Quantum Mechanics I (141) Problem Set 1

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I. Solutions overview

In this problem set, we evaluate a Gaussian integral using two methods: using Gamma functions and using polar coordinates. We also derive a 3D expression for the probability current.

II. Wavefunction Normalization

The task is to normalize $\Psi(x) = Ae^{(-\alpha x^2)}$. That is,

$$\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)\mathrm{d}x = 1 \tag{1}$$

Letting A, α be real, equation (1) gives us

$$A^2 \int_{-\infty}^{\infty} e^{(-2\alpha x^2)}\mathrm{d}x = 1 \tag{2}$$

A. Gamma Function Approach

Defining, for convenience, $B \equiv A^2, \beta \equiv 2\alpha$,

$$B \int_{-\infty}^{\infty} e^{(-\beta x^2)}\mathrm{d}x = 1 \tag{3}$$

Executing a change of variable $t = \beta x^2$, $\mathrm{d}t = 2\beta x \mathrm{d}x$. Observe that there are two branches of solutions stemming from the quadratic nature of x. That is, $x = \pm\sqrt{\frac{t}{\beta}}$. To constrict x into the real domain, it must be that $\alpha \geq 0$. Before completing t substitution, we must divide the integral

$$B\left(\int_{-\infty}^{0} e^{(-\beta x^2)}\mathrm{d}x + \int_{0}^{\infty} e^{(-\beta x^2)}\mathrm{d}x\right) = 1 \tag{4}$$

As x approaches $-\infty$ and $+\infty$, t approaches $+\infty$ while both approaches zero together. Changing variables and limits,

$$\frac{B}{2\beta}\left(\int_{\infty}^{0} -\sqrt{\frac{\beta}{t}}e^{-t}\mathrm{d}t + \int_{0}^{\infty} \sqrt{\frac{\beta}{t}}e^{-t}\mathrm{d}t\right) = 1 \tag{5}$$

Switching limits of the first term and combining the integrals,

$$\frac{B}{\beta}\left(\int_{0}^{\infty} \sqrt{\frac{\beta}{t}}e^{-t}\mathrm{d}t\right) = \frac{B}{\sqrt{\beta}}\int_{0}^{\infty} t^{1/2-1}e^{-t}\mathrm{d}t = 1 \tag{6}$$

The integral in Eq. (6) can be simplified into a Gamma function expression

$$\frac{B}{\sqrt{\beta}}\int_{0}^{\infty} t^{1/2-1}e^{-t}\mathrm{d}t = \frac{B}{\sqrt{\beta}}\Gamma\left(\frac{1}{2}\right) = 1 \tag{7}$$

Hence,

$$B = \sqrt{\frac{\beta}{\pi}} \tag{8}$$

Evaluating back to original forms A and α,

$$A = \left(\frac{2\alpha}{\pi}\right)^{1/4}, \qquad \alpha \geq 0 \tag{9}$$

Therefore, the normalized wavefunction with unit magnitude is

$$\Psi(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{(-\alpha x^2)} \tag{10}$$

Observe that even if α is generally complex, the imaginary parts will cancel out leaving us with Eq. (2) to solve.

B. Integration via Polar Coordinates

We proceed on evaluating the integral on Eq. (2) using polar coordinates. Multiplying it with itself and changing the other factor from x into y, we get

$$A^4 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{(-2\alpha x^2)}e^{(-2\alpha y^2)}\mathrm{d}x\mathrm{d}y = 1 \tag{11}$$

$$A^4 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{(-2\alpha(x^2+y^2))}\mathrm{d}\Omega = 1 \tag{12}$$

where $\mathrm{d}\Omega$ represents the area element. To evaluate, we use the polar coordinate system and use the substitution $r^2 = x^2+y^2$ transforming the area element using the polar Jacobian: $\mathrm{d}\Omega = r\mathrm{d}r\mathrm{d}\phi$. Integral becomes

$$A^4 \int_{0}^{2\pi}\int_{0}^{\infty} e^{(-2\alpha(r^2))}r\mathrm{d}r\mathrm{d}\phi = 1 \tag{13}$$

Making a substitution $u = -2\alpha r^2$, $\mathrm{d}u = -4\alpha r\mathrm{d}r$, u approaches $-\infty$ as r approaches ∞ and both approaches zero together. The integral becomes

$$-\frac{A^4}{4\alpha}\int_{0}^{2\pi}\int_{0}^{-\infty} e^{u}\mathrm{d}u\mathrm{d}\phi = 1 \tag{14}$$

The double integral is trivial and direct evaluation yields

$$\frac{A^4\pi}{2\alpha} = 1 \tag{15}$$

This gives us the same normalization constant as Eq. (9).

$$A = \left(\frac{2\alpha}{\pi}\right)^{1/4}, \qquad \alpha \geq 0 \tag{16}$$

III. Three Dimensional Probability Current

We derive the 3D expression for the probability current. To do so, we use the time-dependent Schrödinger equation and the continuity equation. The former is

$$\hat{H}\left|\Psi\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi\right\rangle \tag{17}$$

Representing in position basis and assuming a time-independent potential, this is expressed as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(r,t) + V(r)\Psi(r,t) = i\hbar\frac{\partial\Psi(r,t)}{\partial t} \tag{18}$$

It is also useful to derive its complex-conjugated version

$$-\frac{\hbar^2}{2m}\nabla^2\Psi^*(r,t) + V(r)\Psi^*(r,t) = -i\hbar\frac{\partial\Psi^*(r,t)}{\partial t} \tag{19}$$

The continuity equation is expressed as

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0 \tag{20}$$

Integrating the first term of the continuity equation over all of space

$$\iiint \frac{\partial\rho}{\partial t}\mathrm{d}^3r = \iiint \frac{\partial}{\partial t}(\Psi^*\Psi)\mathrm{d}^3r \tag{21}$$

Product rule gives us

$$\iiint \Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi*}{\partial t}\mathrm{d}^3r \tag{22}$$

Using Eq. (18) and Eq. (19), we can express the time derivatives as

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\nabla^2\Psi - \frac{iV(r)}{\hbar}\Psi \tag{23}$$

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\nabla^2\Psi^* + \frac{iV(r)}{\hbar}\Psi^* \tag{24}$$

Plugging these derivatives into Eq. (22), the potential terms cancel giving us

$$\iiint \Psi^*\left(\frac{i\hbar}{2m}\nabla^2\Psi\right) + \Psi\left(-\frac{i\hbar}{2m}\nabla^2\Psi^*\right)\mathrm{d}^3r \tag{25}$$

Throwing the constants out the integral, we arrive at

$$\frac{i\hbar}{2m}\iiint \Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\mathrm{d}^3r \tag{26}$$

Recall that Laplace operator is simply the divergence of a gradient

$$\frac{i\hbar}{2m}\iiint \Psi^*\vec{\nabla}\cdot\vec{\nabla}\Psi - \Psi\vec{\nabla}\cdot\vec{\nabla}\Psi^*\mathrm{d}^3r \tag{27}$$

We claim that Eq. (27) can be expressed as

$$\frac{i\hbar}{2m}\iiint \vec{\nabla}\cdot(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*)\mathrm{d}^3r \tag{28}$$

Proof. Recall the the divergence operator is distributive. That is,

$$\frac{i\hbar}{2m}\iiint \vec{\nabla}\cdot\Psi^*\vec{\nabla}\Psi - \vec{\nabla}\cdot\Psi\vec{\nabla}\Psi^*\mathrm{d}^3r \tag{29}$$

For each term, we can execute the product rule for divergences leaving the integrand with the form

$$(\Psi^*\vec{\nabla}\cdot\vec{\nabla}\Psi + \vec{\nabla}\Psi^*\cdot\vec{\nabla}\Psi) - (\Psi\vec{\nabla}\cdot\vec{\nabla}\Psi^* + \vec{\nabla}\Psi\cdot\vec{\nabla}\Psi^*) \tag{30}$$

By commutativity of the dot product, the second terms of each parentheses cancel out leaving us with

$$(\Psi^*\vec{\nabla}\cdot\vec{\nabla}\Psi) - (\Psi\vec{\nabla}\cdot\vec{\nabla}\Psi^*) \tag{31}$$

which we observe to be the integrand of Eq. (27) and thus proving the claim. QED

Using divergence theorem, we can turn a volume integral of a divergence of a vector over a region into a closed surface integral of that vector over the surface enclosing that region. Hence, the divergence theorem converts Eq. (28) into

$$\frac{i\hbar}{2m}\oiint(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*)\cdot\mathrm{d}^2\vec{r} \tag{32}$$

where the surface encloses all of space. Expressing the volume integral in cartesian coordinates $x = q_1, y = q_2, z = q_3$, we can see that Eq. (28) decomposes into

$$\frac{i\hbar}{2m}\sum_{i=1}^{3}\int\frac{\mathrm{d}}{\mathrm{d}q_i}(\Psi^*\frac{\mathrm{d}\Psi}{\mathrm{d}q_i} - \Psi\frac{\mathrm{d}\Psi^*}{\mathrm{d}q_i})\mathrm{d}q_i\iint\mathrm{d}q_j\mathrm{d}q_k \tag{33}$$

where $i \neq j,k$ and $j \neq k$. Since $\Psi = 0$ at the boundaries ($r = \pm\infty$), fundamental theorem says first integral must vanish and, hence, Eq. (32) must also vanish. Rearranging the continuity equation and integrating over all of space,

$$\iiint \frac{\partial\rho}{\partial t}\mathrm{d}^3r = -\iiint \nabla\cdot\vec{J}\mathrm{d}^3r \tag{34}$$

Using Eq. (32) for the left hand side and divergence theorem for the right hand size, we can convert Eq. (34) into an equation of closed surface integrals as follows

$$\frac{i\hbar}{2m}\oiint \Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\mathrm{d}^2r = -\oiint\vec{J}\mathrm{d}^3r \tag{35}$$

To make it more suggestive,

$$\oiint\left(\frac{i\hbar}{2m}(\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi)\right)\cdot\mathrm{d}^2\vec{r} = \oiint\vec{J}\cdot\mathrm{d}^2\vec{r} \tag{36}$$

which implies that

$$\vec{J} = \frac{i\hbar}{2m}(\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi) \tag{37}$$