(x) \end{bmatrix}$$

where k_y is the wave number in the y direction, L_y is a normalization length used to set the probability of finding the particle somewhere in space equal to one, and $\psi_A(x)$ and $\psi_B(x)$ are two different spin states of

the particle. Applying the Hamiltonian containing all of the SOI (spin-orbit interaction) terms to the above wave function gives two coupled differential equations. The Hamiltonian and the two differential equations are as follows:

$$(2) \qquad \hat{H} = \frac{\mathbf{p}^2}{2m^*} + \frac{\alpha_R}{\hbar}(\boldsymbol{\sigma} \times \mathbf{p})_z + i\beta F(x)\sigma_z \frac{\partial}{\partial y}$$

$$(3) \qquad -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dx^2} - k_y^2\right)\psi_A(x) + \alpha\left(\frac{d}{dx} + k_y\right)\psi_B(x) - \beta k_y F(x)\psi_A(x) = \varepsilon\psi_A(x)$$

$$(4) \qquad -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dx^2} - k_y^2\right)\psi_B(x) - \alpha\left(\frac{d}{dx} - k_y\right)\psi_A(x) + \beta k_y F(x)\psi_B(x) = \varepsilon\psi_B(x)$$

where the Hamiltonian is comprised of the free particle contribution, the α contribution that arises from the asymmetry of the quantum well (Rashba mechanism), and the β contribution that arises from the lateral confining electric field. m^* is the reduced mass of the electron, $\hbar$ is the reduced Planck's constant, ε is the eigenenergy of the particle and

$$F(x) = \left(\frac{W}{l_0}\right)\left\{\exp\left[-\frac{(x-W)^2}{2l_0^2}\right] - \exp\left[-\frac{x^2}{2l_0^2}\right]\right\}.$$ $F(x)$ is related to the lateral confinement field in the x-y plane, where l_0 is a measure of the steepness of the potential at the edges of the nanowire. A small value of l_0 means that the the particle hits a very steep potential at the edge of the wire. We needed to find ε-, the energies that satisfy these two equations simultaneously.

Solving the Problem

Our first task was to cast the equations in dimensionless form. We made our unit of length dimensionless by changing x to $X = \dfrac{x}{W}$, and adjusting the derivatives and the function $F(x)$ accordingly. We introduced

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$$l_\alpha = \frac{\hbar^2}{2m^*\alpha}, \quad l_\beta = \frac{\hbar^2}{2m^*\beta}, \quad K_y = k_y W \text{ and } E = \frac{2m^*w^2\varepsilon}{\hbar^2}$$

. Finally, we made the l_α, l_β and l_0 parameters dimensionless by setting $\tau_\alpha = \frac{W}{l_\alpha}$, $\tau_\beta = \frac{W}{l_\beta}$ and $\tau_0 = \frac{W}{l_0}$.

Equations 1 and 2 became:

(5) $\left(K_y^2 - \frac{d^2}{dX^2}\right)\psi_A(X) + \tau_\alpha\left(K_y + \frac{d}{dX}\right)\psi_B(X) - \tau_\beta K_y F(X)\psi_A(X) = E\psi_A(X)$

(6) $\left(K_y^2 - \frac{d^2}{dX^2}\right)\psi_B(X) - \tau_\alpha\left(\frac{d}{dX} - K_y\right)\psi_A(X) + \tau_\beta K_y F(X)\psi_B(X) = E\psi_B(X)$

where

$$F(X) = \tau_0\left\{\exp\left[-\frac{\tau_0^2}{2}(X-1)^2\right] - \exp\left[-\frac{\tau_0^2}{2}X^2\right]\right\}$$

and typical values were $\tau_\alpha \approx 5-10$, $\tau_\beta \approx .5-1$ and $\tau_0 \approx 1000$. It became clear that while these equations did not look very daunting, they could not be solved by elementary functions. We used a central difference approximation to replace the derivatives in the two equations:

$$\frac{d\psi(X)}{dX} = \frac{\psi(X+\delta) - \psi(X-\delta)}{2\delta}$$

$$\frac{d^2\psi(X)}{dX^2} = \frac{\psi(X+\delta) + \psi(X-\delta) - 2\psi(X)}{\delta^2}$$

where δ is a small distance in the x-direction. The derivative of the wave function at each point can be approximated by using the values of the function around the point of interest. The smaller the increment, the better the approximation. We first thought that we could write the two equations at X=0, setting $\psi_{A/B}(X-\delta) = \psi_{A/B}(X) = 0$, and solve for $\psi_{A/B}(X+\delta)$. We would then plug these values into the two equations as the current values of the wave functions and solve for the wave functions at the next step of X. We soon realized that the values of the wave functions at each point would be in terms of E and K_y and we would have no way to solve for the energies. This method also did not take into account the second boundary condition $\psi_A(1) = \psi_B(1) = 0$. Since the electron could not leave the nanowire, its wave function had to go to zero at both ends of the wire. It became clear that we had to write the two equations at each X value between 0 and 1 in steps of δ and solve them simultaneously. At

$X = \delta$, $\psi_A(X-\delta)$ and $\psi_B(X-\delta)$ would be $\psi_A(0)$ and $\psi_B(0)$ and could be set equal to 0. At $X = 1-\delta$ the same could be done for $\psi_A(X+\delta)$ and $\psi_B(X+\delta)$ and in this way the boundary conditions at both sides were addressed. Several equations of this kind can be written at once as one matrix equation in the following way:

(7)
$$x + 3y - 4z = Ex$$
$$2x - 7y + 6z = Ey$$
$$y - z = Ez$$

becomes

(8) $\begin{bmatrix} 1 & 3 & -4 \\ 2 & -7 & 6 \\ 0 & 1 & -1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = E\begin{bmatrix} x \\ y \\ z \end{bmatrix}$

or $\mathbf{M}\cdot\mathbf{r} = E\mathbf{r}$. In our case, $\mathbf{M}$ was a large matrix of mostly zeroes, since for any given equation, only the current, previous and next values of the wave functions were present, and had non-zero coefficients. The matrix $\mathbf{r}$ became $\mathbf{\Psi}$, a long column matrix containing the two wave functions at each x coordinate between 0 and 1:

(9) $\mathbf{\Psi} = \begin{bmatrix} \psi_A(\delta) \\ \psi_B(\delta) \\ \psi_A(2\delta) \\ \psi_B(2\delta) \\ \vdots \\ \psi_A(1-\delta) \\ \psi_B(1-\delta) \end{bmatrix}$

We could solve an equation of the form $\mathbf{M}\cdot\mathbf{\Psi} = E\mathbf{\Psi}$ for E, the eigenvalues of $\mathbf{M}$, by setting the determinant of equal to zero without having to know the value of the wave functions at each point. These eigenvalues are the energies of the electrons in units of $\frac{2m^*w^2}{\hbar^2}$. We assigned values to τ_α, τ_β and τ_0, leaving K_y as the only undefined variable in the matrix. When we solved for the eigenvalues of $\mathbf{M}$ we obtained as many eigenvalues as there were equations. For example, when $\delta = .01$, there are 99 X coordinates, giving 198 equations and 198 eigenvalues. We solved for these eigenvalues in terms of K_y, but the computing power needed became too much beyond a step size of .01. Since Mathematica could handle a purely numerical calculation much more easily, we assigned values to K_y from -20 to 20 in increments of .1 and solved for all of the eigenvalues at each value of K_y. In this way, we were able to produce graphs of E vs. K_y, or $\frac{2m^*w^2\varepsilon}{\hbar^2}$ vs. $k_y W$. Figures 1, 2,

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and 3 are graphs of the first ten energy bands with δ values of 0.1, 0.001 and 0.0005, respectively.
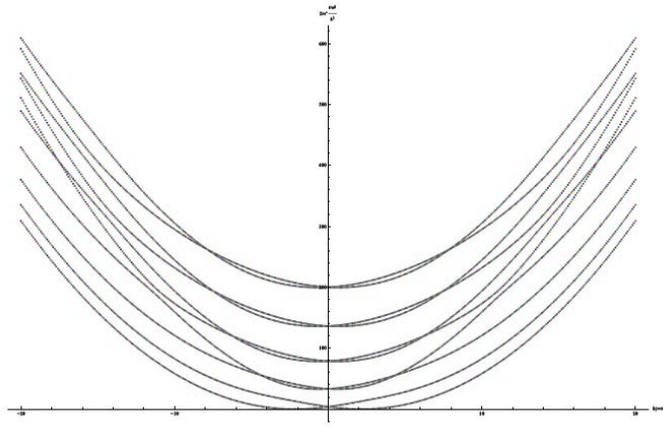
Figure 1: The first ten energy bands of $\frac{2m^*w^2\varepsilon}{\hbar^2}$ vs. $k_y W$ with an X step size of 0.1. This step size was not small enough to take into account the edges of the potential. $\tau_\alpha = 5$, $\tau_\beta = 1$ and $\tau_0 = 1000$. These values remained consistent for Figures 2 and 3 as well. (Plotting E vs. K_y)
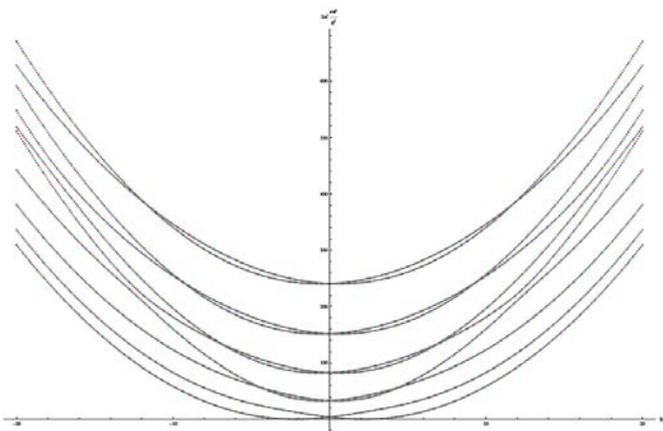
Figure 2: The first ten energy bands with an X step size of 0.001. The bands are much different as our calculation became more accurate. (Plotting E vs. K_y)
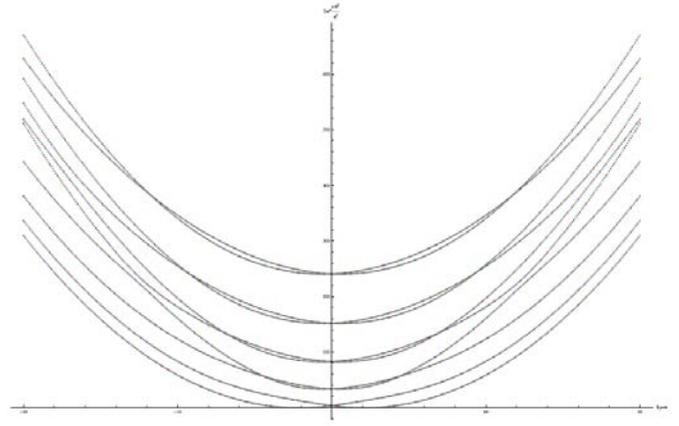
Figure 3: The first ten energy bands with an X step size of 0.0005. This graph and the last graph were very similar as they both take into account change in potential at the edges of the nanowire. (Plotting E vs. K_y)

Possibilities for Further Research

As our step size for X got smaller and smaller, we began to push the boundaries of what our computers could do. Now that we have access to more powerful computers, we would like to get even more accurate approximations by creating larger matrices. We can also now take our eigenvalues and plug them back into our equations and solve for the wave functions of the electrons in the nanowire. This project may aid us in doing similar work on the carbon allotrope graphene. Graphene is a one-atom-thick plane of carbon atoms in a honeycomb-shaped lattice which has become a popular research topic because of its unique conduction properties. We hope to do a similar project on this interesting substance in the near future.

Reference

1. Balassis A, Gumbs G, Huang, D. Energybands, conductance and thermo-electric power for ballistic electrons in a anowire with spin-orbit interaction. *Forthcoming.*