

Problem Set 5
Physics 480 / Fall 1999
Professor Klaus Schulten

Problem 1: Energies of the Bound States of the Morse Potential in the Semiclassical Approximation

Prove that the semiclassical approximation (Bohr-Sommerfeld quantization condition) applied to the Morse potential

$$U(y) = D[e^{-2ay} - 2e^{-ay}]. \quad (1)$$

reproduces the exact energy values

$$\begin{aligned} E_n &= -D + a\hbar\sqrt{\frac{2D}{m}}\left(n + \frac{1}{2}\right) - \frac{a^2\hbar^2}{2m}\left(n + \frac{1}{2}\right)^2, \\ n &= 0, 1, 2, \dots \leq \frac{\sqrt{2mD}}{a\hbar} - \frac{1}{2}. \end{aligned} \quad (2)$$

Problem 2: Electron at Surface of a Semiconductor

The structure of a metal-oxide semiconductor (MOS) device is usually a metal plate insulated from the surface of the semiconductor by silicon dioxide. From the metal layer, an electrostatic field can be applied in a direction normal to the interface between the semiconductor and oxide insulator. The potential of an electron atop the interface can be approximated by the one-dimensional function

$$U(x) = \begin{cases} \infty, & \text{for } x < 0 \text{ (insulator)} \\ e\mathcal{E}x, & \text{for } x \geq 0 \text{ (semiconductor)} \end{cases} \quad (3)$$

where e is the charge of the electron; \mathcal{E} is the added electric field, which is chosen typically 500 KeV/cm; x is the distance away from the interface.

(a) Determine the energies associated with the stationary states characterized in the semiclassical approximation by the Bohr-Sommerfeld condition.

(b) Show that the exact stationary states of an electron with energy E for $x \geq 0$ are given by

$$\phi_E(x) = \text{const} \times \text{Ai}\left[\sqrt[3]{2me\mathcal{E}/\hbar^2}\left(x - \frac{E}{e\mathcal{E}}\right)\right] \quad (4)$$

where Ai is the Airy function.

The stationary states must also obey the boundary condition

$$\phi_E(0) = 0. \quad (5)$$

Figure 1: There are three sets of materials in the surface layer of MOS transistor. By adding an electric field \mathcal{E} , the electron in the semiconductor region is in a linear potential well.

(c) Employ the `Mathematica` built-in function `AiryAi[x]` to test the accuracy of the semiclassical energies $E_n^{(semi)}$ determined in (a). For that purpose, first plot the *Airy function* $\text{Ai}(x)$, estimate from the plot the first ten solutions x_n of $\text{Ai}(x) = 0$, and use the `Mathematica` built-in function `FindRoot` to evaluate the exact solution for the zeros of the Airy function. Calculate the corresponding energies of the stationary states, compare the resulting energies with those obtained in (a). Plot the percentage error as a function of quantum numbers.

(d) Plot $\phi_{E_n}(x)$ as defined in (??) for $n = 0, 2, 4, 6, 8$ using both the semiclassical energies obtained in (a) and the exact energies obtained in (c).

(e) Calculate for an electron in a stationary state with $n = 0, 1, 2, \dots, 9$ (i) the probabilities to penetrate into the classically forbidden region and (ii) the mean values of x . Plot the results as a function of the quantum numbers n .

Problem 3: Semiclassical Tunneling

Consider the scattering of a particle of mass m and energy E by a potential barrier $U(x)$. We consider a barrier which is localized, i.e., $U(x \rightarrow \pm\infty) = 0$ and assume that there exist a region where E is less than $U(x)$.

In the classical case a particle moving in region I cannot move past the barrier. In quantum mechanics, however, there exist a finite probability that such a particle will tunnel through the barrier. We want to calculate this probability in the semiclassical approximation.

We consider the situation that particles come from the left and that the top

Figure 2: A localized potential barrier. The points $x = a$ and $x = b$ are the turning points, i.e., $U(a) = U(b) = E$. We define the regions: $I = \{x, x < a\}$, $II = \{x, a \leq x \leq b\}$, $III = \{x, b < x\}$.

of the barrier is much higher than the energy of the particles. We expect then that most of the particles will be reflected and only a very small fraction will tunnel through the barrier. Accordingly, the wave function to the left of the barrier will be

$$\psi_I(x) = \frac{d}{\sqrt{k(x)}} \exp\left(i \int_x^a k(x') dx'\right) + \frac{d^*}{\sqrt{k(x)}} \exp\left(-i \int_x^a k(x') dx'\right) \quad (6)$$

where $k(x) = \sqrt{2m(E - U(x))/\hbar^2}$, $x = a$ is the left turning point, i.e., $U(a) = E$, d is an arbitrary constant and the asterisk $*$ denotes the operation of complex conjugation.

(a) Show that for wave function (??) the reflected current is equal to the incident current.

For $d = \frac{c}{2i} \exp(i\pi/4)$ wave function (??) can be written

$$\psi_I(x) = \frac{c}{\sqrt{k(x)}} \sin\left(\int_x^a k(x') dx' + \frac{\pi}{4}\right) \quad (7)$$

Below you will see that this peculiar choice of d is convenient.

(b) Using the definition of regions I and II in the caption of Fig.1 prove

that the form of the wave function in region II is

$$\psi_{II}(x) = \frac{c}{2\sqrt{|k(x)|}} \exp\left(\int_a^x -|k(x')| dx'\right). \quad (8)$$

For this purpose follow the derivation presented in class. Approximate $U(x)$ near $x = a$ as $U(x) \approx U_a(x) = E + F_a(x - a)$. A solution of the corresponding Schrödinger equation for $U(x) = U_a(x)$ is

$$\psi_{I,II}(x) = c' \text{Ai}\left[\left(\frac{2mF_a}{\hbar^2}\right)^{1/3} (x - a)\right], \quad (9)$$

where $\text{Ai}(z)$ is the regular Airy function. You will need to use the asymptotic properties of $\text{Ai}(\pm z)$ given in (??) and (??) below to show that $\psi_{I,II}(x)$ smoothly connects to (??) as well as to (??).

(c) Argue why the wave function in region III has the form

$$\psi_{III}(x) = \frac{d'}{\sqrt{k(x)}} \exp\left(i \int_b^x k(x') dx'\right) \quad (10)$$

For later convenience we will substitute $d' = g \exp(i\pi/4)$ and rewrite (??) as

$$\psi_{III}(x) = \frac{g}{\sqrt{k(x)}} \exp\left(i \int_b^x k(x') dx' + i\frac{\pi}{4}\right) \quad (11)$$

In order to connect wave function (??) to (??) and thereby determine the constant g we will apply a similar type of argument as applied for the connection of (??) and (??). For this purpose we consider the wave function near the right turning point $x = b$. We approximate $U(x) \approx U_b(x) = E + F_b(b - x)$, $F_b > 0$. A solution of the corresponding Schrödinger equation for $U(x) = U_b(x)$ is

$$\psi_{II,III}(x) = c'' \text{Ai}\left[\left(\frac{2mF_b}{\hbar^2}\right)^{1/3} (b - x)\right] \quad (12)$$

It is important to note here that there exists another solution of the Schrödinger equation for $U(x) = U_b(x)$, namely the irregular Airy function which is linearly independent of (??)

$$\psi_{II,III}(x) = c''' \text{Bi}\left[\left(\frac{2mF_b}{\hbar^2}\right)^{1/3} (b - x)\right] \quad (13)$$

(d) Use `Mathematica` to plot $Ai(z)$ and $Bi(z)$. The built-in functions are called `AiryAi[z]` and `AiryBi[z]` respectively. The asymptotic behavior of $Bi(z)$ is given in (??) and (??) below.

(e) Why is

$$\psi_{II,III}(x) = g \left(\text{Bi} \left[\left(\frac{2mF_b}{\hbar^2} \right)^{1/3} (b-x) \right] + i \text{Ai} \left[\left(\frac{2mF_b}{\hbar^2} \right)^{1/3} (b-x) \right] \right) \quad (14)$$

also a solution of the Schrödinger equation? Show that (??) smoothly connects to (??) for $x \rightarrow \infty$.

(f) Prove that for the choice

$$g = \frac{c}{2} \exp \left(- \int_a^b |k(x)| dx \right) \quad (15)$$

one can smoothly connect (??) to (??). (Note that in region *II* the contribution of $Ai(z)$ to (??) can be neglected.) Now we have expressed the wave function in *I*, *II* and *III* in terms of a single multiplicative constant c .

(g) Show that the transmission coefficient $T = j_t/j_i$, where j_t is the current of the transmitted particles and j_i is the current of the incident particles, is given by

$$T = \exp \left(-2 \int_a^b |k(x)| dx \right) \quad (16)$$

(h) Calculate the transmission coefficient $T = T(E)$ as a function of the energy E of incoming particles of mass m , scattered by a potential

$$U(x) = \begin{cases} 0, & \text{for } x < -a \\ U_0 - \alpha x^2, & \text{for } -a < x < a, \quad a = \sqrt{U_0/\alpha} \\ 0, & \text{for } a < x \end{cases} \quad (17)$$

where U_0 and α are constants. Plot $T(E/U_0)$ using `Mathematica` for $\alpha = 2mU_0^2/\hbar^2$.

Here we give the asymptotic form of $Ai(z)$ and $Bi(z)$ for $z \rightarrow \pm\infty$. For $z \rightarrow +\infty$, ($\xi = \frac{2}{3}z^{3/2}$)

$$Ai(z) \approx \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-\xi} \quad (18)$$

$$Bi(z) \approx \pi^{-1/2} z^{-1/4} e^{\xi} \quad (19)$$

For $z \rightarrow -\infty$, ($\xi = \frac{2}{3}(-z)^{3/2}$)

$$Ai(z) \approx \pi^{-1/2} (-z)^{-1/4} \sin\left(\xi + \frac{\pi}{4}\right) \quad (20)$$

$$Bi(z) \approx \pi^{-1/2} (-z)^{-1/4} \cos\left(\xi + \frac{\pi}{4}\right) \quad (21)$$

The problem set needs to be handed in by Tuesday, October 26.
The web page of Physics 480 is at
<http://www.ks.uiuc.edu/Services/Class/PHYS480/>