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## FY2045 Problem set 2 fall 2023

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### 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

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

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:

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

**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  $\langle \bar{A}^2 \rangle = \langle (A - \langle A \rangle)^2 \rangle = (\Delta A)^2$  etc., where  $\Delta A$  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

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

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

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

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  $\beta$ , and use this to derive the generalized uncertainty relation

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

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

$$V(x) = \beta \delta(x), \quad (5)$$

where  $\beta$  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 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

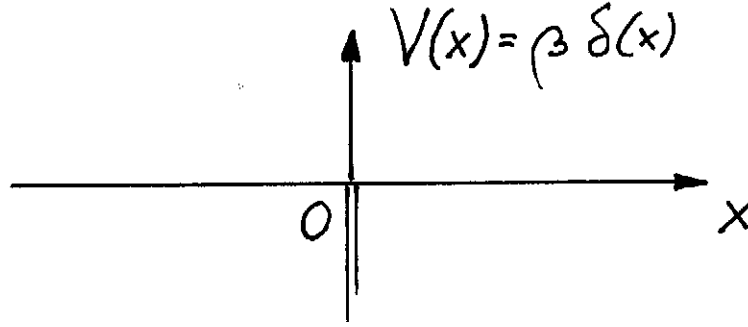


Figure 1: Delta-function potential.

$te^{ikx}$  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

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

where,  $\psi_i(x) = \frac{1}{t}e^{ikx}$ ,  $\psi_r(x) = be^{-ikx}$ ,  $\psi_t(x) = e^{ikx}$ , 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  $\psi_{\text{II}}$  for  $x > 0$ ? Hint: The probability current density is defined as

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

**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  $\psi'(x) = d\psi(x)/dx$ ,

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

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

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

is not necessarily an eigenfunction. But here we have an exception: Check that if  $\text{Im}(k) > 0$ , then  $\psi$  approaches zero when  $x \rightarrow \infty$ , while in the limit  $x \rightarrow -\infty$  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

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

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

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

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

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

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  $\psi_{420}$  or the state  $\psi_{430}$ ?
- 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  $\psi_{320}$  or into  $\psi_{410}$ .