Quantum Molecular Dynamics **Autumn 2001-2002**

Project 3

I. REFLECTION AND TRANSMISSION COEFFICIENTS FROM WAVEPACKET AUTOCORRELATION FUNCTIONS

1. Program name:ref_tra_a.m
2. What program does: Calculates the reflection and transmission coefficients, R(E) and T(E), for a 1-d asymmetric Eckart potential via three different methods. The Eckart potential is:

$$V(x) = -V_1\xi/(1-\xi) - V_0\xi/(1-\xi)^2, \tag{1}$$

where $\xi = -e^{(x-q_0)/a}$.

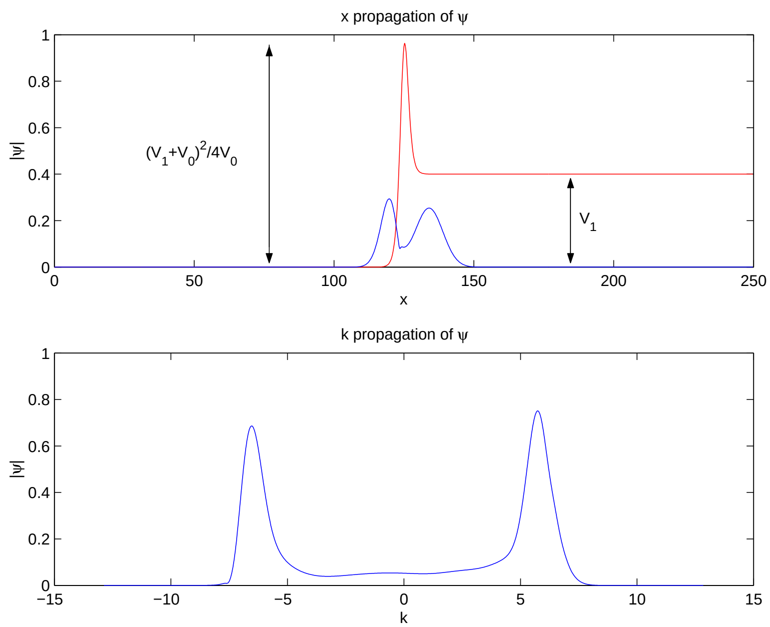

FIG. 1: Wavepacket traversing Eckart barrier in real and fourier space.

(a) **Calculation via wavepacket autocorrelation functions**
The first method calculates R(E) and T(E) by first calculating a 'spectrum' for the incident, reflected and transmitted wavepackets via Fourier transform of their respective autocorrelation functions:

$$\begin{aligned}
\sigma_R(E) &= \int_{-\infty}^{\infty} C_R(t)e^{iEt/\hbar}dt \quad \text{(spectrum of reflected wp)} \\
\sigma_T(E) &= \int_{-\infty}^{\infty} C_T(t)e^{iEt/\hbar}dt \quad \text{(spectrum of transmitted wp)} \\
\sigma_I(E) &= \int_{-\infty}^{\infty} C_I(t)e^{iEt/\hbar}dt \quad \text{(spectrum of incident wp)}
\end{aligned}$$

The reflection and transmission coefficients are then computed as the ratio of the spectra of the reflected/transmitted wavepacket to that of the incident wavepacket:

$$R(E) = \sigma_R(E)/\sigma_I(E); \quad \text{(reflection coefficient)} \tag{2}$$
$$T(E) = \sigma_T(E)/\sigma_I(E); \quad \text{(transmission coefficient)} \tag{3}$$

(Note that both $0 \leq T(E), R(E) \leq 1$).

(b) **Calculation via overlap of the reflected and transmitted wavepackets with plane waves** The second method calculates $R(E)$ and $T(E)$ via overlap of the reflected and transmitted wavepackets with energy normalized plane waves that are outgoing in the reactant/product channel, respectively.

$$R(E(k)) = \frac{|<\psi_{-k}(E)|\Psi_R>|^2}{|<\psi_k(E)|\Psi>|^2} = \frac{|\int_\infty^\infty \Psi_R(x,t)e^{ikx}dx|^2}{|\int_\infty^\infty \Psi(x,t)e^{-ikx}|^2} \quad (eq.7.19)$$

$$T(E(k')) = \frac{k}{k'}\frac{|<\psi_{k'}(E)|\Psi_T>|^2}{|<\psi_k(E)|\Psi>|^2} = \frac{k}{k'}\frac{|\int_\infty^\infty \Psi_T(x,t)e^{-ik'x}dx|^2}{|\int_\infty^\infty \Psi(x,t)e^{-ikx}|^2}. \quad (eq.7.21),$$

where

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2(-k)^2}{2m} = V_0 + \frac{\hbar^2 k'^2}{2m}. \tag{4}$$

(c) **Analytical expressions for $R(E)$, $T(E)$ for the Eckart potential.** The analytic expressions for the reflection and transmission coefficients are:

$$R(E) = A/B, \quad T(E) = 1 - R(E), \tag{5}$$

where

$$A = \cosh(2\pi(\alpha-\beta)) + \cosh(2\pi\delta) \tag{6}$$
$$B = \cosh(2\pi(\alpha+\beta)) + \cosh(2\pi\delta) \tag{7}$$

where $\alpha = 1/2\sqrt{E/C}$, $\beta = 1/2\sqrt{(E-V_1)/C}$, $\delta = 1/2\sqrt{(V_0-C)/C}$, and $C = a^2/8$.

3. References in text: Section 7.1a,b.

4. Assignments:

   (a) Check eqs. 7.91, 7.92 against your numerical results. Are the transmitted and reflected wavepackets approximate replicas (scaled and unscaled respectively) of the incident wavepacket?

   (b) Show numerically that the transmission coefficient, $T(E)$, is identical for a wavepacket incident from the left or from the right. (This property is discussed in two places in the text: a) below exerc. 7.2; b) exerc. 7.6b.

   (c) Replace the Eckart potential in the program by a symmetric double-barrier potential of the type in Ex. 7.eoc.6. Show numerically that near the energies of quasibound states of the region between the barriers, there is an energy of 100% transmission, as discussed in Ex. 7.eoc.6.

   (d) Replace the Eckart potential in the program by a cosine potential with 10 wavelengths, constant everywhere else. Watch the behavior of the wavepacket as parts of it migrate from well to well. Calculate $R(E)$ and $T(E)$, and try to correlate features in these quantities with the dynamics. Explore the dependence on well depth and wavelength.

II. SCATTERING AMPLITUDES VIA WAVEPACKET CROSS-CORRELATION FUNCTIONS

1. Program name: ref_tra_b.m

2. What program does: Program ref_tra_b.m calculates the 4 elements of the scattering matrix for one-dimensional barrier scattering.

$$S_{\alpha\alpha}(E) = \frac{(2\pi\hbar)^{-1}}{\eta(E)\eta^*(E)}\int_\infty^\infty <\phi_\alpha^-|e^{-iHt/\hbar}|\phi_\alpha^+> e^{iEt/\hbar}dt \tag{8}$$

and

$$S_{\beta\alpha}(E) = \frac{(2\pi\hbar)^{-1}}{\eta(E)\mu^*(E)}\int_\infty^\infty <\phi_\beta^-|e^{-iHt/\hbar}|\phi_\alpha^+> e^{iEt/\hbar}dt \tag{9}$$

and similarly $S_{\alpha\beta}$ and $S_{\beta\beta}$.

As opposed to the autocorrelation function approach in the previous project, which gives only scattering *probabilities*, i.e. reflection and transmission coefficients, the cross-correlation approach gives scattering *amplitudes*.

3. References in text: Ch. 7.2, Ch. 18

4. Assignments:

   (a) **Symmetry of the S-matrix**
   Use ref_tra_b.m to calculate the four elements of the S-matrix for scattering from a simple step function. Verify that the S-matrix is symmetric and unitary, i.e. that $S_{\alpha\beta} = S_{\beta\alpha}$, and that the rows and columns of the S-matrix are orthonormal.

   (b) **Reflection and Transmission Coefficients**
   Note that for a wavepacket incident from the right,

$$R(E) = |S_{\alpha\alpha}(E)|^2 \tag{10}$$

$$T(E) = |S_{\beta\alpha}(E)|^2 \tag{11}$$

   Compare the reflection and transmission coefficients for the step potential, calculated using ref_tra_b.m with those calculated using the autocorrelation function approach in the previous project (ref_tra_a.m).

III. SCATTERING AMPLITUDES VIA TIME-INDEPENDENT QUANTUM MECHANICS; PHASE SHIFTS AND TIME DELAY

1. Program name: wall_well.m, double_barrier.m (two_wells_boundary.m is a utility function that you will need as well, that matches the plane wave and its first derivative at a position where the potential is discontinuous.)

2. What program does: Calculates reflection and transmission amplitudes $r(k)$ and $t(k')$, respectively, using time independent quantum mechanics. (two_well_boundary.m can be used for a simple step potential (A); wall_well.m is single barrier separated by a well from a wall (B), double_barrier.m is a symmetric double barrier (C).)

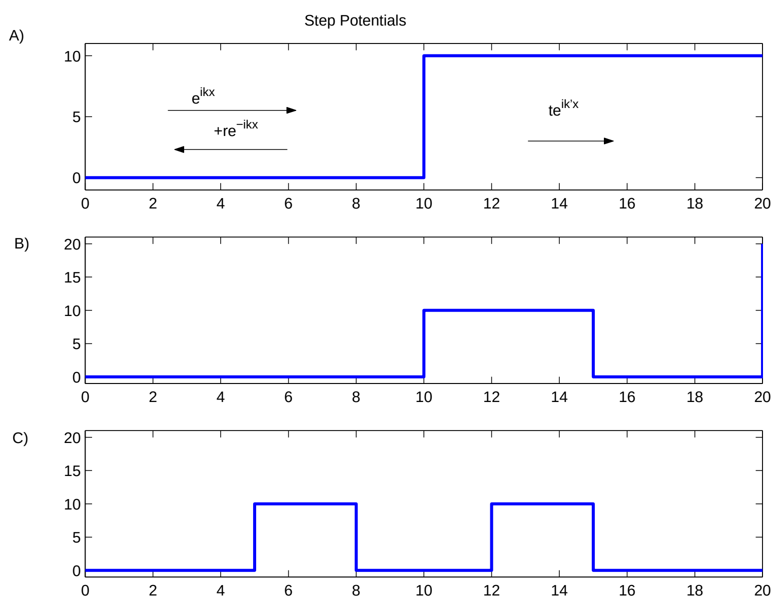

FIG. 2: The three different scattering potentials referred to for this project.

3. References in text: Sections 7.3-7.5

4. Assignments:

   (a) **Symmetry of the scattering amplitudes**
   Calculate the reflection and transmission coefficients for the step potential from two_wells_boundary.m for a wave incident both from the left and from the right. (For an incident wave from the left, implement

two_wells_boundary.m starting from the RIGHT, with amplitudes (1, 0); after solving the equations at the boundary, divide through by the coefficient of e^{ikx} to get the values of t and r. Make the appropriate substitutions for an incident wave from the right.) Verify the symmetry rules eqs. 7.67-7.70. Calculate the four S-matrix elements for the same potential from ref_tra_b.m, and compare with the time-independent calculation. Use the relations $S_{\alpha\alpha} = r$, $S_{\beta\alpha} = \sqrt{\frac{k'}{k}}t$, $S_{\alpha\beta} = \sqrt{\frac{k}{k'}}t'$, $S_{\beta\beta} = r'$.

(b) **Resonances and Time Delay**
Consider the potentials in fig. 7.7 and in ex. 7.eoc.6. Calculate the phase shift, χ, as a function of energy, using both ref_tra_b.m and wall_well.m (or double_barrier.m). Note the dramatic changes in phase shift around the energies of quasibound states of the potential. Use eq. 7.104 to calculate the time delay, τ, as a function of energy. Compare your result with the one you obtain from the following standard formula for the time delay: the expression:

$$\tau(E) = -i\hbar(S^{\dagger}(E)\frac{d}{dE}S(E)). \tag{12}$$

where $S(E) = e^{i\chi(E)}$.