NTNU – Trondheim
Norwegian University of
Science and Technology

NTNU, Department of Physics

FY2045 Problem set 2 fall 2023

Professor Jens O. Andersen, updated by Henning G. Hugdal

Last updated: September 11, 2023

Problem 1

In quantum mechanics, one learns that commuting operators have **simultaneous eigenfunctions**. This can be seen from the fact that if $\hat{F}\psi = f\psi$ and $\hat{G}\psi = g\psi$, we must have

$$[\hat{G}, \hat{F}]\psi = \hat{G}\hat{F}\psi - \hat{F}\hat{G}\psi = f\hat{G}\psi - g\hat{F}\psi = (fg - gf)\psi = 0. \tag{1}$$

When the system is prepared in such a simultaneous eigenstate, the corresponding observables will have sharp values. The observables are then called *compatible*.

On the other hand, when two operators do *not* commute, as for $\hat{x}$ and $\hat{p}$,

$$[\hat{x}, \hat{p}_x] \equiv \hat{x}\hat{p}_x - \hat{p}_x\hat{x} = i\hbar,$$

then the two observables *cannot* have sharp values simultaneously; there are no simultaneous eigenfunctions of the two operators. The observables are then **non-compatible**. One consequence of this is **Heisenberg's uncertainty relation** for the two observables:

$$\Delta x \, \Delta p_x \geq \frac{1}{2}|i[x, \hat{p}_x]| = \frac{1}{2}\hbar.$$

The overall goal of this problem is to derive the **generalized uncertainty relation**, and show that one special case is the above Heisenberg uncertainty relation.

a) Let A and B be two observables, and $\hat{A}$ and $\hat{B}$ the corresponding Hermitian operators. Show first that the operator $i[\hat{A}, \hat{B}]$ is Hermitian (implying that its expectation values and eigenvalues are real).

b) When $\hat{A}$ and $\hat{B}$ are Hermitian, then also the operators $\bar{A} \equiv \hat{A} - \langle A \rangle$ and $\bar{B} \equiv \hat{B} - \langle B \rangle$ are Hermitian. Here, $\langle A \rangle$ and $\langle B \rangle$ are the expectation values of the observables A and B in an arbitrary state. Note that $\langle \bar{A}^2 \rangle = \langle (A - \langle A \rangle) \rangle^2 = (\Delta A)^2$ etc., where ΔA is the uncertainty in the observable A. Verify that $[\bar{A}, \bar{B}] = [\hat{A}, \hat{B}]$.

c) The crucial trick in this problem is to consider the non-negative integral

$$I(\beta) \equiv \int |(\bar{A} + i\beta\bar{B})\Psi|^2 d\tau = \int (\bar{A}\Psi + i\beta\bar{B}\Psi)^* (\bar{A}\Psi + i\beta\bar{B}\Psi) d\tau \geq 0 \, , \tag{2}$$

where Ψ is an arbitrary (normalized) wavefunction and β is a real parameter that we are free to choose. Show that the right-hand side can be written as

$$I(\beta) = (\Delta A)^2_\Psi + \beta^2 (\Delta B)^2_\Psi + \beta \langle i[\hat{A}, \hat{B}] \rangle_\Psi \, , \tag{3}$$

where all three terms are real. Remember that $\bar{A}$ and $\bar{B}$ are Hermitian and can be moved as in the first equation above.

d) Find the minimum of $I(\beta)$ by calculating the derivative with respect to β, and use this to derive the generalized uncertainty relation

$$(\Delta A)_\Psi (\Delta B)_\Psi \geq \frac{1}{2} |\langle i[\hat{A}, \hat{B}] \rangle_\Psi| \, . \tag{4}$$

e) When the two operators satisfy the relation $[\hat{A}, \hat{B}] = i\hbar$, they are said to be **canonically conjugate**. Show that the resulting uncertainty relation has as a special case Heisenberg's uncertainty relation for x and p_x.

f) What value must the integral $I(\beta)$ have if the uncertainty product $\Delta x \, \Delta p_x$ is to have its minimal value $\frac{1}{2}\hbar$? Find the wavefunction in this particular case.

Problem 2

Consider the delta-function potential

$$V(x) = \beta\delta(x) \, , \tag{5}$$

where β can be either positive or negative. See Fig. 1. This potential is a simplified model of a potential that is zero everywhere, except for a thin layer close to (and including) the yz-plane. Suppose that an electron is moving perpendicularly towards this layer, in the

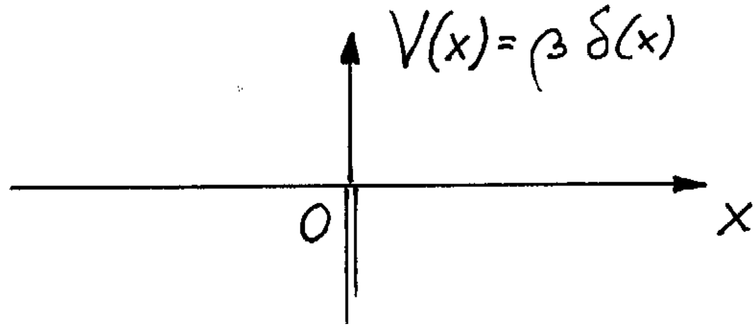

Figure 1: Delta-function potential.

positive x-direction, with the energy $E = (\hbar k)^2/2m_e$. This is a scattering problem that can be treated using an energy eigenfunction, which has the form $e^{ikx} + re^{-ikx}$ for $x < 0$ and te^{ikx} for $x > 0$. In the following, we make a slight modification by dividing by the complex factor t everywhere. Thus energy eigenfunction takes the form

$$\psi_k(x) = \begin{cases} \psi_{\rm I}(x) = \psi_i(x) + \psi_r(x) & \text{for} \quad x < 0, \\ \psi_{\rm II}(x) = \psi_t(x) & \text{for} \quad x > 0 \end{cases} , \tag{6}$$

where, $\psi_i(x) = \frac{1}{t}e^{ikx}$, $\psi_r(x) = b\, e^{-ikx}$, $\psi_t(x) = e^{ikx}$, and $b = r/t$. The three wavefunctions represent the incoming (i), reflected (r) and transmitted wave t, respectively.

a) The general solution of the time-independent Schrödinger equation for $x > 0$ also contains a term De^{-ikx}. Why have we dropped this term in the expression for $\psi_{\rm II}$ for $x > 0$? Hint: The probability current density is defined as

$$j = \mathrm{Re}\left(\Psi^* \frac{\hbar}{im} \frac{d}{dx} \Psi \right) . \tag{7}$$

b) Show that the ratio between the transmitted and incoming waves is unaltered by the above modification, and that the transmission probability $T \equiv \frac{j_t}{j_i} = |t|^2$.

c) Use the continuity condition for $\psi(x)$ and the discontinuity condition for $\psi'(x) = d\psi(x)/dx$,

$$\psi'(0^+) - \psi'(0^-) = \frac{2m\beta}{\hbar^2}\psi(0) , \tag{8}$$

to show that $t = \left[1 + \frac{im\beta}{\hbar^2 k}\right]^{-1}$. Hint: Eliminate the coefficient b.

Let E_B be the binding energy found in the previous problem set for $\beta < 0$, $E_B = \frac{m\beta^2}{2\hbar^2}$. Find the transmission coefficient T expressed in terms of the ratio E/E_B. Consider the results for the cases (i) $E \ll E_B$, (ii) $E = E_B$ and (iii) $E \gg E_B$, and sketch T as a function of E/E_B. Is it reasonable to state that the binding energy is a *natural energy scale* when we are discussing the behaviour of T as a function of E?

d) An interesting point is that the calculation of $1/t$ is valid not only for positive real k $(= \sqrt{2mE/\hbar^2})$, but also if we take k to be complex. However, for such k-values, the resulting wavefunction

$$\psi = \begin{cases} \frac{1}{t}e^{ikx} + be^{-ikx} & \text{for } x < 0, \\ e^{ikx} & \text{for } x > 0 \end{cases} \tag{9}$$

is not necessarily an eigenfunction. But here we have an exception: Check that if $\mathrm{Im}(k) > 0$, then ψ approaches zero when $x \to \infty$, while in the limit $x \to -\infty$ we see that e^{-ikx} approaches zero whereas e^{ikx} becomes infinite. The only way to escape this problem and get an acceptable eigenfunction is if the transmission amplitude t becomes infinite: Find the (imaginary) k-value which makes t infinite.

Problem 3

First let us repeat the measurement postulate: A measurement of an observable F must give one of the eigenvalues f_n, and will leave the system in an eigenstate corresponding to the measured eigenvalue. This means that the part of the wavefunction *before* the measurement which is not consistent with the measured value f_n is removed by the measurement process. This is often called the collapse of the wavefunction.

a) Suppose that a hydrogen atom is prepared in the state

$$\psi_A = 0.8\,\psi_{100} + 0.5\,\psi_{210} + 0.3\,\psi_{310} + 0.1\,\psi_{420} + 0.1\,\psi_{430}\ , \tag{10}$$

where ψ_{nlm} are the energy eigenstates of the hydrogen atom with principal quantum number n and energy E_n, and orbital angular momentum quantum numbers $l = 0, 1, 2, \ldots, n-1$ and $m = 0, \pm 1, \pm 2, \ldots, \pm l$.

Check that this state is normalized. (Hint: The set of eigenfunctions ψ_{nlm} is orthonormalized.)

b) The states ψ_{nlm} are also eigenstates of the operators for the total angular momentum squared, $\hat{\mathbf{L}}^2$, and the z-component of the angular momentum, $\hat{L}_z$,

$$\hat{\mathbf{L}}^2\psi_{nlm} = \hbar^2 l(l+1)\psi_{nlm},$$
$$\hat{L}_z\psi_{nlm} = \hbar m\psi_{nlm}.$$

What is the result if the z-component L_z of the angular momentum is measured for this atom? What is the state of the atom *after* the measurement of L_z?

c) What is the probability P_4 that a measurement of the energy of this atom gives the result E_4, and what is the state after a measurement giving this result? (Remember to normalize this state.)

d) How can we proceed to prepare either the state ψ_{420} or the state ψ_{430}?

e) Suppose now that we have a hydrogen atom prepared in the state $\psi_B = 0.8\,\psi_{320} + 0.6\,\psi_{410}$. Explain why it is impossible to prepare this state using measurements of the compatible observables $E, \mathbf{L}^2$, and L_z. Explain also why it is sufficient to measure one of the observables E or $\mathbf{L}^2$ in order to make this state collapse either to ψ_{320} or into ψ_{410}.