Quantum dynamics, NWI-SM295, computer assignment 2

Gerrit C. Groenenboom, theoretical chemistry, Radboud University Nijmegen, 22-May-2012

Question 1: Tunneling through the Eckart barrier

In 1930, Carl Eckart reported an analytic solution for the reflection coefficient for an electron tunneling through a one-dimensional potential of the form [1]

$$V(x) = -A\frac{\xi}{1-\xi} - B\frac{\xi}{(1-\xi)^2}, \text{ with } \xi = -e^{2\pi x/l}. \tag{1}$$

Here, we will study the problem numerically for these parameters:

$$l = 1 \tag{2}$$
$$A = 0 \tag{3}$$
$$B = 10 \tag{4}$$

1a. Plot the potential $V(x)$ for x in the interval $[-10, 10]$.

The Hamiltonian for this problem

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x), \tag{5}$$

where the mass of the electron in atomic units $\mu = 1$. The Schrödinger equation for the scattering wave function $\Psi_E(x)$ at energy E is given by

$$(\hat{H} - E)\Psi_E(x) = 0 \tag{6}$$

The boundary conditions for an incoming electron from the left are

$$\Psi(x) = \begin{cases} \sim e^{ikx} + e^{-ikx}R & \text{for } x \ll 0 \\ \sim e^{ikx}T & \text{for } x \gg 0 \end{cases} \tag{7}$$

1b. Write a program to compute the wave function $\Psi(x)$ on a grid. Choose an equally spaced grid for the interval $[-10, 10]$ with a step size of $\Delta = 0.1$.

1c. Plot the real and the imaginary part together with the potential (scale Ψ to make the amplitude of Ψ about the same as the maximum of the potential).

1d. Determine R (complex!) and the reflection coefficient $|R|^2$.

1e. Compute the reflection coefficient $|R|^2$ for a range of energies: $0 < E < 5$ and plot the result

1f. Repeat the calculation with the step size reduced to $\Delta = 0.05$ to check convergence of the result.

References

[1] C. Eckart, Phys. Rev. **35**, 1303 (1930).