Semiclassical Scattering Through an Obstruction in a Microwire

A thesis submitted in partial fulfillment of the requirement for the degree of Bachelor of Science in Physics from the College of William and Mary in Virginia,

by

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Abstract

We develop a model of electron interference patterns in a partially blocked microwire with a constant, orthogonal magnetic field. We use the semiclassical theory developed by Maslov and Fedorinuk.
I would first like to thank advisor Professor Delos for spending so much time helping me learn about my project finding errors in my program. I would also like to thank Kevin Mitchell for also helping me learn concepts about my project as well as giving me tips on computer programming.
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1 Introduction

The study of semiconductor systems with reduced dimensions has been one of many ways to understand the transition from classical mechanics to the quantum realm. One of the main models used in this regime is the semi-classical theory. This theory in one dimension is the WKB approximation, which was extended to n-dimensions by Maslov and Fedoriuk [1]. The quantum wave is constructed from classical trajectories as described in Appendix C. The semi-classical theory could give a reasonable account when a travelling wave travels classically and encounters an obstacle where quantum effects could take place. The work by Kirczenow et. al. [2] verified experimentally that certain quantum effects occur in a wire-like cavity when a travelling electron wave encounters an impenetrable obstruction in a high constant magnetic field perpendicular to the long axis of the wire. More specifically, they found that the conductance does not vary as the magnetic field is changed except for a region between $0.2T$ and $0.27T$. The paper also states that as the obstruction is changed in height an additional spurt of conductance will show under certain circumstances, and when the obstruction is further changed, the conductance will return to normal. They claim that at high magnetic fields these effects are purely quantum mechanical. In our model the classical wave travels until it encounters the obstruction. The obstruction leaves two small gaps, about 0.2 microns, near the top and bottom of the microwire. Then there will be a portion of the wave that scatters and a portion that conducts through. The basic content of the theory [3] states that when an electron approaches the obstruction or junction most of the electron wave is reflected while some is conducted through one of the gaps. The portion of the wave that goes through is diffracted. Meanwhile the magnetic field pulls the scattered electron wave, which follows classical paths, back towards the junction. If the magnetic field is tuned just right the trajectory will lead the electron through the other gap. Then there are two paths the electron might follow to get past the obstruction, and one would expect to
find an interference pattern on the other side of the junction. The phase is calculated using the classical action of the wave on each path while the wave amplitude is the square root of the classical density. The important assumptions are that the wire should be large compared to the size of the de Broglie wavelength and that the gaps between the barrier and the edges of the wire have a small width compared to the size of the wire.

Our paper describes a theoretical model based on semiclassical theory, which we hope will explain the interference patterns found by Kirczenow. If successful, this will also show that the interference patterns, proposed by Kirczenow to be of a purely quantum nature, can be described by semiclassical methods. Computer simulations will be done using a straight barrier with different magnetic fields. Trajectories and interference patterns will be calculated. These interference patterns will be written in terms of the conductance. Thus the theory can be related to experiment.

2 Model

The Hamiltonian for an electron in a magnetic field is

\[ H_q = \frac{1}{2\mu}( -i\hbar \nabla - q\vec{a})^2 + V, \]

Here \( \mu \) is the effective mass, \( q \) is the electron charge, \( \vec{a} \) is the vector potential, and \( V \) is the potential energy. It can be shown that a particle moving under this Hamiltonian satisfies the Lorentz force equation

\[ \vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) \]

(See Appendix A). For a particle in potential \( V \) a wave function is used with the phase amplitude \( A \) and phase \( S \).

\[ \text{2} \]
\[ \Psi(\mathbf{r}) = A(\mathbf{r})\exp\left(\frac{i}{\hbar}S(\mathbf{r})\right). \] \hfill (3)

When this wave function is substituted in the Hamiltonian without magnetic field and the solution is expanded to 1st order in \( \hbar \) one gets

\[ \frac{\left| \nabla S(\vec{R}) \right|^2}{2\mu} + V(\vec{R}) - E = 0, \] \hfill (4)
\[ 2\vec{\nabla}A \cdot \vec{\nabla}S + \nabla^2SA = 0 \] \hfill (5)

(See Appendix B to get derivation with magnetic field). To find the classical trajectories, Hamilton’s equations and an equation for \( S(\vec{R}) \) (see Appendix C) are used

\[ \dot{p}_i = -\frac{\partial H}{\partial q_i}, \]
\[ \dot{q}_i = \frac{\partial H}{\partial p_i}, \]
\[ \dot{S} = p \cdot \dot{q} = \sum_{i=1}^{n} p_i dq_i / dt. \] \hfill (6)

The amplitude \( A \) comes from the continuity equation, and it can be calculated by

\[ A(\vec{R}) = A_0 \frac{J(0, w^0)}{J(t, w^0)} \] \hfill (7)

where \( J \) is the jacobian, which is defined as

\[ J(t, w^0) = \frac{\partial q(t, w^0)}{\partial (t, w^0)} \] \hfill (8)

[5]. \( q \) is defined as the coordinates in phase space and \( t, w^0 \) are the generalized coordinates.

The wave function of the electron wave is found by adding all the wavefunctions due to the different trajectories at the end of the wire where the current is to be measured. This point will be just far enough away from the obstruction to make sure
the trajectories that reflect back to the entrance do not reach the measured segment. What is needed for the wavefunction determination is the amplitude and the phase at the measured place.

![Trajectories for particle in a magnetic field](image)

Figure 1: A set of trajectories of an electron wave function going through a wire

3 Simulation

The magnetic field needs to be perpendicular to the two dimensional wire. Hence a vector potential that satisfies such a condition would be \( \vec{a} = B_0 \vec{x} \vec{j} \). The trajectories of an electron travelling in a wire with an obstruction and a magnetic field were calculated using a computer simulation. A preliminary understanding of what is going on is done by calculating the transmission amplitude with sample magnetic field strengths applied. We take arbitrary parameters just to show that interference patterns are possible. The wire has width of 2, the charge is 1 and the mass is 1. The magnetic field is also 1. Finally the obstruction has a width of 1.6 centered at 0. The initial conditions are \( y = 0 \) and \( p_x = 1, p_y = 0 \), and \( x = 0.2R \). \( R \) is the cyclotron radius calculated from \( qB = \frac{mv}{R} \). Some trajectories passing through the wire would
In this hypothetical situation, where the wire is the height of the Landau orbits, three main families of trajectories passing through the obstruction are present as shown in Figure 2.

One mode goes right through the lower gap, not touching the obstruction. A second bounces off the obstruction on the left and circles forwards till the electron goes through the other gap. A third mode bounces off both sides of the obstruction creating shapes between the other two modes. The wave amplitude and phase are calculated at the end of the trajectory. The sum of partial wavefunctions calculated from the amplitude and phase is the total wave-function. Then the conductance would be proportional to the square of the wavefunction. The magnetic field will be changed, which will create different eigenvalues. A new conductance will then be calculated. Thus a variation in conductance can be observed as the magnetic field changes. Once interference patterns are shown, parameters that simulate the experiments of Kirczenow et al. will be placed. Hopefully the qualitative results of the experiment will be duplicated.
Table 1: Transition amplitudes as function of magnetic field

<table>
<thead>
<tr>
<th>Magnetic Field</th>
<th>Proportional to Transmission Amplitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.400</td>
<td>2.32</td>
</tr>
<tr>
<td>1.200</td>
<td>0.101</td>
</tr>
<tr>
<td>1.100</td>
<td>0.04129</td>
</tr>
<tr>
<td>1.007</td>
<td>40.186</td>
</tr>
<tr>
<td>1.006</td>
<td>62.99</td>
</tr>
<tr>
<td>1.005</td>
<td>75.71</td>
</tr>
<tr>
<td>1.004</td>
<td>86.4</td>
</tr>
<tr>
<td>1.003</td>
<td>86.84</td>
</tr>
<tr>
<td>1.001</td>
<td>83.20</td>
</tr>
<tr>
<td>1.000</td>
<td>85.41</td>
</tr>
<tr>
<td>0.900</td>
<td>8.91</td>
</tr>
<tr>
<td>0.800</td>
<td>8.04</td>
</tr>
</tbody>
</table>

4 Results

The Transmission amplitude changed as the magnetic field changed (See Table 1).

From the table there may be some hint of interference patterns since the Transmission amplitude goes increases and decreases at some points. Unfortunately the conductance goes up instead of down around the cyclotron frequency, which was not what was found experimentally. Also interference patterns are not at all obvious. A plot of the conductance as a function of magnetic field is shown.

5 Conclusions

The wavefunctions were calculated for different magnetic fields, but no notable interference patterns were found. There was not enough information to tell whether the
Figure 3: Conductance as a function of magnetic field in arbitrary units

semiclassical model compared well with experiment. If anything, it seems that the semiclassical model did not agree with experiment. The model should be improved by adding the hermite polynomials, and adding phase changes due to boundary conditions. Also there were only about 10-30 trajectories going through the obstruction out of about 2000 trajectories. These may not have been enough trajectories. Maybe the step size of the initial x-coordinate should be made smaller.
A Appendix

We show the proof for the x component only since for the other components the proof is done the same way.

\[ \vec{F} = \frac{1}{2\mu} (\vec{P} - q\vec{A})^2 + V \]

\[ = \frac{1}{2\mu} ((P_x - qA_x)i + (P_y - qA_y)j + (P_z - qA_z)k)^2 + V \]

\[ = \frac{1}{2\mu} [(P_x - qA_x)^2 + (P_y - qA_y)^2 + (P_z - qA_z)^2] + V \]

Let \( \nabla \times \vec{A} = \vec{B} \) and \( \vec{E} = -\nabla V - \frac{\partial A}{\partial t} \). We then use hamilton equations, which are defined in the model section of the paper, to calculate the velocity. \( \frac{\partial H}{\partial P_x} = \frac{P_x - qA_x}{\mu} = v_x \)

We see that the momentum has a new meaning from the usual one. We also have

\[ \frac{-\partial H}{\partial x} = \frac{P_x - qA_x}{\mu} (q \frac{\partial A_x}{\partial x}) + \frac{P_y - qA_y}{\mu} (q \frac{\partial A_y}{\partial x}) + \frac{P_z - qA_z}{\mu} (q \frac{\partial A_z}{\partial x}) - \frac{\partial V}{\partial x} \]

\[ = \frac{dP_x}{dt} \]

From the definition of force \( F_x = \mu a_x \). Then

\[ a_x = \frac{dv_x}{dt} = (\frac{dP_x}{dt} - q \frac{dA_x}{dt}) \]

\[ \rightarrow \frac{dA_x}{dt} = \frac{\partial A_x}{\partial x} \frac{dx}{dt} + \frac{\partial A_x}{\partial y} \frac{dy}{dt} + \frac{\partial A_x}{\partial z} \frac{dz}{dt} + \frac{\partial A_x}{\partial t} \]

Now we can find the force using the new found equations from the hamiltonian equations. First we use the chain rule...

\[ F_x = \frac{1}{\mu} (\frac{dP_x}{dt} - q \frac{\partial A_x}{\partial x} \frac{dx}{dt} - q \frac{\partial A_y}{\partial y} \frac{dy}{dt} - q \frac{\partial A_z}{\partial z} \frac{dz}{dt} - q \frac{\partial A_x}{\partial t}) \]

\[ = \frac{q}{\mu} ((\frac{P_x - qA_x}{\mu} (q \frac{\partial A_x}{\partial x}) + \frac{P_y - qA_y}{\mu} (q \frac{\partial A_y}{\partial x}) + \frac{P_z - qA_z}{\mu} (q \frac{\partial A_z}{\partial x}) - \frac{\partial V}{\partial x} \]

\[ - (\frac{\partial A_x}{\partial x} \frac{dx}{dt} + \frac{\partial A_x}{\partial y} \frac{dy}{dt} + \frac{\partial A_x}{\partial z} \frac{dz}{dt} + \frac{\partial A_x}{\partial t})] \]

We now deal with the cross products

\[ \nabla \times \vec{A} = (\frac{\partial}{\partial y} A_z - \frac{\partial}{\partial z} A_y)i + (\frac{\partial}{\partial z} A_x - \frac{\partial}{\partial x} A_z)j + (\frac{\partial}{\partial x} A_y - \frac{\partial}{\partial y} A_x)k \quad (9) \]
and
\[ (\vec{v} \times \vec{B})_x = v_y \left( \frac{\partial}{\partial x} A_y - \frac{\partial}{\partial y} A_x \right) - v_z \left( \frac{\partial}{\partial z} A_x - \frac{\partial}{\partial x} A_z \right) \]

For \( \vec{v} \) we have
\[
\vec{v} = \frac{dx}{dt} \hat{i} + \frac{dy}{dt} \hat{j} + \frac{dz}{dt} \hat{k} = \frac{P_x - qA_x}{\mu} \hat{i} + \frac{P_y - qA_y}{\mu} \hat{j} + \frac{P_z - qA_z}{\mu} \hat{k} \tag{10}
\]

So then the force can be written
\[
F_x = q \left[ (v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_x}{\partial y} + v_z \frac{\partial A_x}{\partial z} - \frac{\partial V}{\partial x}) - (\frac{\partial A_x}{\partial x} v_x + \frac{\partial A_x}{\partial y} v_y + \frac{\partial A_x}{\partial z} v_z + \frac{\partial A_x}{\partial t}) \right]
\]
\[
= q \left[ (v_y \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} v_y) + (v_z \frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} v_z) - (\frac{\partial V}{\partial x} + \frac{\partial A_x}{\partial t}) \right]
\]
\[
= q (\vec{v} \times \vec{B} + qE_x)
\]

B Appendix

The Hamilton-Jacobi equation and the continuity equation are derived as approximations from the Schrodinger equation.

The Hamiltonian is \( H = \frac{1}{2\mu} (-i\hbar \nabla - q\vec{a})^2 + V \) where \( \vec{a} \) is the vector potential.

Assume that \( \Psi = A(\vec{R}) e^{i\frac{S(\vec{R})}{\hbar}} \) then \( \nabla \Psi = (\nabla A e^{i\frac{S(\vec{R})}{\hbar}} + A e^{i\frac{\nabla S(\vec{R})}{\hbar}}) e^{i\frac{S(\vec{R})}{\hbar}} \) So \(-i\hbar \nabla - q\vec{a})\Psi = (-i\hbar (\nabla A + \frac{i}{\hbar} A \nabla S) - Aq\vec{a}) \]) e^{i\frac{S(\vec{R})}{\hbar}} \) Let \( B = (-i\hbar (\nabla A + \frac{i}{\hbar} A \nabla S) - Aq\vec{a}) \) so that \( \nabla B = -i\hbar \nabla^2 A + \nabla (A \nabla S) - \nabla (Aq\vec{a}) \) Thus from the first term of the hamiltonian we get
\[
(-i\hbar \nabla - q\vec{a}) B e^{i\frac{S(\vec{R})}{\hbar}} = \left[ (-i\hbar (\nabla B + \frac{i}{\hbar} B \nabla S) - B q\vec{a}) \right] e^{i\frac{S(\vec{R})}{\hbar}}
\]
\[
= \left[ -\hbar^2 \nabla^2 A - i\hbar \nabla (A \nabla S) + i\hbar \nabla (Aq\vec{a}) - i\hbar A \nabla S \cdot \nabla S - Aq\vec{a} \cdot \nabla S \\
+ i\hbar (\nabla A) q\vec{a} - Aq \nabla S \cdot \vec{a} + Aq^2 |\vec{a}|^2 \right] e^{i\frac{S(\vec{R})}{\hbar}}
\]

Now the semiclassical approximation works when the action is large compared to \( \hbar \), or, equivalently, that the variation of the wave amplitude does not vary much
compared to wave amplitude. Since $\hbar$ is small we do a Taylor expansion centered on this small number. We thus sort in order of $\hbar$

For zeroth order $\frac{1}{2\mu}[A(\nabla S)^2 - Aq\ddot{a} \cdot \nabla S - Aq\nabla S \cdot \dddot{a} + Aq^2 |\ddot{a}|^2] + AV = AE$ Hence if we define $\vec{P} = \nabla S$ then $\frac{1}{2\mu}[\vec{P} - q\dddot{a}]^2 + V = E$

C Appendix

The general procedure for calculating classical trajectories associated with wave functions goes as follows:

1. Define an $n - 1$ dimensional surface in an $n$ dimensional space. This is a surface of constant phase $S(\vec{R})$.

2. At each point on the surface construct a vector normal to the surface with magnitude $\vec{P}(\vec{R})$ where $\frac{\vec{P}(\vec{R})^2}{2\mu} + V(\vec{R}) = E$.

3. A group of points $\vec{P}(\vec{R})$ on the original surface is regarded as a collection of initial conditions. So we have $\vec{P}_0 = \vec{P}(\vec{R})$. We then solve Hamilton’s Equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i},$$
$$\dot{q}_i = \frac{\partial H}{\partial p_i},$$

(11)

with initial conditions $\vec{P}(t = 0) = \vec{P}_0$ and $\vec{R}(t = 0) = \vec{R}_0$.

4. Solve

$$\dot{S} = p \cdot \dot{q} = \sum_{i=1}^{n} p_i dq_i / dt.$$

Now I claim that $\vec{S}(\vec{R})$ satisfies the first hamiltonian equation.

Proof:
I need to show that

$$|\nabla S(\vec{R})| = \sqrt{2\mu(E-V)}$$

We will do better and prove that

$$\nabla S(\vec{R}) = \sqrt{2\mu(E-V)}$$

Now to use differential properties in our space we need uniquely defined quantities. We use the original surface, which has dimensions $n-1$ and $t$ for the last dimension [5]. We have

$$S(\vec{R}_2) = \int_0^{t_2} p \cdot \frac{dR_2}{dt} dt$$
$$S(\vec{R}_1) = \int_0^{t_1} p \cdot \frac{dR_1}{dt} dt$$
$$S(\vec{R}_2) - S(\vec{R}_1) = \int_0^{t_2} p \cdot \frac{dR_2}{dt} dt - \int_0^{t_1} p \cdot \frac{dR_1}{dt} dt$$
$$= \int_0^{t_1} (p \cdot \frac{dR_2}{dt} - p \cdot \frac{dR_1}{dt}) dt + \int_{t_1}^{t_2} p \cdot \frac{dR_2}{dt} dt$$

Since difference in paths are small we use the product rule and we have

$$\int_0^{t_1} \Delta(p \cdot \frac{d\vec{R}}{dt}) dt = \int_0^{t_1} [\Delta p \cdot \frac{d\vec{R}}{dt} + p \cdot \frac{d\Delta \vec{R}}{dt}] dt$$

and

$$p \cdot \frac{d\Delta \vec{R}}{dt} = p \cdot \Delta \vec{R} \bigg|_0^{t_1} - \int_0^{t_1} \Delta \vec{R} \cdot \frac{dp}{dt} dt$$

So

$$\int_0^{t_1} \Delta(p \cdot \frac{d\vec{R}}{dt}) dt = \int_0^{t_1} [\Delta p \cdot \frac{d\vec{R}}{dt} - \Delta \vec{R} \cdot \frac{dp}{dt}] dt$$
$$= \int_0^{t_1} [\Delta p \cdot \frac{\partial H}{\partial p} - \Delta \vec{R} \frac{\partial H}{\partial \vec{R}}] dt$$

Since a surface is defined such that a change in the Hamiltonian is 0 and $\vec{R}$ is perpendicular to the original surface we get

$$p(\vec{R}_f) \cdot (\vec{R}_3 - \vec{R}_1) + p(\vec{R}_2) \cdot (\vec{R}_2 - \vec{R}_3) = p \cdot (\vec{R}_2 - \vec{R}_1)$$
where $\vec{R}_3$ is $R$ in the path between the end of $\vec{R}_1$ and $\vec{R}_2$ as $R$ goes along the surface of constant $S$.

D Appendix

This appendix contains all the programs used. The program $dpodrt.f$ was used, which is a publically available numerical integrator.

PROGRAM 1

Main program

c Calculates poincare’s orbits for a 2-d magnetic field.
c There are nine neqns to calculate wave amplitudes. This program uses
c $dpodrt$ to integrate Hamilton’s equations. Initial conditions
c are $\mu=1, q=1$. The vector potential is $a$ and $a_y = B*x$ where $B$ is
c initial magnitude of magnetic field. Obstruction is added at $5=x$,
c and there are walls at $y=-1, 1$. $y(n)$ are positions $x,y$, momentum
c in the x and y directions and the action respectively for $n=1,2,3,4,5$.
c The magnetic field is $B=1.00$.

c MAIN

c BEGIN

c
IMPLICIT REAL*8(a-h,o-z)
INTEGER kuest, inc
PARAMETER (neqn=5, nw=100+21*neqn, li=3000, pl=2)
DIMENSION y(neqn), yp(neqn), work(nw), iwork(5), val(li,pl)

EXTERNAL hamilton, g, g1, g2

OPEN(11, file='traj.d')
OPEN(13, file='jac.d')
OPEN(15, file='trajpass.d')

! Necessary parameters.
relerr = 1.0D-10
abserr = 1.0D-10
reroot = 100*relerr
aeroot = 100*abserr
ord = 0.00001
B0 = 1.00 ! Value of initial magnetic field. Also defined in hamilton.
kuest = 0
grail = 0
avt = 0
av = 0
inc = 0
step = 0.1 ! Step size of time increments

! Loop for the trajectories where j is the trajectory number.
DO 200 j = 1, 2000

! Initial values

t = 0.
inc = 0
y(1) = 0.001*(j+1) ! x coordinate
y(2) = 0. ! y coordinate
y(3) = 1. ! momentum in x direction
y(4) = B0*y(1) ! momentum in y direction
y(5) = 1. ! initial value of action
coor = 0.001*(j+1) ! x coordinate
coor1 = 0.001*(j+1) + ord ! x coordinate used to calculate the amplitude.
tout = 0.1 ! time step for integration.

Integration of each trajectory where i is the step number.

103 CONTINUE
DO 110 i=1,400
inc = inc + 1
c preval gives value of the x value at one step earlier in time
preval = y(1)
IF (y(1) .lt. -0.1) GO TO 140 ! Trajectory must move forwards
iflag = 1
CALL dpodrt(hamilton,neqn,y,t,tout,relerr,abserr,
* iflag,work,iwork,g,reroot,aeroot)
104 CONTINUE
IF ((iflag .eq. 2 .or. iflag .eq. 7) .and. y(1)
* .ge. 7.999) THEN ! This is where trajectory reaches end of wire
val(inc,1) = y(1)
val(inc,2) = y(2)
x0 = y(1)
y0 = y(2)
GO TO 120
ENDIF

IF (iflag .ne. 2 .and. iflag .ne. 7) THEN
   WRITE (11, 108) iflag, y(1), y(2), y(3), y(4)
   GO TO 120
ENDIF

c
Electron hits a boundary
c

IF(iflag .eq. 7) THEN

c
   WRITE (11,105) t, y(1), y(2), y(3), y(4), iflag
   val(inc,1) = y(1)
   val(inc,2) = y(2)
   iflag = 1

c   Kuest counts the number of passing through abstruction.
c   If kuest is 1 or greater then it is a passed trajectory.

IF(y(1) .gt. 5.) THEN
   kuest = 1
ENDIF

c  Boundary condition for obstruction

IF (y(2) .ge. -0.8 .and. y(2) .le. 0.8) THEN

c Bouncing off obstruction?

   IF(kuest .ge. 1) THEN
      grail = 1
ENDIF

c
vx = y(3)
y(3) = -vx

ENDIF

c Boundary condition for edge of wire
IF (y(2) .lt. -0.8 .or. y(2) .gt. 0.8) THEN
    IF(y(2) .gt. -0.999 .and. y(2) .lt. 0.999) THEN
        c Counts average number of passages through holes
        kuest = kuest + 1
    ELSE
        vy = y(4) - B0*y(1)
y(4) = -vy + B0*y(1)
    ENDIF
ENDIF
ENDIF

tout = tout + 1.0d-01
iflag = 1

c This ensures that electron stays inside wire
CALL dpodrt(hamilton,neqn,y,t,tout,relerr,abserr,
* iflag,work,iwork,g1,reroot,aeroot)
WRITE (11, 105) t, y(1), y(2), y(3), y(4), iflag
tout = tout + step

c
IF(preval .gt. 5. .or. y(1) .lt. 5. .or. (y(2) .lt. 1 .and. y(2) .gt. -1)) GOTO 103

c
ENDIF

c
Sees whether code fails to see boundary going through obstruction
and edge of wire. If it does integration goes back in time and
then forwards with a simpler boundary condition just for edge of wire.
c
IF (preval .lt. 5. .and. y(1) .gt. 5. .and. (y(2) .gt. 1 .or. y(2) .lt. -1)) THEN

   tout = tout - 2*step
   iflag = 1
   CALL dpodrt(hamilton,neqn,y,t,tout,relerr,abserr, * iflag,work,iwork,g1,reroot,aeroot)
   iflag = 1
   tout = tout + step
   CALL dpodrt(hamilton,neqn,y,t,tout,relerr,abserr, * iflag,work,iwork,g2,reroot,aeroot)
   WRITE (11,105) t, y(1), y(2), y(3), y(4), iflag
   val(inc,1) = y(1)
   val(inc,2) = y(2)
   GO TO 104

ENDIF

c
IF (y(2) .lt. -1. .or. y(2) .gt. 1) GO TO 120
WRITE (11,105) t, y(1), y(2), y(3), y(4), iflag
val(inc,1) = y(1)
val(inc,2) = y(2)
105 format (1h ,5g14.7 ,i5)
107 format (1h,i5, 7g14.7)
108 format (’ WARNING. iflag =’, i5, ’ y=’,4g14.7)
    tout = tout + step
    IF (tout .ge. 50.) go to 120

110 CONTINUE

c

120 CONTINUE

c

c Counts in each adjacent trajectory.

c

c Initial values for adjacent trajectory
    y(1) = 0.001*(j+1) + ord
    y(2) = 0.
    y(3) = 1.
    y(4) = B0*y(1)
    t = 0.
    tout = 0.1

c

c
127 CONTINUE

DO 130 i = 1, 400
    preval = y(1)
    IF (y(1) .lt. -0.1) GO TO 140
    iflag = 1
    CALL dpodrt(hamilton,neqn,y,t,tourel,relerr,abserr,
                 * iflag,work,iwork,g,root,aeroot)

128 CONTINUE
IF ((iflag .eq. 2 .or. iflag .eq. 7) .and. y(1) * .ge. 7.999) THEN
   x1 = y(1)
y1 = y(2)
   GO TO 140
ENDIF

IF (iflag .ne. 2 .and. iflag .ne. 7) THEN
   PRINT *, 'WARNING IFLAG = 8'
   GO TO 140
ENDIF

IF (iflag .eq. 7) THEN
  c
  c Boundary condition for abstraction
  IF (y(2) .ge. -0.8 .and. y(2) .le. 0.8) THEN
     vx = y(3)
y(3) = -vx
  ENDIF
  c
  IF (y(2) .lt. -0.8 .or. y(2) .gt. 0.8) THEN
     IF (y(2) .lt. -0.999 .or. y(2) .gt. 0.999) THEN
        vy = y(4) - B0*y(1)
y(4) = -vy + B0*y(1)
     ENDIF
  ENDIF
  tout = tout + 1.0d-01
  iflag = 1
  CALL dpodrt (hamilton, neqn, y, t, tout, relerr, abserr,

19
* iflag, work, iwork, g1, reroot, aeroot

tout = tout + step

c
IF (preval .gt. 5. .or. y(1) .lt. 5. .or. (y(2) .lt. 1 .and. y(2) .gt. -1)) GOTO 127

c
ENDIF

c
IF (preval .lt. 5. .and. y(1) .gt. 5. .and. (y(2) .gt. 1 .or. y(2) .lt. -1)) THEN

tout = tout - 2*step

iflag = 1

CALL dpodrt (hamilton, neqn, y, t, tout, relerr, abserr,
* iflag, work, iwork, g1, reroot, aeroot)

tout = tout + step

iflag = 1

CALL dpodrt (hamilton, neqn, y, t, tout, relerr, abserr,
* iflag, work, iwork, g2, reroot, aeroot)

GO TO 128

ENDIF

c
IF (y(2) .lt. -1. .or. y(2) .gt. 1) GO TO 140

tout = tout + step

IF (tout .ge. 50.) go to 140

c
iflag set to 1 for the next trajectory

iflag = 1

c
Jacobian evaluation

IF (y(1) .ge. 7.999) THEN

delx = (x1-x0)/(coor1 - coor)
dely = (y1-y0)/(coor1 - coor)
ajac = y(3)*dely - (y(4)-B0*y(1))*delx
ampl = 1/SQRT(ABS(ajac))
WRITE (13,107) j,ampl, delx,dely,ajac,y(5), x0, y0
ENDIF

IF(kuest .ge. 1) THEN
    DO 150 dum=1, inc
        WRITE (15, 170) val(dum,1), val(dum,2)
    150    CONTINUE
ENDIF

IF(kuest .gt. 1) THEN
    av = av + kuest
    avt = avt + 1
ENDIF

kuest = 0
grail = 0

format (1h ,5g14.7)
av = (av)/(avt)  
PRINT *, 'number of curvy paths are', avt  
PRINT *, 'Average number of passages through the '  
PRINT *, 'holes before getting through is', av  
235 FORMAT(a)  
  
STOP  
  
END  
  
  
This is hamilton equations  
  
SUBROUTINE hamilton(t, y, yp)  
  
IMPLICIT REAL*8(a-h,o-z)  
PARAMETER (neqn = 9, nw = 100+21*neqn)  
DIMENSION y(neqn), yp(neqn), work(nw), iwork(5)  
  
magnetic field parameter  
  
B0 = 1.00  
  
  
yp(1) = y(3)  
yp(2) = y(4) - B0*y(1)  
yp(3) = B0*(y(4) - B0*y(1))  
yp(4) = 0.  
  

yp(5) = y(3)*yp(1) + y(4)*yp(2)

c
102 format (1h,5(g14.7,2x))
RETURN

c
END

c
This are the boundary conditions used by dpodrt.f

c
FUNCTION g(t, y, yp)

c
IMPLICIT real*8(a-h,o-z)
PARAMETER (neqn = 5, nw = 100+21*neqn)
DIMENSION y(neqn), yp(neqn), work(nw), iwork(5)

c
IF (y(2) .ge. 0.0d0) THEN
   g = (y(2) - 1.)*1.0d4
ENDIF

IF (y(2) .lt. 0.0d0) THEN
   g = -(y(2) + 1.)*1.0d4
ENDIF

IF (y(1) .ge. 4.9) THEN
   g = -(y(1) - 5.)*g
ENDIF

IF (y(1) .ge. 7.999) THEN
   g = -(y(1) - 8.)*g
ENDIF

FUNCTION g1(t, y, yp)
IMPLICIT real*8(a-h,o-z)
PARAMETER (neqn = 5, nw = 100+21*neqn)
DIMENSION y(neqn), yp(neqn), work(nw), iwork(5)

IF (y(2) .ge. 0.0d0) THEN
    g1 = 1.0d0
    ENDIF

IF (y(2) .lt. 0.0d0) THEN
    g1 = 1.0d0
    ENDIF

RETURN
END

FUNCTION g2(t, y, yp)
IMPLICIT real*8(a-h,o-z)
PARAMETER (neqn = 5, nw = 100+21*neqn)
DIMENSION y(neqn), yp(neqn), work(nw), iwork(5)
IF (y(2) .ge. 0.0d0) THEN
  g2 = (y(2) - 1.)*1.0d4
ENDIF
IF (y(2) .lt. 0.0d0) THEN
  g2 = -(y(2) + 1)*1.0d4
ENDIF

RETURN
END

PROGRAM 2

This program reads data pertaining to the wavefunction of the
semiclassical theory. It gets the amplitude and the phase. The files
come from finalprog.f. It then calculates the transition coefficient(conduction)
c by squaring the wavefunction. The first column of the file is the amplitude, an
c the second column is the action.

MAIN

REAL*8 wreal, wim, amp, s, lps
INTEGER iostatus, inc
DIMENSION Amp(3000), S(3000)
OPEN (11,file='mf12.d')
lps = 1666. ! lps is total trajectories which changes as B changes.
inc =0
wreal = 0.
wim = 0.

DO WHILE (iostatus .eq. 0)
    inc = inc + 1
    READ(11,107,iostat=iostatus) j,amp(inc),s(inc),x0,y0,x1,y1
    PRINT *,j,amp(inc),s(inc)
    wreal = wreal+amp(inc)*cos(s(inc))
    wim = wim+amp(inc)*sin(s(inc))
END DO

cond = (wreal*wreal + wim*wim)/lps

107 FORMAT (1h ,i5, 7g14.7)

PRINT *,amp(1),s(1)
PRINT *, 'The conduction is proportional to',cond

END
References


