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FY2045 Solutions Problem set 2 fall 2023

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September 1, 2023

Problem 1

a) When $\hat{A}$ and $\hat{B}$ are Hermitian (self-adjoint, $\hat{A}^\dagger = \hat{A}$), we find that the adjoint of the operator

$$\left(i[\hat{A},\hat{B}]\right)^\dagger = (i)^* \left[(\hat{A}\hat{B})^\dagger - (\hat{B}\hat{A})^\dagger\right] = -i\left[\hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger\right] = -i\left[\hat{B}\hat{A} - \hat{A}\hat{B}\right] = i[\hat{A},\hat{B}]\ , \quad (1)$$

which shows that the operator is self-adjoint, or Hermitian. This ensures that this operator has real expectation values and also real eigenvalues. Here we have used the fact that the adjoint of a scalar is simply the complex conjugate, and the rule $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{B}^\dagger$ — analogous to the transpose of a product of two matrices.

b) Since the real numbers $\langle A\rangle$ and $\langle B\rangle$ commute with anything (the commutator is zero), we see that

$$\begin{aligned}[\bar{A},\bar{B}] &= [\hat{A} - \langle A\rangle, \hat{B} - \langle B\rangle] \\ &= [\hat{A},\hat{B}] - [\hat{A},\langle B\rangle] - [\langle A\rangle,\hat{B}] + [\langle A\rangle,\langle B\rangle] \\ &= \underline{\underline{[\hat{A},\hat{B}]}}\ , \end{aligned} \quad (2)$$

Between the first and second line, we have used the commutator identity $[A+B,C] = [A,C] + [B,C]$.

c) This expression is non-negative for all real β, including the value of β that minimizes the integral $I(\beta)$. (Note that the original integrand is non-negative in the entire region of integration.) By moving the Hermitian operators $\bar{A}$ and $\bar{B}$, we can rewrite the integral $I(\beta)$ as follows

$$\begin{aligned} I(\beta) &= \int \left[(\bar{A}\Psi)^*(\bar{A}\Psi) + (i\beta)^*(i\beta)(\bar{B}\Psi)^*(\bar{B}\Psi) + (i\beta)^*(\bar{B}\Psi)^*(\bar{A}\Psi) + i\beta(\bar{A}\Psi)^*(\bar{B}\Psi)\right] d\tau \\ &= \int \Psi^* \left[\bar{A}^2 + \beta^2\bar{B}^2 + i\beta(\bar{A}\bar{B} - \bar{B}\bar{A})\right] \Psi d\tau \\ &= \langle \bar{A}^2\rangle_\Psi + \beta^2\langle \bar{B}^2\rangle_\Psi + \beta\langle i[\bar{A},\bar{B}]\rangle_\Psi \\ &= \underline{\underline{(\Delta A)^2_\Psi + \beta^2(\Delta B)^2_\Psi + \beta\langle i[\hat{A},\hat{B}]\rangle_\Psi \geq 0}} \; . \end{aligned} \tag{3}$$

Between the first and second lines we have used the fact that for a Hermitian operator $\hat{F}$ we have

$$\int (\hat{F}\Psi)^*\Phi \; d\tau = \int \Psi^*\hat{F}\Phi \; d\tau, \tag{4}$$

inserting $\hat{F} = \bar{A}$ or $\bar{B}$ and $\Phi = \bar{A}\Psi$ or $\bar{B}\Psi$.

d) We next calculate the derivative of Eq. (3),

$$\frac{dI(\beta)}{d\beta} = 2\beta(\Delta B)^2 + \langle i[\hat{A},\hat{B}]\rangle \; . \tag{5}$$

This means that $I(\beta)$ is a minimum for [1]

$$\beta_{\min} = -\frac{\langle i[\hat{A},\hat{B}]\rangle}{2(\Delta B)^2} \; . \tag{6}$$

Inserting this, we find the minimum of $I(\beta)$

$$0 \leq I(\beta_{\min}) = (\Delta A)^2 - \frac{\langle i[\hat{A},\hat{B}]\rangle^2}{4(\Delta B)^2} \; . \tag{7}$$

Multiplication by $(\Delta B)^2$ then gives the inequality $0 \leq (\Delta B)^2 I(\beta_{\min}) = (\Delta A)^2(\Delta B)^2 - \frac{1}{4}\langle i[\hat{A},\hat{B}]\rangle^2$, i.e.

$$(\Delta A)_\Psi(\Delta B)_\Psi \geq \frac{1}{2}|\langle i[\hat{A},\hat{B}]_\Psi\rangle| \; . \tag{8}$$

Note that this uncertainty relation holds for an arbitrary wavefunction Ψ. Note also that the *equality sign* in this inequality holds only if the integral $I(\beta_{\min})$ is equal to zero.

[1] In order to show it is a minimum, examine the second derivative. Since it given by $2(\Delta B)^2 > 0$, it follows.

e) When the two operators satisfy the same commutator relation as $\hat{x}$ and $\hat{p}_x$, that is, when $[\hat{A}, \hat{B}] = i\hbar$, then the inequality simplifies to

$$(\Delta A)_\Psi (\Delta B)_\Psi \geq \frac{1}{2}\hbar \tag{9}$$

which we may call a generalized Heisenberg's uncertainty relation. With $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}_x$, we obtain Heisenberg's original uncertainty relation,

$$(\Delta x)_\Psi (\Delta p_x)_\Psi \geq \frac{1}{2}\hbar \; . \tag{10}$$

f) From the derivation in **e**) we see that the inequality is saturated (so that the uncertainty product becomes minimal) when the integral $I(\beta_{\min})$ is equal to zero. This puts severe restrictions on the wavefunction Ψ, since it requires that $\bar{A}\Psi + i\beta_{\min}\bar{B}\Psi = 0$. With $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}_x$, $\bar{A} = x - \langle x \rangle$ etc., this is a first-order differential equation for the function Ψ. We first calculate

$$\beta_{\min} = -\frac{\langle i[\hat{A}, \hat{B}]\rangle}{2(\Delta B)^2} = \frac{\hbar}{2(\Delta p_x)^2} = \frac{2(\Delta x)^2}{\hbar} \; . \tag{11}$$

where the last step follows from the uncertainty relation which now (by assumption) has the form $\Delta x \Delta p_x = \frac{1}{2}\hbar$, i.e. $\frac{1}{(\Delta p_x)^2} = \frac{4(\Delta x)^2}{\hbar^2}$. Inserting $\beta_{\min}$ into the first order differential equation, we obtain

$$\bar{A}\Psi + i\beta_{\min}\bar{B}\Psi = \left[(x - \langle x \rangle) + \frac{2i}{\hbar}(\Delta x)^2(\hat{p}_x - \langle p_x \rangle)\right]\Psi = 0 \; . \tag{12}$$

Dividing by $2(\Delta x)^2$ and inserting $\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$, we can write this in the form

$$\frac{d\Psi}{dx} = \left[-\frac{x - \langle x \rangle}{2(\Delta x)^2} + i\langle p_x/\hbar \rangle\right]\Psi \; , \tag{13}$$

or

$$\frac{d\Psi}{\Psi} = \left[-\frac{x - \langle x \rangle}{2(\Delta x)^2} + i\langle p_x \rangle/\hbar\right] dx \; . \tag{14}$$

Integrating this we have

$$\begin{aligned} \ln\Psi &= \ln C' - \frac{1}{4(\Delta x)^2}\left[x^2 - 2x\langle x \rangle + \langle x^2 \rangle - \langle x^2 \rangle\right] + i\langle p_x/\hbar \rangle x \\ &= \ln C - \frac{1}{4(\Delta x)^2}\left(x - \langle x \rangle\right)^2 + i\langle p_x/\hbar \rangle x \; , \end{aligned} \tag{15}$$

where we have added and subtracted a term proportional to $\langle x^2 \rangle$ to complete the square.

The conclusion is that the uncertainty relation is saturated, so that $\Delta x \Delta p_x = \frac{1}{2}\hbar$ for the following *class* of functions:

$$\Psi = C \exp\left[-\frac{(x-\langle x\rangle)^2}{4(\Delta x)^2} + \frac{i\langle p_x\rangle x}{\hbar}\right] . \tag{16}$$

Here, the quantities $\langle x\rangle$, $\langle p_x\rangle$ and Δx are arbitrary. Note that $|\Psi|^2 \propto \exp\left[-\frac{(x-\langle x\rangle)^2}{2(\Delta x)^2}\right]$ here becomes a Gaussian with a maximum at $x = \langle x\rangle$ and with a form that corresponds to the uncertainty Δx. Therefore, we may very well call this class of functions Gaussian wave packets.

Problem 2

a) The term $\psi_t = C\exp(ikx)$ for $x > 0$ corresponds to a transmitted wave with a probability current density $j_t = |C|^2\hbar k/m$. A term $D\exp(-ikx)$ for $x > 0$ would correspond to particles coming in from the right, which is unphysical. Thus, the condition is that for $x > 0$, we have only a transmitted wave. One could also argue from the sign of the momentum eigenvalue: the term De^{-ikx} has momentum $-\hbar k$, i.e. towards negative x. Such a solution does not make physical sense for $x > 0$.

b) Before the modification we have $\psi_t^0/\psi_i^0 = t$ (superscript 0 denoting prior to the modification), and after the modification we have $\psi_t/\psi_i = 1/t^{-1} = t$. Hence, the ratio between the transmitted and incoming waves is unaltered by the modification.

The transmitted (probability) current density is

$$j_t = \mathrm{Re}\left[\psi_t \frac{\hbar}{im_e}\frac{d\psi_t}{dx}\right] = \mathrm{Re}\left[e^{-ikx}\frac{\hbar}{im_e}\, ik\, e^{ikx}\right] = \frac{\hbar k}{m_e} . \tag{17}$$

For the incoming one we find in the same manner that

$$j_i = \mathrm{Re}\left[\frac{1}{t^*}e^{-ikx}\frac{\hbar}{im_e}ik\,\frac{1}{t}\,e^{ikx}\right] = \frac{1}{|t|^2}\frac{\hbar k}{m_e} . \tag{18}$$

It follows that the transmission probability (also called the transmission coefficient) as before is the absolute square of the transmission amplitude t,

$$T = \frac{j_t}{j_i} = \underline{\underline{|t|^2}} . \tag{19}$$

Before the modification we would have $j_t^0 = |t|^2\hbar k/m_e$ and $j_i^0 = \hbar k/m_e$, which would give the same transmission probability $T = |t|^2$.

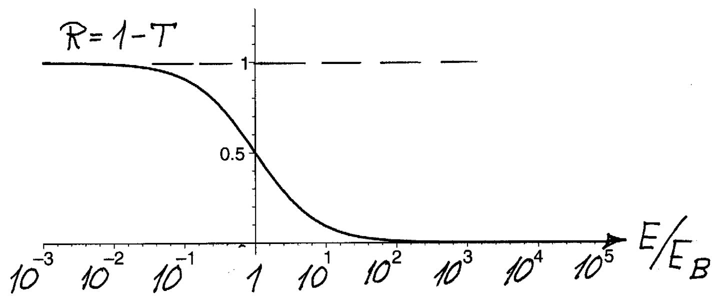

Figure 1: The reflection coefficient $R = 1 - T$ as a function of the dimensionless ratio $\frac{E}{E_B}$.

c) With ψ equal to $\frac{1}{t}e^{ikx} + be^{-ikx}$ for $x < 0$ and equal to e^{ikx} for $x > 0$, continuity of ψ at $x = 0$ gives the condition $1/t + b = 1$, that is, $b = 1 - 1/t$. This can be used to eliminate b from the given discontinuity condition for ψ', which is

$$\psi'(0^+) - \psi'(0^-) = ik - ik\left(\frac{1}{t} - b\right) = \frac{2m\beta}{\hbar^2}\ . \tag{20}$$

Inserting he result for b and rearranging the terms, we get

$$\boxed{\tfrac{1}{t} = 1 + \tfrac{im\beta}{\hbar^2 k}.} \tag{21}$$

Thus the transmission coefficient is

$$T = |t|^2 = \frac{1}{1 + \frac{m^2\beta^2}{\hbar^4 k^2}} = \frac{1}{1 + \frac{E_B}{E}}\ , \tag{22}$$

where $E_B = \frac{m\beta^2}{2\hbar^2}$. We consider the three cases:

(i) For $E \ll E_B$, we see that $T \approx E/E_B \ll 1$ (and $R = 1 - T \approx 1$).

(ii) For $E = E_B$ we find that $T = \frac{1}{2}$.

(iii) For $E \gg E_B$ we see that $T \approx 1$ (and $R = 1 - T \ll 1$).

Figure 1 shows that the change from $T \ll 1$ to $T \sim 1$ takes place roughly for $0.1E_B \leq E_k \leq 10E_B$ Thus, we may state that the binding energy E_B sets the scale when one wants to discuss the energy dependence of the transmission coefficient T and the reflection coefficient $R = 1 - T$.

d) Provided that $\mathrm{Im}(k) > 0$, it follows that $\lim_{x\to\infty} e^{ikx} = 0$, $\lim_{x\to-\infty} e^{-ikx} = 0$, while $\exp(ikx)$ becomes infinite in the limit $x \to -\infty$. To avoid the latter problem, we must therefore in addition require that t is infinite, or $1/t = 0$. Solving $1 + im\beta/\hbar^2 k = 0$ for k, we get

$$k = -\frac{im\beta}{\hbar^2}, \tag{23}$$

which has a positive imaginary part when $\beta < 0$, which is necessary for bounds states to occur. This value of k corresponds to $E = -E_B$, for which T diverges. The conclusion is that poles in the scattering amplitude corresponds to bound states.

Problem 3

a) Since the eigenfunctions ψ_{nlm} are both normalized and orthogonal, the squared norm of ψ_A is

$$||\Psi||^2 = 0.8^2 + 0.5^2 + 0.3^2 + 0.1^2 + 0.1^2 = 1.00 \ , \tag{24}$$

showing that ψ_A is normalized.

b) We note that all the terms in ψ_A have magnetic quantum number $m = 0$ so that ψ_A is an eigenfunction of $\hat{L}_z$ with the eigenvalue $L_z = 0$. A measurement then gives $L_z = 0$, and will leave the atom in an unaltered state; the measurement does not remove any part of the wavefunction.

c) A measurement of the energy E_4 removes the first three terms in ψ_A, with the probability $P_4 = 0.1^2 + 0.1^2 = 0.02$. The state of the atom after this measurement becomes

$$\psi_4 = \frac{0.1\,\psi_{420} + 0.1\,\psi_{430}}{\sqrt{P_4}} = \frac{1}{\sqrt{2}}(\psi_{420} + \psi_{430}) \ . \tag{25}$$

d) If we go on and measure $\mathbf{L}^2$, we will either get $6\hbar^2$ and leave the atom in the state ψ_{420}, or $12\hbar^2$ leaving the atom in ψ_{430}. The probability for each of these measurements is $P = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$, cf, Eq. (25).

e) As you will realize from the above, a measurement of the three compatible observables E, $\mathbf{L}^2$ and L_z will leave the atom in a simultaneous eigenstate of the type ψ_{nlm} (or in a continuum state with $E > 0$ and well-defined l and m). In order to prepare a state of the type $\psi_B = 0.8\,\psi_{320} + 0.6\,\psi_{410}$, one must therefore figure out some other clever way to obtain the desired result. Assuming that this has been done, we may state that a measurement of E only, or of $\mathbf{L}^2$ only, will remove either ψ_{410} or ψ_{320}, so that the atom is left either in ψ_{320} or in ψ_{410}. The probality for each measurement is $P = (0.8)^2 = 0.64$ and $P = (0.6)^2 = 0.36$, respectively, cf, Eq. (24).