

Problem Set 6
Physics 480 / Fall 1999
Professor Klaus Schulten

Problem 1: The Group SO(3)

Do exercises 5.1.1 through 5.2.3 in the notes "Theory of Angular Momentum and Spin".

Problem 2: Two-dimensional Potential Well with Variable Width

Consider an electron in a plane which contains regions $D_i, i = 1, 2, 3$ of dimensions L_i and H_i with $L_1 = L_3 = 20\text{\AA}$, $L_2 = 3.75\text{\AA}$, $H_1 = H_3 = 2H_2 = 8\text{\AA}$ (see Fig.1). The electron experiences the potential

$$V(\vec{x}) = \begin{cases} 0 & \text{for } \vec{x} \in D = D_1 \cup D_2 \cup D_3 \\ \infty & \text{else} \end{cases} \quad (1)$$

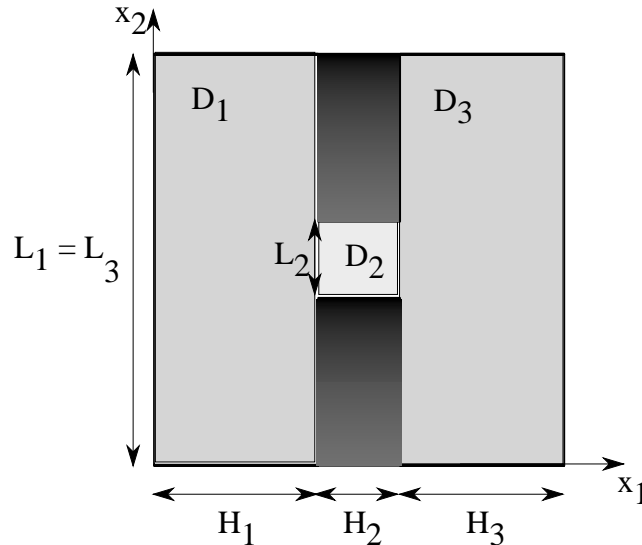


Figure 1: Two-dimensional Potential Well with Variable Width

We would like to describe electron transfer from region D_1 into region D_3 through region D_2 .

(a) First, compute the energy levels and eigenstates in each of the boxes D_j under the assumption that the electron experiences the potential

$$V_j(\vec{x}) = \begin{cases} 0 & \text{for } \vec{x} \in D_j \\ \infty & \text{else} \end{cases} \quad (2)$$

Show that in the case of potentials (2) the eigenfunctions of an electron in each of the regions D_j

are given by

$$\psi_{n_1, n_2}^{(j)}(x_1, x_2) = \phi_{n_1}^{(j)}(x_1; H_j) \phi_{n_2}^{(j)}(x_2; L_j), \quad (3)$$

where $\phi_n(x; a)$ describes the eigenstate of a particle in a one-dimensional box of length a . Determine the corresponding energies $E_{n_1, n_2}^{(j)}$.

(b) Now consider the motion of an electron under the influence of potential (1). Assume the electron to be in an initial state

$$\psi(x_1, x_2, t = 0) = \begin{cases} \psi_{n_1, n_2}^{(1)}(x_1, x_2) & \text{for } (x_1, x_2) \in D_1 \\ 0 & \text{else} \end{cases} \quad (4)$$

Provide the explicit form for the initial function.

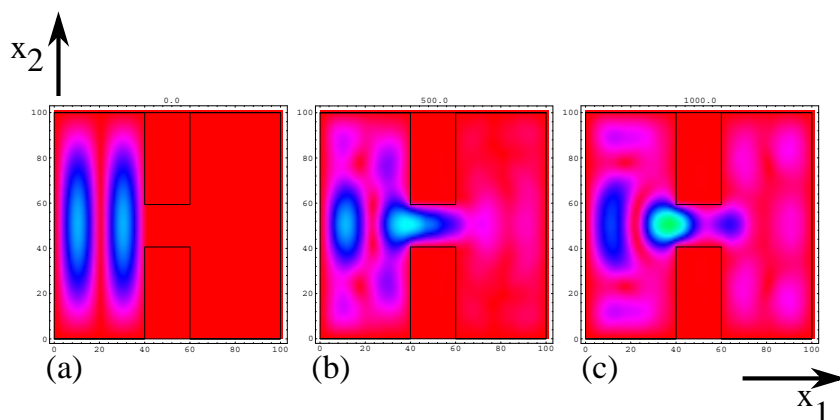


Figure 2: Absolute value of $\psi(x_1, x_2, t)$ at $t = 0, 1.5 \times 10^{-15} s$, and $3 \times 10^{-15} s$ corresponding to the initial values $n_1 = 2, n_2 = 1$. The units in the graph correspond to a box of size 20 \AA .

(c) Figures 2a,b,c show the absolute value of the wavefunction $\psi(x_1, x_2, t)$ at time $t = 0$ (a), $t = 1.5 \times 10^{-15} s$ (b), $t = 3 \times 10^{-15} s$ (c), for $n_1 = 2$ and $n_2 = 1$ in the initial state as given by (4). What prevents the particle described by $\psi(x_1, x_2, t)$ to freely propagate across D_2 ? (Hint: Compare the energy eigenvalues for the eigenstates $\psi_{n_1, n_2}^{(j)}(x_1, x_2)$ for each D_j to the energy of the initial state $\psi(x_1, x_2, t = 0)$. Note, that for the region D_2 only the x_2 degree of freedom is relevant, since there is no wall restriction in the direction of x_1 for this region.)

Figures 3a,b,c show the absolute value of the wavefunction $\psi(x_1, x_2, t)$ at time $t = 0$ (a), $t = 7.5 \times 10^{-16} s$ (b), $t = 1.5 \times 10^{-15} s$ (c), for $n_1 = 3$ and $n_2 = 1$ in the initial state as given by (4). For this case, you can follow visually the time evolution of the amplitude of the wave function of the particle, by using the animation feature of *Mathematica*, in the notebook provided on the course website. The snapshots were obtained by numerically solving the corresponding time-dependent 2D Schrödinger equation.

Explain why in case of Fig.3 the particle crosses region D_2 very easily.

The probability $P(D_3)$ of finding the particle in the area D_3 as a function of time for $n_1 = 2, n_2 = 1$ and for $n_1 = 3, n_2 = 1$ is given graphically in Fig. 4. The plots were obtained by using the numerical solution to the corresponding Schrödinger equation.

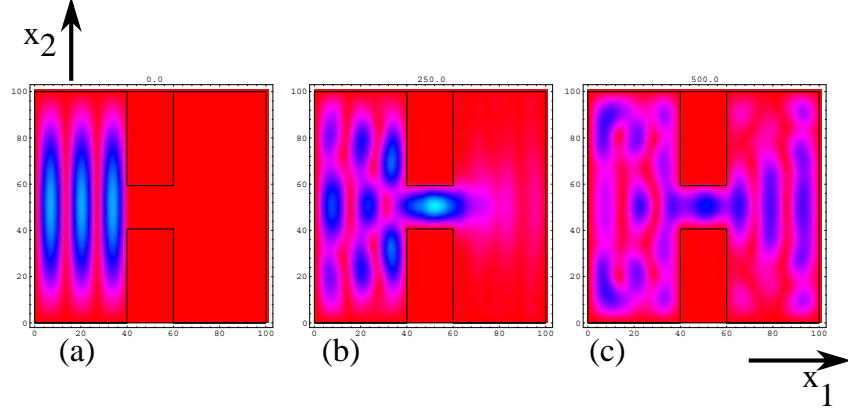


Figure 3: Absolute value of $\psi(x_1, x_2, t)$ at $t = 0, 7.5 \times 10^{-16} s$, and $1.5 \times 10^{-15} s$ corresponding to the initial values $n_1 = 3, n_2 = 1$. The units in the graph correspond to a box of size 20 \AA .

By using the data in Fig. 4, calculate (approximately) and plot the rate $K(t) \equiv dP(D_3)/dt$ for the transition from D_1 to D_3 .

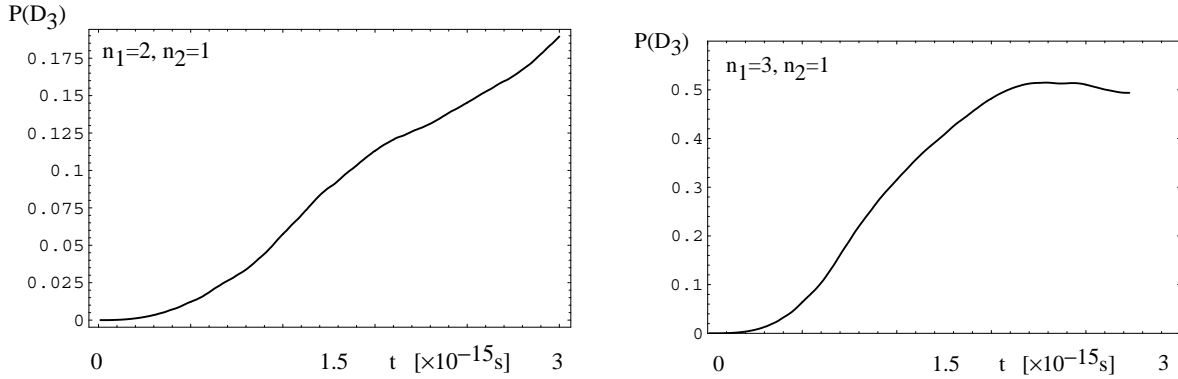


Figure 4: Time dependence of the probability of finding the particle in the region D_3

(d) In the case of low excitations in region D_1 the transfer to region D_3 occurs through tunneling. In this case one can use a simple 1-dimensional approximation and apply the quasiclassical tunneling theory which gives for the tunneling rate K

$$K \approx \nu \exp \left[-\frac{2}{\hbar} \int_{x_1=H_1}^{x_1=H_1+H_2} \sqrt{2m_e(U - E)} dx_1 \right]. \quad (5)$$

Here E is the total energy of a particle initially located in region D_1 . U is the height of the barrier which equals the energy of the ground state of a particle in area D_2 . ν can be estimated according to the formula

$$\nu \approx \frac{n_1 \hbar \pi}{2mH_1^2}. \quad (6)$$

Compute K analytically for $n_1 = 2$ and $n_2 = 1$ using the formula given above and compare it with the results obtained at (c).

The problem set needs to be handed in by Tuesday, November 2.

The web page of Physics 480 is at <http://www.ks.uiuc.edu/Services/Class/PHYS480/>