WAVE PROPAGATION

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1. **A square barrier.** In this first task you test the transfer and scattering matrix methods on a standard textbook problem, the square potential barrier. Start from the one-dimensional Schrödinger equation

$$E\psi(x) + \frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - V(x)\psi(x) = 0; \quad x \in (-\infty;\infty).$$

We use scaled units $\lambda = E/V_0$, $y = x/x_0$, with $x_0 = \hbar/\sqrt{2mV_0}$, and $W(y) = V(x)/V_0$ to obtain

$$\lambda\psi(y) + \frac{d^2\psi(y)}{dy^2} - W(y)\psi(y) = 0; \quad y \in (-\infty;\infty).$$

Define a square potential barrier: $W(y) = 1;\ -\frac{1}{2}a \leq y \leq \frac{1}{2}a;\ \ W(y) = 0;\ y < -\frac{1}{2}a$ or $y > \frac{1}{2}a$. The analytical expression for the transmission of a wave is given by[1]

$$T_{\text{ana}}(\lambda) = \left[1 + \left(\frac{k^2+\eta^2}{2k\eta}\right)^2 \sinh^2(\eta a)\right]^{-1}; \quad k = \sqrt{\lambda};\ \eta = \sqrt{1-\lambda};\ 0 < \lambda < 1.$$

(a) *Description:* Choose $a = 1$. Using the *transfer matrix algorithm*, calculate the transmission $T(\lambda)$ for $0 < \lambda < 1$ and compare it to results obtained with the analytical expression $T_{\text{ana}}(\lambda)$.
Deliverables: A plot of $T(\lambda)$, compared with $T_{\text{ana}}(\lambda)$, and a small discussion.

(b) *Description:* The transfer matrix not only gives access to the transmission, but also to the reflection, as well as to the transmission and reflection of a wave coming from the right side of the barrier,. However, not all these quantities will be equally accurate due to an intrinsic numerical instability in the transfer matrix method (LN Sec. 2.3).[2] For instance, the transmission coefficients of a wave coming from the left and from the right of the barrier are given respectively by

$$T = \frac{1}{|M_{11}|^2} \quad \text{and} \quad T' = \left|M_{22} - \frac{M_{21}M_{12}}{M_{11}}\right|^2,$$

in terms of the matrix elements of the transfer matrix, see LN Eqs. 20, 21, 27 and 31, and Fig. 4.
To investigate this in more detail, choose $\lambda = 0.01$ and calculate the transmission

[1] See Griffiths, problem 2.32.
[2] LN stands for "lecture notes".

$T(a)$ with the transfer matrix method as a function of barrier thickness a with $0 < a < 30$. Now calculate $T'(a)$ using the same transfer matrix over the same range of a. Plot $T(a)$ and $T'(a)$ on a logarithmic scale. Ideally the two should be idential because of symmetry. Are they?
Deliverables: A logarithmic plot of $T(a)$ and $T'(a)$ (the function "semilogy" in matlab). Why should ideally the two be identical? Discuss why they are not in this case.

(c) *Description:* Alternatively, one can use the scattering matrix, and the composition rule for scattering matrices, LN Eqs. 34, 40. The transmission coefficients in terms of the matrix elements of the scattering matrix are given by

$$T = |S_{21}|^2 \quad \text{and} \quad T' = |S_{12}|^2 \,,$$

see LN Eqs. 42 and 46. Repeat (b), but calculate $T(a)$ and $T'(a)$ using the scattering matrix approach.
Deliverables: A logarithmic plot of $T(a)$ and $T'(a)$. What is different from (b)? Discuss why this is.

(d) *Description:* Choose $\lambda = 0.5$ and repeat the calculations of (b) using the transfer matrix method.
Deliverables: A logarithmic plot of $T(a)$ and $T'(a)$. What is different from (b)? Discuss why this is. Which method do you recommend for calculating the transmission and why?

2. **A distorted barrier.** The second task deals with barriers that are triangularly distorted. There is some physics in this shape. Applying an electric field $\mathcal{E} = \Delta V/a$ across a square barrier of height V_1, it obtains a slope, and becomes $W(y) = V_1 - \mathcal{E}\left(y + \frac{1}{2}a\right);\ -\frac{1}{2}a \leq y \leq \frac{1}{2}a;\quad W(y) = 0;\ y < -\frac{1}{2}a\quad W(y) = -\mathcal{E}a;\ y > \frac{1}{2}a$.

   (a) *Description:* Choose $V_1 = 1$, $a = 1$, $\Delta V = 0.5$ and $\lambda = 0.5$. The task is to find a minimal y-grid that converges the transmission to within 10^{-5}. Try the midpoint rule.
   Deliverables: A description of the minimal y-grid and proof that it does the task.

   (b) *Description:* same as (a), but use the rule shown in LN Fig. 3(a).
   Deliverables: same as (a). Which of the grids is best, the one you used in (a), or the present one?

   (c) *Description:* Again $V_1 = 1$, $a = 1$, $\Delta V = 0.5$. Calculate the transmission $T(\lambda)$ for $0 < \lambda < V_1$.
   Deliverables: A plot of $T(\lambda)$ as a function of $0 < \lambda < V_1$. Plot $T_{\text{ana}}(\lambda)$ of the previous problem in the same figure, and explain qualitatively the difference between the two curves.

3. **The WKB approximation.** By now you have a working program for calculating the transmission of any potential barrier. We use it to test the accurary of the so-called WKB approximation,[3] which is absolutely worshipped by experimentalists. WKB states that

[3] WKB stands for Wenzel, Kramers, Brillouin, the inventors of the approximation. The English call it the JWKB approximation, where J stands for Jeffreys. After brexit, the J will possibly be split off. For a background see LN Sec. 4.

the transmission through a barrier can be approximated by

$$T_{\mathrm{WKB}}(\lambda) = \frac{v_R}{v_L} D(\lambda) \exp\left[-2 \int_{y_{\mathrm{in}}}^{y_{\mathrm{out}}} \sqrt{W(y) - \lambda} dy\right],$$

The exponent marks the essential WKB approximation, see LN Eqs. 56-58. In the barrier $W(y) \geq \lambda$, and y_{in} and y_{out} mark the outer boundaries of the barrier, the points where $W(y_{\mathrm{in}}) = \lambda$ and $W(y_{\mathrm{out}}) = \lambda$. [4] A prefactor $D(\lambda)$ needs to be added if the potential is discontinuous, see LN Eq. 59.

We consider the triangularly distorted potential of problem 2 in the regime $0 < \lambda < V_1 - \Delta V$. Then $y_{\mathrm{in}} = -\frac{1}{2}a$, $y_{\mathrm{out}} = +\frac{1}{2}a$, and

$$D(\lambda) = \frac{16\lambda\,(V_1 - \Delta V - \lambda)}{V_1^2}.$$

(a) *Description:* This time we take a high barrier: choose $V_1 = 10$, $a = 1$, $\Delta V = 0.5$
Deliverables: A logarithmic plot containing $T(\lambda)$ and $T_{\mathrm{WKB}}(\lambda)$ for $0 < \lambda < V_1 - \Delta V$. Discuss the similarities and the differences between the two curves.

(b) *Description:* Same as (a), but for a stronger field: choose $V_1 = 10$, $a = 1$, $\Delta V = 2.5$
Deliverables: A logarithmic plot containing $T(\lambda)$ and $T_{\mathrm{WKB}}(\lambda)$ for $0 < \lambda < V_1 - \Delta V$. Discuss the similarities and the differences between the two curves.

(c) *Description:* Same as (a), but for a low barrier (and corresponding weak field): choose $V_1 = 1$, $a = 1$, $\Delta V = 0.05$
Deliverables: A logarithmic plot containing $T(\lambda)$ and $T_{\mathrm{WKB}}(\lambda)$ for $0 < \lambda < V_1 - \Delta V$. Discuss the similarities and the differences between the two curves.

(d) Based on your results, discuss under which circumstances the WKB approximation is useful.

4. **MIM diode.** Consider a metal-insulator-metal (MIM) diode (LN Sec. 8). The potential steps between the metals and the insulator are Φ_1 and Φ_2, respectively, see LN figures 19 and 20. The thickness of the insulator is 3 nm, the electron mass m is equal to that of an electron in free space and the Fermi energy $E_F = 1$ eV for both metals. [We are essentially redoing some of the calculations of Tuomisto *et al.*, J. Appl. Phys. **121**, 134304 (2017).]

(a) *Deliverables:* Assume an asymmetric barrier with $\Phi_1 = 0.4$ eV and $\Phi_2 = 1.8$ eV. What is the build-in potential of this structure? Set $x_0 = 1$ nm. Determine the scaling constant V_0 in eV.

(b) *Description:* Assume a symmetric barrier with $\Phi_1 = \Phi_2 = 1.1$ eV. Assume we have a purely one-dimensional system, such that we can calculate the tunnel current according to LN Sec. 6.3. Calculate the tunnel current I_T as a function of applied bias potential ΔV, for biases between -2 eV and 2 eV. [Hints: (1) the most critical here is the energy grid used for calculating LN eq. 101. In any case, the matlab function “trapz” gives better results than “sum”. (2) Watch the boundaries of the integral: read LN Sec. 6.3.]
Deliverables: A logarithmic plot of I_T as a function of voltage difference U (in SI units, i.e., in A and V). Give a short explanation of the qualitative behavior of this curve.

[4] A classical particle would bounce back from the barrier here, hence y_{in} and y_{out} mark classical turning points.

(c) *Description:* Assume an asymmetric barrier with $\Phi_1 = 0.4$ eV and $\Phi_2 = 1.8$ eV. Repeat for this asymmetric MIM the calculation of (b).
Deliverables: A logarithmic plot of I_T as a function of voltage difference U (in SI units, i.e., in A and V). Give a short explanation of the differences between this curve and that of (b). Does this device function as a diode?

(d) *Description:* Same situation as in (c), but now assume we have a three-dimensional layered material (which is actually much closer to an experimental MIM diode). We have to calculate the tunnel current density $\mathcal{J}_T$ as described in the LN Sec. 7.3. Assume that the MIM diode has a surface area of 1 μm^2, and the current density is uniform across this surface area. Calculate the tunnel current I_T as a function of applied bias potential ΔV, for biases between -2 eV and 2 eV. [Hint: Watch the sign of ΔV and the boundaries of the integrals: read LN Sec. 7.3.]
Deliverables: A logarithmic plot of I_T as a function of voltage difference U (in SI units, i.e., in A and V). Discuss the differences with the one-dimensional case of (c). Does this device function as a diode?

5. **RTD.** Resonant-tunneling diodes can be constructed from layers of GaAs and $Ga_{0.5}Al_{0.5}As$, as explained in LN Sec. 9. The barrier height is then $V_1 = 0.5$ eV. The outer GaAs regions are heavily n-type doped, such that the Fermi level is inside the conduction band with $E_F = 0.005$ eV. The effective mass of the electrons is $m = 0.067m_0$, where m_0 is the mass of an electron in free space. We make a double-barrier structure ABA'BA, where A is n-doped GaAs, B is $Ga_{0.5}Al_{0.5}As$, and A' is undoped GaAs. The B regions are 2 nm wide, whereas the A' region is 5 nm wide. Set $x_0 = 1$ nm.

   (a) *Deliverables:* Determine the scaling constant V_0 in eV.

   (b) *Description:* Calculate the transmission T_{1D} as a function of electron energy $0 < E < 1.5$ eV.
   Deliverables: Plot T_{1D} as a function of E. How do the quasi-bound states emerge in this plot? Plot the wave function that belongs to a quasi-bound state.

   (c) *Description:* Calculate the tunnel current I_T as a function of applied bias U for $0 < U < 1.5$ V.
   Deliverables: Plot I_T as a function of U. One observes the phenomenon of negative differential resistance (see LN Sec. 9). Give a short explanation of this effect.