Semiclassical Scattering Through an Obstruction in a Microwire

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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 Fedoriuk.

Acknowledgements

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.

Contents

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 obtruction 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 buttom 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

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

Here μ 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

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) \tag{2}$$

(See Appendix A). For a particle in potential V a wave function is used with the phase amplitude A and phase S[4],

$$\Psi(\mathbf{r}) = A(\mathbf{r})exp(\frac{i}{\hbar}S(\mathbf{r})). \tag{3}$$

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

$$\begin{aligned} \frac{|\nabla S(\vec{R})|^2}{2\mu} + V(\vec{R}) - E &= 0, && (4) \\ 2\vec{\nabla} A \cdot \vec{\nabla} S + \vec{\nabla}^2 SA &= 0 && (5) \end{aligned}$$

(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

$$\begin{aligned} \dot{p}_i &= \frac{-\partial H}{\partial q_i,} \\ \dot{q}_i &= \frac{\partial H}{\partial p_i,} \\ \dot{S} &= p \cdot \dot{q} = \sum_{i=1}^{n} p_i dq_i/dt. && (6) \end{aligned}$$

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

$$A(\vec{R}) = A_0 \frac{J(0, w^0)}{J(t, w^0)} \tag{7}$$

where J is the jacobian, which is defined as

$$J(t, w^0) = \frac{\partial q(t, w^0)}{\partial(t, w^0)} \tag{8}$$

[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.

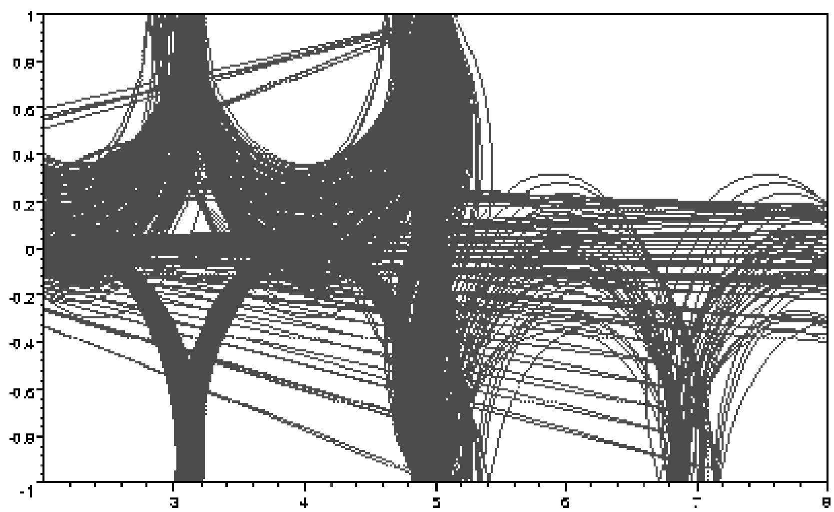

Figure 1: A set of trajectories of an electron wave function going through a wire

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 $\vec{a} = B_0 x \mathbf{j}$. 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

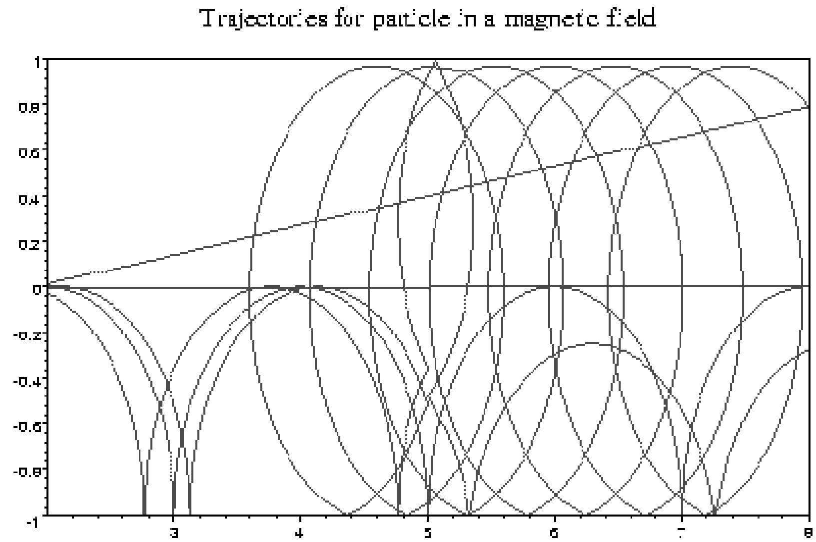

Figure 2: Three main families of trajectories by the electron

look like Figure 1.

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

Magnetic Field	Proportional to Transmission Amplitude
1.400	2.32
1.200	0.101
1.100	0.04129
1.007	40.186
1.006	62.99
1.005	75.71
1.004	86.4
1.003	86.84
1.001	83.20
1.000	85.41
0.900	8.91
0.800	8.04

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 Transission 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

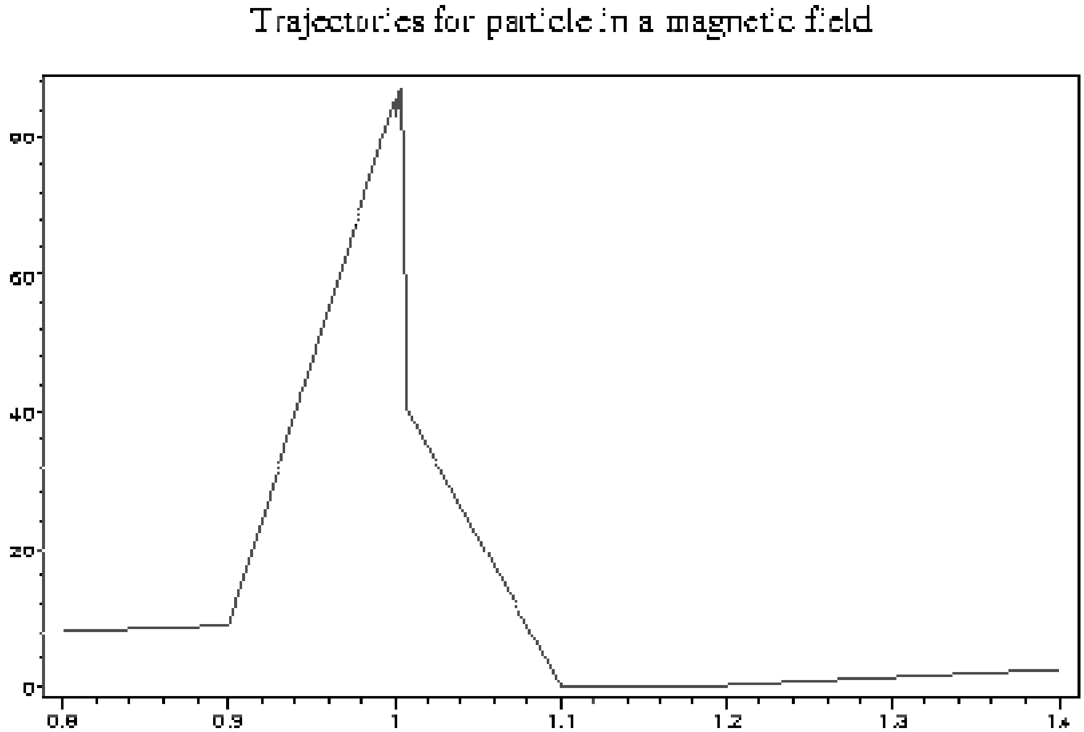

Figure 3: Conductance as a function of magnetic field in arbitrary units

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.

$$\begin{aligned}
\vec{E} &= \frac{1}{2\mu}(\vec{P} - q\vec{A})^2 + V \\
&= \frac{1}{2\mu}((P_x - qA_x)\mathbf{i} + (P_y - qAy)\mathbf{j} + (P_z - qA_z)\mathbf{k})^2 + V \\
&= \frac{1}{2\mu}[(P_x - qA_x)^2 + (P_y - qA_y)^2 + (P_z - qAz)^2] + V
\end{aligned}$$

Let $\nabla \times \vec{A} = \vec{B}$ and $\vec{E} = -\nabla\frac{V}{q} - \frac{\partial A}{\partial t}$ 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

$$\begin{aligned}
\frac{-\partial H}{\partial x} &= \frac{P_x - qA_x}{\mu}(q\frac{\partial A_x}{\partial x}) + \frac{P_y - qA_y}{\mu}(q\frac{\partial A_y}{\partial x}) + \frac{P_z - qA_z}{\mu}(q\frac{\partial A_z}{\partial x}) - \frac{\partial V}{\partial x} \\
&= \frac{dP_x}{dt}
\end{aligned}$$

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

$$\begin{aligned}
a_x &= \frac{dv_x}{dt} = (\frac{dP_x}{dt} - q\frac{dA_x}{dt}) \\
&\longrightarrow \frac{dA_x}{dt} = \frac{\partial A_x}{\partial x}\frac{dx}{dt} + \frac{\partial A_x}{\partial y}\frac{dy}{dt} + \frac{\partial A_x}{\partial z}\frac{dz}{dt} + \frac{\partial A_x}{\partial t}
\end{aligned}$$

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

$$\begin{aligned}
F_x &= \frac{1}{\mu}(\frac{dP_x}{dt} - q\frac{\partial A_x}{\partial x}\frac{dx}{dt} - q\frac{\partial A_x}{\partial y}\frac{dy}{dt} - q\frac{\partial A_x}{\partial z}\frac{dz}{dt} - q\frac{\partial A_x}{\partial t}) \\
&= q[(\frac{P_x - qA_x}{\mu}(q\frac{\partial A_x}{\partial x}) + \frac{P_y - qA_y}{\mu}(q\frac{\partial A_y}{\partial x}) + \frac{P_z - qA_z}{\mu}(q\frac{\partial A_z}{\partial x}) - \frac{\partial V}{\partial x}) \\
&\quad - (\frac{\partial A_x}{\partial x}\frac{dx}{dt} + \frac{\partial A_x}{\partial y}\frac{dy}{dt} + \frac{\partial A_x}{\partial z}\frac{dz}{dt} + \frac{\partial A_x}{\partial t})]
\end{aligned}$$

We now deal with the cross products

$$\nabla \times \vec{A} = (\frac{\partial}{\partial y}A_z - \frac{\partial}{\partial z}A_y)\mathbf{i} + (\frac{\partial}{\partial z}A_x - \frac{\partial}{\partial x}A_z)\mathbf{j} + (\frac{\partial}{\partial x}A_y - \frac{\partial}{\partial y}A_x)\mathbf{k} \tag{9}$$

and

$$(\vec{v}\times\vec{B})_x = v_y(\frac{\partial}{\partial x}A_y - \frac{\partial}{\partial y}A_x) - v_z(\frac{\partial}{\partial z}A_x - \frac{\partial}{\partial x}A_z)$$

For $\vec{v}$ we have

$$\begin{aligned}\vec{v} &= \frac{dx}{dt}\mathbf{i} + \frac{dy}{dt}\mathbf{j} + \frac{dz}{dt}\mathbf{k} \\ &= \frac{P_x - qA_x}{\mu}\mathbf{i} + \frac{P_y - qA_y}{\mu}\mathbf{j} + \frac{P_z - qA_z}{\mu}\mathbf{k} \end{aligned} \tag{10}$$

So then the force can be written

$$\begin{aligned} F_x &= q[(v_x\frac{\partial A_x}{\partial x} + v_y\frac{\partial A_y}{\partial x} + v_z\frac{\partial A_z}{\partial x} - \frac{\partial V}{\partial x}) - (\frac{\partial A_x}{\partial x}v_x + \frac{\partial A_x}{\partial y}v_y + \frac{\partial A_x}{\partial z}v_z + \frac{\partial A_x}{\partial t})] \\ &= q[(v_y\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}v_y) + (v_z\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}v_z) - (\frac{\partial V}{\partial x} + \frac{\partial A_x}{\partial t})] \\ &= q(\vec{v}\times\vec{B} + qE_x) \end{aligned}$$

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 $\Psi = A(\vec{R})e^{\frac{i}{\hbar}S(\vec{R})}$ then $\nabla\Psi = (\nabla A e^{\frac{i}{\hbar}S(\vec{R})} + A\frac{i}{\hbar}\nabla S)e^{\frac{i}{\hbar}S(\vec{R})}$ So $(-i\hbar\nabla - q\vec{a})\Psi = (-i\hbar(\nabla A + \frac{i}{\hbar}A\nabla S) - Aq\vec{a})e^{\frac{i}{\hbar}S(\vec{R})}$ 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

$$\begin{aligned} &(-i\hbar\nabla - q\vec{a})Be^{\frac{i}{\hbar}S(\vec{R})} = [(-i\hbar(\nabla B + \frac{i}{\hbar}B\nabla S) - Bq\vec{a})]e^{\frac{i}{\hbar}S(\vec{R})} \\ = \; &[-\hbar^2\nabla^2 A - i\hbar\nabla(A\nabla S) + i\hbar\nabla(Aq\vec{a}) - i\hbar\nabla A\nabla S + A\nabla S\cdot\nabla S - Aq\vec{a}\cdot\nabla S \\ &+ i\hbar(\nabla A)q\vec{a} - Aq\nabla S\cdot\vec{a} + Aq^2|\vec{a}|^2]e^{\frac{i}{\hbar}S(\vec{R})} \end{aligned}$$

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

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

$$\begin{aligned} \dot{p}_i &= \frac{-\partial H}{\partial q_i,} \\ \dot{q}_i &= \frac{\partial H}{\partial p_i,} \end{aligned} \tag{11}$$

   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

$$\begin{aligned}
S(\vec{R_2}) &= \int_0^{t_2} p \cdot \frac{dR_2}{dt} dt \\
S(\vec{R_1}) &= \int_0^{t_1} p \cdot \frac{dR_1}{dt} dt \\
S(\vec{R_2}) - S(\vec{R_1}) &= \int_0^{t_2} p \cdot \frac{dR_2}{dt} dt - \int_0^{t_1} p \cdot \frac{dR_1}{dt} dt \\
&= \int_0^{t_1} (p \cdot \frac{dR_2}{dt} - p \cdot \frac{dR_1}{dt}) dt + \int_{t_1}^{t_2} p \cdot \frac{dR_2}{dt}
\end{aligned}$$

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

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

So

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

Since a surface is defined such that a change in the Hamiltonian is 0 and 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
c      MAIN
c
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')

c     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.
c     kuest =1 says that it passed 5, grail=1 says that it bounced off obstructio
      kuest = 0
      grail = 0
      avt = 0
      av = 0
      inc = 0
      step = 0.1 !  Step size of time increments
c
c     Loop for the trajectories where j is the trajectory number.
       DO 200 j= 1,2000
c
c    Initial values
c
       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.
c
c
c      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
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
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 though holes
            kuest = kuest + 1
          ELSE
           vy = y(4) - B0*y(1)
           y(4) = -vy + B0*y(1)
          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
c      Sees whether code fails to see boundary going through obstruction
c      and edge of wire.  If it does integration goes back in time and
c      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,tout,relerr,abserr,
     * iflag,work,iwork,g,reroot,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 abstruction
            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,
```

```
     *    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
```

```
 130  CONTINUE
 140  CONTINUE
c
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
c
c
        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
 170    format (1h ,5g14.7)
 200   CONTINUE
c
```

```
      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)
c
      STOP
c
      END
c
c
c   This is hamilton equations
c
      SUBROUTINE hamilton(t, y,   yp)
c
      IMPLICIT REAL*8(a-h,o-z)
      PARAMETER (neqn = 9, nw = 100+21*neqn)
      DIMENSION y(neqn), yp(neqn), work(nw), iwork(5)
c
c     magnetic field parameter
     B0 = 1.00
c
      yp(1) = y(3)
      yp(2) = y(4)-B0*y(1)
      yp(3) = B0*(y(4)-B0*y(1))
      yp(4) = 0.
c
```

```
      yp(5) = y(3)*yp(1) + y(4)*yp(2)
c
 102  format (1h ,5(g14.7,2x))
      RETURN
c
      END
c
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
c
c
      RETURN
      END
c
      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)
c
      IF (y(2) .ge. 0.0d0) THEN
            g1 = 1.0d0
             ENDIF
c
      IF (y(2) .lt. 0.0d0) THEN
         g1 = 1.0d0
          ENDIF
c
      RETURN
      END
c
      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)
c
```

```
       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
c
c
       RETURN
       END
```

PROGRAM 2

```
c      This program reads data partaining to the wavefunction of the
c semiclassical theory. It gets the amplitude and the phase.  The files
c 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, a
c the second column is the action.
c
c     MAIN
c
       REAL*8 wreal,wim, amp, s, lps
       INTEGER iostatus, inc
       DIMENSION Amp(3000), S(3000)
       OPEN (11,file='mf12.d')
c
c     INITIALIZE
```

```
      lps = 1666. ! lps is total trajectories which changes as B changes.
      inc =0
      wreal = 0.
      wim = 0.
c
      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
c
      cond = (wreal*wreal + wim*wim)/lps
c
 107  FORMAT (1h ,i5, 7g14.7)
c
      PRINT *,amp(1),s(1)
      PRINT *, 'The conduction is proportional to',cond
c
c
     END
```

References

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