

Quantum Mechanics

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Problem Set 1

Problem 1. The wave function of this particle is,

$$\psi(x, 0) = N \exp \left(- \left(\frac{x - x_0}{2\sigma} \right)^2 \right) \quad (1)$$

(1) From the normalization of the wave function,

$$\int |\psi(x, 0)|^2 dx = N^2 \int \exp \left(-2 \left(\frac{x - x_0}{2\sigma} \right)^2 \right) dx = 1 \quad (2)$$

Since a range of integration is entire of real, the translation about x can be negligible. To make a convenient form, change a integral variable.

$$N^2 \int \exp \left(-2 \left(\frac{x - x_0}{2\sigma} \right)^2 \right) dx = \sqrt{2}\sigma N^2 \int e^{-x^2} dx \quad (3)$$

We know how to calculate this. Easy way is using a idea of double integration. So,

$$\int e^{-x^2} dx = \sqrt{\pi}, \quad \sqrt{2}\sigma N^2 = 1 \quad (4)$$

Finally,

$$N = \left(\frac{1}{2\pi\sigma^2} \right)^{\frac{1}{4}} \quad (5)$$

(2) First, we have to find $\phi(p, 0)$. It is a fourier transformation of ψ .

$$\phi(p, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x, 0) e^{-\frac{i}{\hbar}px} dx = \frac{N}{\sqrt{2\pi\hbar}} \int \exp \left(- \left(\frac{x - x_0}{2\sigma} \right)^2 \right) e^{-\frac{i}{\hbar}px} dx \quad (6)$$

$$= \frac{N}{\sqrt{2\pi\hbar}} \int \exp \left(- \left(\frac{x - x_0}{2\sigma} \right)^2 - \frac{i}{\hbar}px \right) dx \quad (7)$$

As we did, operate translation and change of variable. And transform a exponential of integrated function into the complete square one about x .

$$-x^2 - 2\frac{i}{\hbar}\sigma px = - \left(x + \frac{i}{\hbar}\sigma p \right)^2 - \frac{\sigma^2}{\hbar^2} p^2 \quad (8)$$

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In term of integration of x , there is a translation term and it can be negligible with the same reason in previous. So,

$$\phi(p, 0) = \frac{2\sigma N}{\sqrt{2\pi\hbar}} \exp\left(-\frac{\sigma^2}{\hbar^2}p^2 - \frac{i}{\hbar}x_0p\right) \int e^{-x^2} dx = \sqrt{\frac{2\sigma}{\hbar}} \left(\frac{1}{2\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{\sigma^2}{\hbar^2}p^2 - \frac{i}{\hbar}x_0p\right) \quad (9)$$

Then, $\phi(0, 0)$ is,

$$\phi(0, 0) = \sqrt{\frac{2\sigma}{\hbar}} \left(\frac{1}{2\pi}\right)^{\frac{1}{4}} \quad (10)$$

(3) Because it is a free particle, the time evolution of $\phi(x, 0)$ is $\phi(x, t) = e^{-i\omega t} \phi(p, 0)$ and $\omega = \frac{p^2}{2m\hbar}$.

$$\phi(p, t) = \sqrt{\frac{2\sigma}{\hbar}} \left(\frac{1}{2\pi}\right)^{\frac{1}{4}} \exp\left(-\alpha\left(p + \frac{ix_0}{2\alpha\hbar}\right)^2 - \frac{x_0^2}{4\alpha\hbar^2}\right), \quad \alpha = \frac{2m\sigma^2 + i\hbar t}{2m\hbar^2} \quad (11)$$

(4) $\psi(x, t)$ is a fourier transformation of $\phi(p, t)$,

$$\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p, t) e^{\frac{i}{\hbar}px} dp = \frac{1}{\hbar} \sqrt{\frac{\sigma}{\pi}} \left(\frac{1}{2\pi}\right)^{\frac{1}{4}} \int \exp\left(-\alpha\left(p + \frac{ix_0}{2\alpha\hbar}\right)^2 - \frac{x_0^2}{4\alpha\hbar^2} + \frac{i}{\hbar}px\right) dp \quad (12)$$

A exponential of a integrated function can be changed into the complete square form about p .

$$-\alpha\left(p + \frac{ix_0}{2\alpha\hbar}\right)^2 - \frac{x_0^2}{4\alpha\hbar^2} + \frac{i}{\hbar}px = -\alpha\left(p + i\frac{x_0 - x}{2\alpha\hbar}\right)^2 - \frac{(x_0 - x)^2}{4\alpha\hbar^2} \quad (13)$$

So,

$$\psi(x, t) = \frac{1}{\hbar} \sqrt{\frac{\sigma}{\pi}} \left(\frac{1}{2\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{(x_0 - x)^2}{4\alpha\hbar^2}\right) \int e^{-\alpha p^2} dp \quad (14)$$

$$= \frac{1}{\hbar} \sqrt{\frac{\sigma}{\alpha}} \left(\frac{1}{2\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{(x_0 - x)^2}{4\alpha\hbar^2}\right) \quad (15)$$

(5) From a (4), $|\psi(x, t)|^2$ and $|\psi(0, t)|^2$ are,

$$|\psi(x, t)|^2 = \frac{1}{\hbar^2} \frac{\sigma}{\sqrt{\alpha^*\alpha}} \left(\frac{1}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{(x_0 - x)^2}{4\alpha^*\hbar^2} - \frac{(x_0 - x)^2}{4\alpha\hbar^2}\right) \quad (16)$$

$$|\psi(0, t)|^2 = \frac{1}{\hbar^2} \frac{\sigma}{\sqrt{\alpha^*\alpha}} \left(\frac{1}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{x_0^2}{4\alpha^*\hbar^2} - \frac{x_0^2}{4\alpha\hbar^2}\right) \quad (17)$$

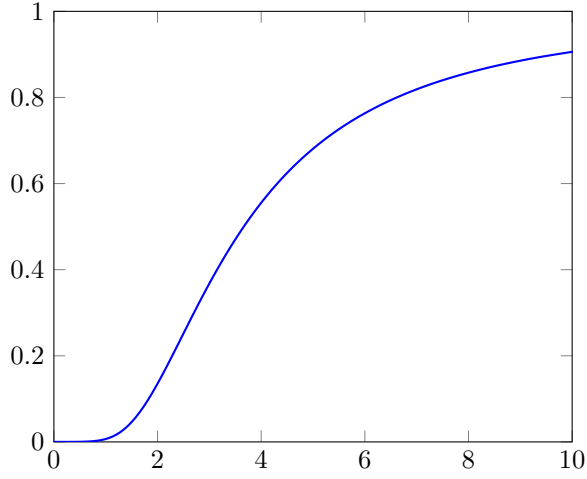
Since coefficients are canceled, there remains only exponential term.

$$\mathcal{S}(t) = \frac{|\psi(x, t)|^2}{|\psi(0, t)|^2} = \exp\left(-\frac{x^2 - 2xx_0}{4\hbar^2} \left(\frac{\alpha^* + \alpha}{|\alpha|^2}\right)\right) \quad (18)$$

We want to know that is the spread increases with time t . Since only α is dependent to time and time is a imaginary part of α , all of what is need to us is in $e^{-\frac{1}{|\alpha|^2}}$.

$$\frac{1}{|\alpha|^2} = \frac{4m^2\hbar^4}{4m^2\sigma^4 + \hbar^2 t^2}, \quad \mathcal{S}(t) = A \exp\left(-\frac{4m^2\hbar^4}{4m^2\sigma^4 + \hbar^2 t^2}\right) \quad (19)$$

A is a constant about t . The form of $\mathcal{S}(t)$ is $\exp\left(-\frac{k_1}{k_2 + t^2}\right)$. The derivative of $\mathcal{S}(t)$ is $\frac{2k_1 t}{(k_2 + t^2)^2} \mathcal{S}(t)$, being positive in all positive time t . This is a graph of $\exp(-\frac{10}{1+x^2})$ with $4m^2\hbar^2 = 10$, $4\frac{m^2\sigma^4}{\hbar^2} = 1$.



Problem 2. The Hamiltonian of the free particle is,

$$H = \frac{p^2}{2m}. \quad (20)$$

(1) $\langle p_x \rangle$ can be expanded about t .

$$\langle p_x \rangle = \langle p_x \rangle_{t=0} + \frac{1}{1!} \frac{d}{dt} \langle p_x \rangle \Big|_{t=0} t + \dots \quad (21)$$

Calculate $\frac{d}{dt} \langle p_x \rangle$ using Hamiltonian,

$$i\hbar \frac{d}{dt} \langle p_x \rangle = \langle [p_x, H] \rangle + i\hbar \left\langle \frac{\partial p_x}{\partial t} \right\rangle = \frac{1}{2m} \langle [p_x, p_x^2] \rangle = 0 \quad (22)$$

So, there remains only $\langle p_x \rangle_{t=0}$,

$$\langle p_x \rangle = \langle p_x \rangle_{t=0} \quad (23)$$

(2) With the same method,

$$\langle x \rangle = \langle x \rangle_{t=0} + \frac{1}{1!} \frac{d}{dt} \langle x \rangle \Big|_{t=0} t + \frac{1}{2!} \frac{d^2}{dt^2} \langle x \rangle \Big|_{t=0} t^2 + \dots \quad (24)$$

We have to calculate two time derivatives.

$$\frac{d}{dt} \langle x \rangle = \frac{1}{2im\hbar} \langle [x, p^2] \rangle + \left\langle \frac{\partial x}{\partial t} \right\rangle = \frac{1}{m} \langle p_x \rangle \quad (25)$$

$$\frac{d^2}{dt^2} \langle x \rangle = \frac{1}{m} \frac{d}{dt} \langle p_x \rangle = 0 \quad (26)$$

Finally,

$$\langle x \rangle = \langle x \rangle_{t=0} + \frac{\langle p_x \rangle_{t=0}}{2m} t \quad (27)$$

(3) From the definition of the deviation,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2, \quad (\Delta p_x)_{t=0}^2 = \langle p_x^2 \rangle_{t=0} - \langle p_x \rangle_{t=0}^2 \quad (28)$$

As we did,

$$\langle p_x^2 \rangle = \frac{1}{2m} \langle [p^2, p^2] \rangle = 0 = \langle p_x^2 \rangle_{t=0} \quad (29)$$

And we know that $\langle p_x \rangle^2 = \langle p_x \rangle_{t=0}^2$ by the result of (1). Therefore, $(\Delta p_x)^2 = (\Delta p_x)_{t=0}^2$.

(4) From the (3),

$$\frac{d}{dt}(\Delta x)^2 = \frac{d}{dt}\langle x^2 \rangle - \frac{d}{dt}\langle x \rangle^2 \quad (30)$$

We have to calculate two time derivatives.

$$\frac{d}{dt}\langle x^2 \rangle = \frac{1}{2im\hbar}\langle [x^2, p_x^2] \rangle = \frac{2}{m}\langle xp_x \rangle \quad (31)$$

$$\frac{d}{dt}\langle x \rangle = \frac{1}{2im\hbar}\langle [x, p_x^2] \rangle = \frac{1}{m}\langle p_x \rangle \quad (32)$$

$\langle xp_x \rangle$ can be approximated a series of time t .

$$\langle xp_x \rangle = \langle xp_x \rangle_{t=0} + \frac{1}{1!} \frac{d}{dt} \langle xp_x \rangle \Big|_{t=0} t + \frac{1}{2!} \frac{d^2}{dt^2} \langle xp_x \rangle \Big|_{t=0} t^2 + \dots \quad (33)$$

Most derivative calculations about expectation value are using the Hamiltonian.

$$\frac{d}{dt}\langle xp_x \rangle = \frac{1}{2im\hbar}\langle [xp_x, p^2] \rangle = \frac{1}{m}\langle p^2 \rangle \quad (34)$$

Since $\frac{d}{dt}\langle xp_x \rangle$ is a multiple of $\langle p^2 \rangle$, the quadratic and higher term will be vanished. So,

$$\langle xp_x \rangle = \langle xp_x \rangle_{t=0} + \frac{1}{m}\langle p^2 \rangle_{t=0} t \quad (35)$$

Substitute these results in $\frac{d}{dt}(\Delta x)^2$,

$$\frac{d}{dt}(\Delta x)^2 = \frac{2}{m}\langle xp_x \rangle - \frac{2}{m}\langle x \rangle \langle p_x \rangle \quad (36)$$

We already know that $\langle x \rangle$ and $\langle p_x \rangle$ can be represented by initial conditions.

$$\frac{d}{dt}(\Delta x)^2 = \frac{2}{m} \left(\langle xp_x \rangle_{t=0} + \frac{\langle p^2 \rangle_{t=0}}{m} t \right) - \frac{2}{m} \langle p_x \rangle_{t=0} \left(\langle x \rangle_{t=0} + \frac{\langle p_x \rangle_{t=0}}{2m} t \right) \quad (37)$$

Problem 3. In this problem, the wave function of a particle is,

$$\psi(x) = C \exp \left[i \frac{p_0 x}{\hbar} - \frac{(x - x_0)^2}{2\sigma^2} \right] \quad (38)$$

(1) The normalization constant is calculable from the normalization.

$$C^2 \int \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx = C^2 \int \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx = C^2 \sigma \sqrt{\pi} \quad (39)$$

The result of the normalization must be 1. So,

$$C = \left(\frac{1}{\sigma \sqrt{\pi}} \right)^{\frac{1}{2}} \quad (40)$$

(2) First, let us find the mean value of x .

$$\langle x \rangle = \int \psi^* x \psi dx = \frac{1}{\sigma \sqrt{\pi}} \int x \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx \quad (41)$$

$$\int x \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx = \int x e^{-\left(\frac{x}{\sigma}\right)^2} dx + x_0 \int e^{-\left(\frac{x}{\sigma}\right)^2} dx \quad (42)$$

The first term of the right side is a zero, because $xe^{-(\frac{x}{\sigma})^2}$ is a even function and this integration is from $-\infty$ to ∞ . The calculation of the second term is simple.

$$x_0 \int e^{-(\frac{x}{\sigma})^2} dx = x_0 \sigma \sqrt{\pi} \quad (43)$$

So, the mean value is a x_0 .

$$\langle x \rangle = \frac{1}{\sigma \sqrt{\pi}} x_0 \sigma \sqrt{\pi} = x_0 \quad (44)$$

The mean value of p is,

$$\langle p \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} dx = \frac{-i\hbar}{\sigma \sqrt{\pi}} \int \left(\frac{i}{\hbar} p_0 - \frac{x - x_0}{\sigma^2} \right) \exp \left(-\left(\frac{x - x_0}{\sigma} \right)^2 \right) dx \quad (45)$$

$$= \frac{-i\hbar}{\sigma \sqrt{\pi}} \left[\frac{i}{\hbar} p_0 \int \exp \left(-\left(\frac{x - x_0}{\sigma} \right)^2 \right) dx - \int \left(\frac{x - x_0}{\sigma^2} \right) \exp \left(-\left(\frac{x - x_0}{\sigma} \right)^2 \right) dx \right] = p_0 \quad (46)$$

Because the second term is a even function about $x = x_0$, it is a zero.

(3) From a (3) in problem 2, we use the definition of the deviation.

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2, \quad (\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 \quad (47)$$

First we calculate $\langle x^2 \rangle$.

$$\langle x^2 \rangle = \frac{1}{\sigma \sqrt{\pi}} \int x^2 \exp \left(-\left(\frac{x - x_0}{\sigma} \right)^2 \right) dx = \frac{1}{\sigma \sqrt{\pi}} \left[\int x^2 e^{-(\frac{x}{\sigma})^2} dx + 2x_0 \int x e^{-(\frac{x}{\sigma})^2} dx + x_0^2 \int e^{-(\frac{x}{\sigma})^2} dx \right] \quad (48)$$

The middle term of the right side is zero from a (2) and the last term is $x_0^2 \sigma \sqrt{\pi}$.

$$\int x^2 e^{-(\frac{x}{\sigma})^2} dx = \sigma^3 \int x^2 e^{-x^2} dx = -\frac{1}{2} \sigma^3 [x e^{-x^2}]_{-\infty}^{\infty} + \frac{1}{2} \sigma^3 \int e^{-x^2} dx = \frac{1}{2} \sigma^3 \sqrt{\pi} \quad (49)$$

So,

$$\langle x^2 \rangle = \frac{1}{\sigma \sqrt{\pi}} \left[x_0^2 \sigma \sqrt{\pi} + \frac{1}{2} \sigma^3 \sqrt{\pi} \right] = \frac{1}{2} \sigma^2 + x_0^2 \quad (50)$$

Then $(\Delta x)^2$ is,

$$(\Delta x)^2 = \frac{1}{2} \sigma^2 + x_0^2 - x_0^2 = \frac{1}{2} \sigma^2 \quad (51)$$

the expectation value of p^2 is,

$$\langle p^2 \rangle = -\hbar^2 \int \psi^* \frac{\partial^2 \psi}{\partial x^2} dx = -\hbar^2 \int \left(\frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} \right) - \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} \right) dx \quad (52)$$

There are two terms that seem complicated. But, some of the integration in calculation will be canceled since these are even functions and the integration range is symmetric.

$$\int \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} \right) dx = \frac{1}{\sigma \sqrt{\pi}} \int \frac{\partial}{\partial x} \left(\left(\frac{i}{\hbar} p_0 - \frac{x - x_0}{\sigma^2} \right) \exp \left(-\left(\frac{x - x_0}{\sigma} \right)^2 \right) \right) dx = 0 \quad (53)$$

$$\int \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} dx = \frac{1}{\sigma \sqrt{\pi}} \int \left(\left(\frac{p_0}{\hbar} \right)^2 + \left(\frac{x - x_0}{\sigma^2} \right)^2 \right) \exp \left(-\left(\frac{x - x_0}{\sigma} \right)^2 \right) dx = \left(\frac{p_0}{\hbar} \right)^2 + \frac{1}{\sigma^2 \sqrt{\pi}} \int x^2 e^{-x^2} dx \quad (54)$$

It is a simple gaussian integration.

$$\int x^2 e^{-x^2} dx = -\frac{1}{2} \left[x e^{-x^2} \right]_{-\infty}^{\infty} + \frac{1}{2} \int e^{-x^2} dx = \frac{\sqrt{\pi}}{2} \quad (55)$$

From these results, we can calculate $\langle p^2 \rangle$.

$$\langle p^2 \rangle = p_0^2 + \frac{\hbar^2}{2\sigma^2} \quad (56)$$

Finally, we can calculate $(\Delta p)^2$,

$$(\Delta p)^2 = p_0^2 + \frac{\hbar^2}{2\sigma^2} - p_0^2 = \frac{\hbar^2}{2\sigma^2} \quad (57)$$

Confirm these result does satisfy Heisenberg's uncertainty principle.

$$\Delta x \Delta p = \sqrt{\frac{\hbar^2}{2\sigma^2} \frac{\sigma^2}{2}} = \frac{\hbar}{2} \quad (58)$$

It is in the sense.

Problem 4.

(a) The initial state is,

$$\psi(\mathbf{x}, 0) = c_1 \psi_1(\mathbf{x}) + c_2 \psi_2(\mathbf{x}) \quad (59)$$

Since this particle is in region Ω_1 , $c_1 = 1$ and $c_2 = 0$. The time evolutoin of this particle is,

$$\psi(\mathbf{x}, t) = c_1 e^{-\frac{i}{\hbar} E_1 t} \psi_1(\mathbf{x}) + c_2 e^{-\frac{i}{\hbar} E_2 t} \psi_2(\mathbf{x}) = e^{-\frac{i}{\hbar} E_1 t} \psi_1(\mathbf{x}) \quad (60)$$

Since the time evolution is dependent to only $\psi_1(\mathbf{x})$, it will stay region Ω_1 , forever.

(b) The time evolution is,

$$\psi(\mathbf{x}, t) = \frac{1}{\sqrt{2}} \left[e^{-\frac{i}{\hbar} E_1 t} \psi_1(\mathbf{x}) + e^{-\frac{i}{\hbar} E_2 t} \psi_2(\mathbf{x}) \right] \quad (61)$$

Consider the probability density of this particle.

$$|\psi(\mathbf{x}, t)|^2 = \frac{1}{2} \left[|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2 + e^{-\frac{i}{\hbar} (E_2 - E_1) t} \psi_1^* \psi_2 + e^{-\frac{i}{\hbar} (E_1 - E_2) t} \psi_1 \psi_2^* \right] \quad (62)$$

Suppose that Ω_3 in \mathbb{R}^3 satisfies that $\Omega_1 \cap \Omega_3 = \emptyset$, $\Omega_2 \cap \Omega_3 = \emptyset$ and $\Omega_1 \cup \Omega_2 \cup \Omega_3 = \mathbb{R}$. If $\mathbf{x} \notin \Omega_1$, then $\psi_1(\mathbf{x}) = 0$. If $\mathbf{x} \notin \Omega_2$, then $\psi_2(\mathbf{x}) = 0$. And $\psi_1^* \psi_2 = \psi_1 \psi_2^* = 0$ any $\mathbf{x} \in \mathbb{R}$ because of following reasons.

- (i) $\mathbf{x} \in \Omega_1 \implies \psi_2 = \psi_2^* = 0$
- (ii) $\mathbf{x} \in \Omega_2 \implies \psi_1 = \psi_1^* = 0$
- (iii) $\mathbf{x} \in \Omega_3 \implies \psi_1 = \psi_2 = 0$

Therefore, $|\psi(\mathbf{x}, t)|^2 = \frac{1}{2} [|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2]$. And the probability density is time-independent.

(c) From a (62), since $E_2 - E_1 = \hbar\Omega$,

$$|\psi(\mathbf{x}, t)|^2 = \frac{1}{2} [|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2 + e^{-i\omega t} \psi_1^* \psi_2 + e^{i\omega t} \psi_1 \psi_2^*] \quad (63)$$

$$= \frac{1}{2} [|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2 + e^{-i\omega t} \psi_1^* \psi_2 + (e^{-i\omega t} \psi_1^* \psi_2)^*] \quad (64)$$

Imaginary parts of the last two terms are canceled.

$$|\psi(\mathbf{x}, t)|^2 = \frac{1}{2} [|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2 + (\psi_1^* \psi_2 + (\psi_1^* \psi_2)^*) \cos \omega t] \quad (65)$$

This result is a periodic function about time because the last term is a periodic function of time and other terms are constant about time.

(d) From the continuity equation, We use the integration of this equation because of the right term.

$$\int_{\Omega_2} \frac{\partial \rho}{\partial t} dr^3 = \int_{\Omega_2} \nabla \cdot \mathbf{J} dr^3 \quad (66)$$

The left term can be calculated using (c),

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t} |\psi(\mathbf{x}, t)|^2 = -\omega \psi_1 \psi_2 \sin \omega t \quad (67)$$

If we integrate this, it will be a zero since ψ_1 and ψ_2 are orthogonal to each other. Consider the right term. This integration is changed into the surface integration following Green's Theorem.

$$\int_{\Omega_2} \nabla \cdot \mathbf{J} dr^3 = \int_{\Omega_2} \mathbf{J} \cdot d\mathbf{S} \quad (68)$$

Because wave functions are isotropic, a current has the same value in a different direction. It means that this integration is replaced by the just inner product.

$$\int_{\Omega_2} \mathbf{J} \cdot d\mathbf{S} = 4\pi R_2^2 \mathbf{J} \cdot \hat{n} \quad (69)$$

\hat{n} is a vector that is vertical to the surface of a sphere Ω_2 . Fianlly,

$$0 = 4\pi R_2^2 \mathbf{J} \cdot \hat{n} \quad (70)$$

This means that there is no probability current between region Ω_1 and Ω_2 .