Homework #3 — Phys622 — Fall 1998
Deadline: Wednesday, September 23, 1998.
Turn in homework in the class or put in
the box on the door of Phys 2314 by 5 p.m.

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Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of Schwabl.
Equation numbers without period, like (5), refer to the equations of this homework.

One-Dimensional Problems (Chapter 3)

1. [**3 points each part**] Schwabl's Problem 3.5, part (a) only. Additional part:

(d) Find the force $F = -\partial E/\partial L$, where $L = 2a$ is the width of the well, exerted by the electron in the n-th energy eigenstate on the walls of the well.

Calculate the force also classically, by considering a classical particle of the energy E_n and finding its velocity, the frequency of collisions with a given wall, and the momentum transfer per collision. Compare with the quantum result obtained above.

2. [**5 points each part**] Schwabl's Problem 3.7, part (a) only. Solve the problem in two different ways:

i. Take the limit $V_0 \to \infty$, $a \to 0$, but $2aV_0 = \text{const} = \lambda$ of the solution found in Section 3.4.
ii. Integrate the Schrödinger equation (3.43) around the position of the δ-function from $-\epsilon$ to $+\epsilon$, where ϵ is infinitesimal: $\int_{-\epsilon}^{+\epsilon} dx$, and find the relations between the values of the wave function $\psi(x)$, its derivative $\psi'(x)$, and the logarithmic derivative $\psi'(x)/\psi(x)$ at $\pm\epsilon$. Use these relations to match the solutions of the Schrödinger equation to the left and to the right of the δ-function.

Additional part:

(c) Consider a one-dimensional potential well of a given (arbitrary) shape $V(x)$, such that

$$\int V(x)\,dx < 0, \tag{1}$$

and $V(x) \to 0$ at $x \to \pm\infty$. The well has the characteristic depth V_0 and the characteristic width a that obey the following inequality:[1)]

$$\hbar^2/ma^2 \gg V_0, \tag{2}$$

where m is the mass of a quantum particle moving in this potential. Such a well is called *shallow*. Find (approximately) the energy E_0 and the wave function $\psi_0(x)$ of a bound state of the particle in this potential. Your answers should be expressed in terms of $\int V(x)\,dx$ (**see Hints**). Compare E_0 with the depth of the potential V_0 and the width of the wave function $\psi_0(x)$ with the width of the potential a. How many bound states does this potential have?

3. [**7 points**] Schwabl's Problem 3.18, part (a) only. *(Similar to Physics Qualifier, Fall 1994 and Spring 1986, Problem II-1.)* The antisymmetric bound state disappears when a decreases below a certain critical value a_0. Find a_0.

Find out whether the two potential wells experience an attractive or a repulsive force when the particle is in the even or in the odd bound state.

[1)] The presence of the parameters V_0 and a does *not* imply that the shape of the potential well is rectangular, as in Section 3.4. The word "characteristic" indicates that these are the parameters that characterize the overall size of the potential $V(x)$, which may have an arbitrary shape.

4. Let us consider transmission through an arbitrary potential $V(x)$ located within $|x| < a$, so that $V(x) = 0$ at $|x| > a$. A wave function of the energy $E = \hbar^2 k^2/2$ has the following forms outside of the potential:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a, \\ Fe^{ikx} + Ge^{-ikx}, & x > a, \end{cases} \tag{3}$$

(compare with Eq. (3.60)). The amplitudes of the *outgoing* waves, B and F, are related to the amplitudes of the *incoming* waves, A and G, by the so-called *scattering matrix* S:

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}. \tag{4}$$

Sometimes it is more convenient to work with the so-called *transfer matrix* M, which gives the amplitudes to the *right* of the potential, F and G, in terms of those to the *left*, A and B:

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}. \tag{5}$$

(a) [**3 points**] Express the four elements of the M-matrix in terms of the elements of the S-matrix and vice versa.

The transmission and reflection coefficients, T_l and R_l, for the wave incoming from the left are

$$T_l = \left.\frac{|F|^2}{|A|^2}\right|_{G=0} = |S_{21}|^2, \qquad R_l = \left.\frac{|B|^2}{|A|^2}\right|_{G=0} = |S_{11}|^2. \tag{6}$$

The transmission and reflection coefficients, T_r and R_r, for the wave incoming from the right are

$$R_r = \left.\frac{|F|^2}{|G|^2}\right|_{A=0} = |S_{22}|^2, \qquad T_r = \left.\frac{|B|^2}{|G|^2}\right|_{A=0} = |S_{12}|^2. \tag{7}$$

Express T_l, R_l, T_r, and R_r in terms of the elements of the M-matrix.

(b) [**3 points**] Suppose the potential consists of two isolated pieces: $V(x) = V_1(x) + V_2(x)$, where $V_1(x)$ is localized within $x_1 < x < x_2$, $V_2(x)$ is localized within $x_3 < x < x_4$, and $x_2 < x_3$. Suppose that the potential $V_1(x)$ has the transfer matrix M_1, and the potential $V_2(x)$ the transfer matrix M_2. Show that the M-matrix for the combination of the potentials is the *product* of the two M-matrices for each section separately:

$$\mathsf{M} = \mathsf{M}_2\mathsf{M}_1. \tag{8}$$

That obviously generalizes to any number of pieces and accounts for the usefulness of the transfer matrix.

5. [**5 points**] Schwabl's Problem 3.19. Find also the S- and the M-matrices of the potential. Consider both $\lambda > 0$ and $\lambda < 0$.

6. [**7 points**] Schwabl's Problem 3.18, part (b). Discuss resonances in transmission.

One possible way to solve this problem is to use Eq. (8) with the transfer matrices of individual δ-functions. Here one needs to be careful. In Problem 5 you found the transfer matrix of a delta-function located *at the origin of coordinates* ($x = 0$). On the other hand, in this problem the scatterers are located at different points $x = \pm a$. In this case one should use a generalization of Eq. (8), namely:

$$\mathsf{M} = \mathsf{M}_{-a}\mathsf{M}_\delta\mathsf{M}_a\mathsf{M}_a\mathsf{M}_\delta\mathsf{M}_{-a}, \tag{9}$$

where M_δ is the transfer matrix of a delta-function potential located at the origin of coordinates, and M_a is the transfer matrix of the empty space of the length a:

$$\mathbf{M}_a = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}. \tag{10}$$

7. *Adapted from Physics Qualifier, Fall 1985, Problem II-5.*

Let us consider a particle subject to a periodic potential:

$$V(x+a) = V(x), \tag{11}$$

where a is the period of the potential.

(a) [**3 points**] Show that, because of the finite translational invariance of the Hamiltonian, the energy eigenfunctions may be selected to obey the following relation:

$$\psi(x+a) = e^{i\varphi}\psi(x), \tag{12}$$

and can be written in the form:

$$\psi_q(x) = e^{iqx}u_q(x), \tag{13}$$

where $u(x)$ is a periodic function of x: $u(x+a) = u(x)$, and q is a parameter, called quasimomentum, that labels the eigenstates and their eigenenergies: $E(q)$.

Eq. (13) is called *Bloch's theorem* in quantum mechanics and *Floquet's theorem* in mathematics.

(b) [**3 points**] What momenta does the state (13) contain? In other words, if the wave function (13) is Fourier-expanded, what wave vectors would be present in the expansion?

(c) [**7 points**] Let us consider a particle in the potential that consists of periodically spaced delta-functions:

$$V(x) = \lambda \sum_{n=-\infty}^{+\infty} \delta(x - na) \tag{14}$$

(the so-called *Dirac comb* or *Kronig-Penney model*).

From the Schrödinger equation for potential (14), obtain an equation that determines a relation between the quasimomentum q and energy E of the eigenfunctions (13), the so-called *dispersion relation* (**see Hints**). Study this equation graphically and show that the energy E may take values only within certain ranges, called the *energy bands*, and may not take value within other ranges, called the *energy gaps*.

Hints

2c Argue that condition (2) allows to use the method of part (a)ii.

7c One possible way to solve this problem is to write the wave function of the energy $E = \hbar^2k^2/2m$ in the form $\psi(x) = Ae^{ikx} + Be^{-ikx}$ and argue that A and B must form an eigenvector of the transfer matrix $\mathsf{M}_a\mathsf{M}_\delta$ (the notation of Eq. (9)) with the eigenvalue e^{iqa}:

$$e^{iqa}\begin{pmatrix} A \\ B \end{pmatrix} = \mathsf{M}_a\mathsf{M}_\delta \begin{pmatrix} A \\ B \end{pmatrix}. \tag{15}$$