Quantum Mechanics
Qualifying Exam–August 2010

Notes and Instructions:

- There are **6** problems and **7** pages.
- Be sure to write your alias at the top of every page.
- Number each page with the problem number, and page number of your solution (e.g. "Problem 3, p. 1/4" is the first page of a four page solution to problem 3).
- **You must show all your work**.

Possibly useful formulas:

Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

One-dimensional simple harmonic oscillator operators:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$$

$$P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$Y_0^0(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_2^2(\theta, \varphi) = \frac{5}{\sqrt{96\pi}} 3 \sin^2\theta \, e^{2i\varphi}$$

$$Y_2^1(\theta, \varphi) = -\frac{5}{\sqrt{24\pi}} 3 \sin\theta \cos\theta \, e^{i\varphi}$$

$$Y_1^1(\theta, \varphi) = -\frac{3}{\sqrt{8\pi}} \sin\theta \, e^{i\varphi} \qquad Y_2^0(\theta, \varphi) = \frac{5}{\sqrt{4\pi}} \left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$Y_1^0(\theta, \varphi) = \frac{3}{\sqrt{4\pi}} \cos\theta \qquad Y_2^{-1}(\theta, \varphi) = \frac{5}{\sqrt{24\pi}} 3 \sin\theta \cos\theta \, e^{-i\varphi}$$

$$Y_1^{-1}(\theta, \varphi) = \frac{3}{\sqrt{8\pi}} \sin\theta \, e^{-i\varphi} \qquad Y_2^{-2}(\theta, \varphi) = \frac{5}{\sqrt{96\pi}} 3 \sin^2\theta \, e^{-2i\varphi}$$

In spherical coordinates, the Laplacian is

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

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PROBLEM 1: Motion of a Particle in One Dimension

Consider a particle of mass m moving along the $+x$ direction in free space.

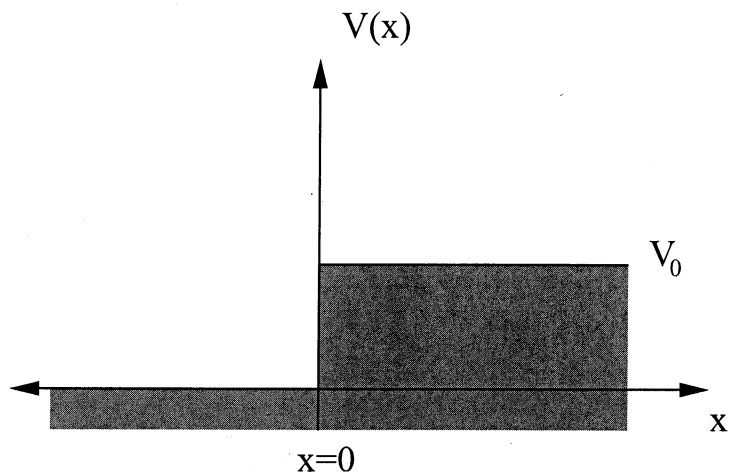
(a) [2 points] Suppose the particle is in a momentum eigenstate where the particles momentum is known precisely to be p_0. Write a wavefunction $\Psi(x, t)$ that describes such a state.

n. (b) [2 points] Suppose the particle is in a state where it is equally probable for the particle to have any momentum between $p_0 - \Delta p/2$ and $p_0 + \Delta p/2$ at time $t = 0$. Construct a wavefunction $\Psi(x, t)$ that describes such a state.

(c) [2 points] Suppose a beam of particles, each in the state described in part (a), encounters an abrupt step in potential energy at $x = 0$. The step height V_0 is less than the particles total energy E. Construct the wavefunction, $\Psi(x, t)$ with $-\infty \leq x \leq \infty$, that describes this situation.

(d) [2 points] Calculate the probability that a particle is reflected by the potential energy step described in part (c).

(e) [2 points] Consider the situation described in part (c), except with V_0 greater than E. Compare the probability of finding a particle at a distance x inside the barrier to the probability of finding a particle at $x = 0$.



P1

$$\hat{P}|p\rangle = p_0|p\rangle \Rightarrow$$

$$\psi(x,t) = \phi(x)\, e^{-iEt/\hbar}$$

$$\rightarrow \phi(x) = \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{ipx/\hbar}\, dp$$

$$\hat{P}|p\rangle = P_0|p\rangle$$

$$\Rightarrow \langle x|\hat{P}|p\rangle = \langle x|P_0|P\rangle$$

$$\Rightarrow \int_{-\infty}^{+\infty} \langle x|\hat{P}|y\rangle\langle y|P\rangle\, dy = P_0\langle x|P\rangle$$

$$\Rightarrow -i\hbar\int_{-\infty}^{+\infty}\frac{d}{dx}\delta(x-y)\underbrace{\langle y|P\rangle}_{\phi_p(y)}\, dy = P_0\langle x|P\rangle$$

$$\Rightarrow -i\hbar\frac{d}{dx}\phi_p(x) = P_0\,\phi_p(x)$$

$$\Rightarrow \frac{d\phi_{p_0}(x)}{dx} = -\frac{P_0}{i\hbar}\phi_p(x)$$

$$\Rightarrow \frac{d\phi_{p_0}(x)}{dx} = \frac{iP_0}{\hbar}\phi_p(x)$$

$$\Rightarrow \underbrace{\phi_{p_0}(x)}_{\langle x|P\rangle} = A e^{iP_0x/\hbar} = A e^{ik_0x}$$

Now for a free particle.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$$K^2 = \frac{2mE}{\hbar^2}$$

$$\Rightarrow E = \frac{\hbar^2K_0^2}{2m}$$

$$\lambda^2 = -k_0^2$$

$$\Rightarrow \psi(x) = Ae^{-iK_0x} + Be^{iK_0x}$$

$$\psi(x,t) = \phi_p(x)\, e^{-iEt/\hbar} = A e^{iK_0x} e^{-iEt/\hbar}$$

$$= A e^{i(K_0x - \frac{\hbar^2K_0^2}{2m}t)}$$

$$=$$

$$\psi(x,0) = Ae^{ikx}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{p_0-\Delta p/2}^{p_0+\Delta p/2} A e^{ikx} e^{-ikx} \, dx$$

$$\psi(x,t) = Ae^{ip_0x/\hbar}$$

$$\cancel{\psi(x,t) = \int_{p_0-\Delta p/2}^{p_0+\Delta p/2} A e^{ipx/\hbar} \, dp}$$

$$= \frac{\hbar}{x}$$

F-10

PROBLEM 2: Harmonic Oscillator with Two Particles

Consider a Hamiltonian for two non-interacting particles:

$$
\begin{aligned}
H(1,2) &= \frac{P_1^2}{2m} + \frac{1}{2}m\omega_1^2 X_1^2 + \frac{P_2^2}{2m} + \frac{1}{2}m\omega_2^2 X_2^2 \\
&= H_1 + H_2
\end{aligned}
$$

where $\omega_2 = 2\omega_1 = 2\omega$.

Defining the raising and lowering operators:

$$
\begin{aligned}
a_n &= \frac{1}{\sqrt{2}}(\bar{X}_n + i\bar{P}_n) \\
a_n^\dagger &= \frac{1}{\sqrt{2}}(\bar{X}_n - i\bar{P}_n)
\end{aligned}
$$

where $n = 1, 2$ and

$$
\begin{aligned}
\bar{X}_n &= \left(\frac{m\omega_n}{\hbar}\right)^{1/2} X_n \\
\bar{P}_n &= \left(\frac{1}{\hbar m\omega_n}\right)^{1/2} P_n
\end{aligned}
$$

$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

such that $[a_m, a_n^\dagger] = \delta_{mn}, m, n = 1, 2$.

Answer the following questions:

(a) [2 points] Write the Hamiltonian in terms of raising and lowering operators.

(b) [2 points] Write the eigenvector $|\psi_{n_1,n_2}\rangle$ in terms of the ground state $|\psi_{0,0}\rangle = |\phi_{n_1=0}\rangle|\phi_{n_2=0}\rangle$ where $|\phi_{n_1}\rangle$ is the eigenvector for particle 1, i.e.,

$$H_1|\phi_{n_1}\rangle = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1|\phi_{n_1}\rangle$$

and similarly for particle 2.

(c) [1 points] Write a formula for the energy levels of this oscillator, E_n with n defined in terms of n_1 and n_2.

(d) [1 points] Determine a formula for the degeneracy, g_n , of an energy level E_n. Need to talk

(e) [2 points] Using your results from part (d) determine the degeneracy g_n for the energy, $E = 15/2\hbar\omega$ and list all the eigenfunctions $|\psi_{n_1,n_2}\rangle$ that have this energy. Need to talk

(f) [2 points] Determine ΔX_1, the uncertainty in X_1 for the state $|\psi_{n_1=1,n_2=2}\rangle$ using raising and lowering operators. Discuss the dependence of ΔX_1, on the frequency ω_1 and explain why it makes sense physically.

Prb2.

a) $$H(1,2) = \frac{\hat{p}_1^2}{2m} + \frac{1}{2}m\omega_1^2\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega_2^2\hat{x}_2^2$$

$$a_n^+ a_n = \frac{1}{2}(\bar{x}_n + i\bar{P}_n)(\bar{x}_n - i\bar{P}_n) = \frac{1}{2}[\hat{x}_n^2 - i\bar{x}_n\bar{P}_n + i\bar{P}_n\bar{x}_n + \bar{P}_n^2]$$

$$= \frac{1}{2}\{\hat{\bar{x}}_n^2 + \hat{\bar{P}}_n^2 - i\underbrace{[\bar{x}_n, \bar{P}_n]}\}$$

$$= \frac{1}{2}(\bar{x}_n^2 + \bar{P}_n^2 - i\hbar) = \frac{m\omega_n}{2\hbar}\hat{x}_n^2 + \frac{1}{2\hbar m\omega_n}\hat{P}_n^2 - \frac{\hbar}{2}$$

$$[\bar{x}_n, \bar{P}_n] = \frac{1}{\hbar}[\hat{x}, \hat{p}] = +i$$

$$H(1,2) = \hbar\omega_n \frac{\hat{P}_n^2}{2\hbar m\omega_n} + \hbar\omega_n \frac{m\omega_n}{2\hbar}\hat{x}_n^2$$

$$= \hbar\omega_n\left(a_n^+ a_n - \frac{m\omega_n}{2\hbar}\hat{x}_n^2 + \frac{1}{2}\right) + \hbar\omega_n \frac{m\omega_n}{2\hbar}\hat{x}_n^2$$

$$= \hbar\omega_n\left(a_n^+ a_n + \frac{1}{2}\right)$$

$$= \hbar\omega_1\left(a_1^+ a_1 + \frac{1}{2}\right) + \hbar\omega_2\left(a_2^+ a_2 + \frac{1}{2}\right)$$

$$= \hbar\omega\left(a_1^+ a_1 + \frac{1}{2}\right) + 2\hbar\omega\left(a_2^+ a_2 + \frac{1}{2}\right) = \hbar\omega\left(a_1^+ a + 2a_2^+ a_2 + \frac{3}{2}\right)$$

b) $$|\psi_{n_1,n_2}\rangle = (a_1^+)^{n_1}(a_2^+)^{n_2}|\psi_{0,0}\rangle = (1\sqrt{2}\sqrt{3}\cdots\cdots\sqrt{n_1})(1\sqrt{2}\sqrt{3}\cdots\sqrt{n_2})|\psi_{00}\rangle$$

~~wrong!~~

$$= (n_1!n_2!)^{1/2}|\psi_{n_1n_2}\rangle \quad \left[\begin{array}{l}(a_1^+)^{n}(a_2^+)^{n_2}[|\Phi_{0_1}\rangle\otimes|\Phi_{0_2}\rangle] \\ \neq 1\end{array}\right]$$

$$\Rightarrow |\psi_{n_1n_2}\rangle = \frac{(a_1^+)^{n_1}(a_2^+)^{n_2}}{\sqrt{n_1!\,n_2!}}$$

c) $$E_n = E_1 + E_2 = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1 + \left(n_2 + \frac{1}{2}\right)\hbar\omega_2 = \left(n_1 + \frac{1}{2}\right)\hbar\omega + \left(n_2 + \frac{1}{2}\right)2\hbar\omega$$

$$= \left(2n_2 + n_1 + \frac{3}{2}\right)\hbar\omega$$

$$= \left(n + \frac{3}{2}\right)\hbar\omega$$

where, $n = 2n_2 + n_1$

d) $$g_n = \binom{n + D - 1}{n}$$

f) $(\Delta x_1) = \sqrt{\langle x_1^2\rangle - \langle x_1\rangle^2}$

$\sqrt{2}\bar{x}_n = a_n + a_n^+$

$\Rightarrow \langle \hat{x}_1\rangle = \langle \psi_{n_1=1, n_2=2} | \hat{x}_1 | \psi_{n_1=1,n_2=2}\rangle$

$\Rightarrow \bar{x}_n = \frac{1}{\sqrt{2}}(a_n + a_n^+)$

$= \langle n_1=1, n_2=2 | \left(\frac{\hbar}{2m\omega_1}\right)^{1/2} (a_1 + a_1^+) | n_1=1 n_2=2\rangle \Rightarrow \hat{x}_n = \left(\frac{\hbar}{2m\omega_n}\right)^{1/2}(a_n + a_n^+)$

$= \sqrt{\frac{\hbar}{2m\omega_1}} \langle n_1=1, n_2=2 | a_1 + a_1^+ | n_1=1, n_2=2\rangle$

$= 0$

$\Rightarrow \langle \hat{x}_1^2\rangle = \frac{\hbar}{2m\omega_1} \langle 1\ 2 | a_1^2 + (a_1^+)^2 + a_1 a_1^+ + a_1^+ a_1 | 1\ 2\rangle$

$= \frac{\hbar}{2m\omega_1}\left[\sqrt{2}\sqrt{2} + \sqrt{1}\sqrt{1}\right] = \frac{3\hbar}{2m\omega_1}$

$(\Delta x_1) = \sqrt{\frac{3\hbar}{2m\omega_1}}$ No explanation!

$\omega_1 \to$ angular velocity it moves faster harder to pin down the pos.!

e) $E = \frac{15}{2}\hbar\omega = (n + \frac{3}{2})\hbar\omega$ $D = 2$

$\Rightarrow \frac{15}{2} = n + \frac{3}{2} \Rightarrow n = 6$

$g_n = \binom{6+2-1}{6} = \binom{7}{6} = \frac{7!}{6!} = 7$

$2n_2 + n_1 = 6$

$\Rightarrow n_2 = \frac{6 - n_1}{2}$

$n_1 = 0 \quad n_2 = 3$

$n_1 = 1 \quad n_2 \neq$

$n_1 = 2 \quad n_2 = 2$

$n_1 = 3$

F-10

PROBLEM 3: Dirac formulation of quantum mechanics

Let $\mathcal{E}_3$ be a three-dimensional Hilbert space that is spanned by the orthonormal basis $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$. The operator Ω acts in $\mathcal{E}_3$ as follows:

$$\Omega|u_1\rangle = 3|u_1\rangle \tag{1}$$
$$\Omega|u_2\rangle = 2|u_2\rangle - |u_3\rangle \tag{2}$$
$$\Omega|u_3\rangle = -|u_2\rangle + 2|u_3\rangle \tag{3}$$

(a) [5 pt] Prove that Ω is Hermitian. Find its eigenvalues, ω_1, ω_2, and ω_3, and write down each of the corresponding eigenvectors in the $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis.

(b) [1 pt] Does $\{\Omega\}$ constitute a complete set of commuting operators for $\mathcal{E}_3$? Why or why not?

(c) [2 pt] According to Eq. (1), $\mathcal{E}_3$ can be partitioned into eigensubspaces by letting $\mathcal{E}_a$ be the subspace spanned by $\{|u_1\rangle\}$ and $\mathcal{E}_b$ be its orthogonal supplement. Construct an orthonormal basis $\{|t_2\rangle, |t_3\rangle\}$ of $\mathcal{E}_b$, and write each basis vector in $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis. (Choose $|t_3\rangle$ to correspond to the *smallest* eigenvalue of Ω.)

??

(d) [2 pt] With $|t_1\rangle = |u_1\rangle$, the set $\{|t_1\rangle, |t_2\rangle, |t_3\rangle\}$ constitutes an alternate basis of $\mathcal{E}_3$. Find the matrix S, with elements $S_{i,k} = \langle u_i \mid t_k\rangle$, that transforms between $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ and $\{|t_1\rangle, |t_2\rangle, |t_3\rangle\}$.

P3.

$$\Omega|u_1\rangle = 3|u_1\rangle$$

$$\Omega|u_2\rangle = 2|u_2\rangle - |u_3\rangle$$

$$\Omega|u_3\rangle = -|u_2\rangle + 2|u_3\rangle$$

a. $$\Omega = \begin{array}{c|ccc} & |u_1\rangle & |u_2\rangle & |u_3\rangle \\ \hline \langle u_1| & & & \\ \langle u_2| & & & \\ \langle u_3| & & & \end{array} \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

it is clear now that $\Omega = \Omega^\dagger$

$$\begin{vmatrix} 3-\lambda & 0 & 0 \\ 0 & 2-\lambda & -1 \\ 0 & -1 & 2-\lambda \end{vmatrix} = 0 \Rightarrow (3-\lambda)\{(2-\lambda)^2 - 1\} = 0$$

$$\Rightarrow (3-\lambda)(2-\lambda-1)(2-\lambda+1) = 0$$

$$\Rightarrow (3-\lambda)(1-\lambda)(3-\lambda) = 0$$

$$\Rightarrow \lambda = 1, 3, 3$$

$\underline{\lambda = 1}$

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$\Rightarrow 2a_1 = 0 \Rightarrow a_1 = 0$ $\quad \rightarrow |\lambda = 1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$

$$\left.\begin{array}{l} \Rightarrow a_2 - a_3 = 0 \\ \Rightarrow -a_2 + a_3 = 0 \end{array}\right\} a_2 = a_3$$

$\underline{\lambda = 3}$

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & -1 & -1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \begin{array}{l} \Rightarrow b_1 \text{ arbitary} \\ \Rightarrow -b_2 - b_3 = 0 \Rightarrow b_3 = -b_2 \end{array}$$

$$|\lambda = 3\rangle = \frac{1}{\sqrt{|b_1|^2 + 2|b_2|^2}} \begin{pmatrix} b_1 \\ b_2 \\ -b_2 \end{pmatrix}$$

$$\langle \lambda = 3, 1| = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

Now,

$$\langle \lambda = 3, 2 | \lambda = 3, 1\rangle = 0$$

$$\begin{pmatrix} b_1 & b_2 & -b_2 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} = 0 \quad \Rightarrow \quad b_2 = 0$$

$$|\lambda = 3, 2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

b) Now, Since Ω is degenerate $\{\Omega\}$ itself cannot constitute a CSCO

c)

PROBLEM 4: Stationary Perturbation Theory

Consider a non-relativistic particle of mass m moving in the three dimensional potential:

$$V(x) = \frac{1}{2}k(x^2 + y^2 + z^2)\,.$$

(a) [1 point] What is the ground state energy and first excited state energy for this potential?

Now there is a perturbation applied so the potential becomes

$$V(x) = \frac{1}{2}k(x^2 + y^2 + z^2) + \lambda xy$$

where λ is a small parameter.

(b) [1 point] Calculate the ground state energy to first order in λ.

(c) [4 point] Calculate the ground state energy to second order in λ.

(d) [4 point] Calculate the first excited state energies to first order in λ.

↑ degenerate?

P4

$$V(x) = \frac{1}{2}k(x^2+y^2+z^2) = \frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

a) Recognize this is a Harmonic Oscillator potential (3 dim)

So, $E_n = (n_x+\frac{1}{2})\hbar\omega_x + (n_y+\frac{1}{2})\hbar\omega_y + (n_z+\frac{1}{2})\hbar\omega_z$

$$= (n_x+n_y+n_z+\tfrac{3}{2})\hbar\omega = (n+\tfrac{3}{2})\hbar\omega$$

$$E_0 = \frac{3}{2}\hbar\omega$$

$$E_1 = (1+\tfrac{3}{2})\hbar\omega = \tfrac{5}{2}\hbar\omega$$

$$\rightsquigarrow V(x) = \frac{1}{2}k(x^2+y^2+z^2) + \lambda xy$$

$$\rightsquigarrow H = H_0 + \lambda xy = H_0 + \lambda H_1$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots = \sum_{m=0}^{\infty} \lambda^m E_n^{(m)}$$

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots = \sum_{m=0}^{\infty} \lambda^m |n^{(m)}\rangle$$

For Harmonic oscillator in stationary state, the EOM becomes eigen value eqn

$$H|n\rangle = E_n|n\rangle$$

$$\Rightarrow (H_0 + \lambda H_1)\left(\sum_{m=0}^{\infty}\lambda^m |n^{(m)}\rangle\right) = \left(\sum_{m=0}^{\infty}\lambda^m E_n^{(m)}\right)\left(\sum_{m=0}^{\infty}\lambda^m |n^{(m)}\rangle\right)$$

To the 1st order in λ

$$H_1 |n^{(0)}\rangle + H_0 |n^{(1)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle$$

$\Rightarrow$ Multiply both sides $\langle n^{(0)}|$

$$\Rightarrow \langle n^{(0)} | H_1 | n^{(0)}\rangle + \underbrace{\langle n^{(0)} | H_0 | n^{(1)}\rangle}_{=0} = \underbrace{\langle n^{(0)} | E_n^{(0)} | n^{(1)}\rangle}_{0} + \langle n^{(0)} | E_n^{(1)} | n^{(0)}\rangle$$

$$\Rightarrow \langle n^{(0)} | H_1 | n^{(0)}\rangle = E_n(1)$$

$$E_n^{(1)} = \langle n^{(0)} | H_1 | n^{(0)}\rangle$$

$(a+a^\dagger)(a-a^\dagger)$

$(a)^2 + aa^\dagger + a^\dagger a - a^{\dagger 2}$

In our case,

$$E_n^{(1)} = \langle n_x n_y n_z | \hat{x}\hat{y} | n_x n_y n_z\rangle$$

$$= \frac{\hbar}{2m\omega}\left(-\frac{m\omega\hbar}{2}\right)\langle n_x n_y n_z | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | n_x n_y n_z\rangle$$

$$= -\frac{\hbar^2}{4}\langle 000 | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | 000\rangle$$

$$E_0^{(1)} = 0$$

$$E_0 = \frac{3}{2}\hbar\omega + E_0^{(1)} = \frac{3}{2}\hbar\omega$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m^{(0)} | H_1 | n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$= \sum_{m_x, m_y, m_z} \frac{|\langle m_x^{(0)} m_y^{(0)} m_z^{(0)} | H_1 | n_x^{(0)} n_y^{(0)} n_z^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\langle m_x^{(0)} m_y^{(0)} m_z^{(0)} | \hat{x}\hat{y} | n_x^{(0)} n_y^{(0)} n_z^{(0)} \rangle$$

$$= \frac{\hbar}{2m\omega} \langle m_x^{(0)} m_y^{(0)} m_z^{(0)} | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | n_x^{(0)} n_y^{(0)} n_z^{(0)} \rangle$$

$$= \frac{\hbar}{2m\omega} \langle m | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | n \rangle$$

$$= \frac{\hbar}{2m\omega} \left\{ \langle m | a_x a_y | n \rangle + \langle m | a_x a_y^\dagger | n \rangle + \langle m | a_x^\dagger a_y | n \rangle + \langle m | a_x^\dagger a_y^\dagger | n \rangle \right\}$$

$$= \frac{\hbar}{2m\omega} \left\{ \sqrt{n_y}\sqrt{n_x}\, \delta_{m_x, n_x - 1} \delta_{m_y, n_y - 1} \delta_{m_z, n_z} + \sqrt{n_x}\sqrt{n_y+1}\, \delta_{m_x, n_x - 1} \delta_{m_y, n_y + 1} \delta_{m_z n_z} + \sqrt{n_x+1}\sqrt{n_y}\, \delta_{m_x, n_x + 1} \delta_{m_y, n_y - 1} \delta_{m_z, n_z} + \sqrt{n_x+1}\sqrt{n_y+1}\, \delta_{m_x, n_x + 1} \delta_{m_y, n_y + 1} \delta_{m_z, n_z} \right\}$$

For Ground state we have $|000\rangle$

$$= \frac{\hbar}{2m\omega} \left\{ 1 \ \langle 110 | 000 \rangle \right\} \qquad |m_x, m_y, m_z\rangle = |110\rangle$$

$$m = 2$$

$$E_0^{(2)} = \frac{\hbar^2 / 4m^2\omega^2}{E_0^{(0)} - E_2^{(0)}}$$

$$\rightsquigarrow E_2^{(0)} = (m + \tfrac{3}{2})\hbar\omega = \tfrac{7}{2}\hbar\omega$$

$$\rightsquigarrow E_0^{(0)} - E_2^{(0)} = -2\hbar\omega$$

$$E_0^{(2)} = \frac{\hbar^2}{4m^2\omega^2 \times (-2\hbar\omega)} = -\frac{\hbar}{8m^2\omega^3}$$

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)}$$

$$= \frac{3}{2}\hbar\omega - \frac{\lambda^2\hbar}{8m^2\omega^3}$$

d) $$E_n^{(1)} = \langle n^{(0)} | H_1 | n^{(0)} \rangle$$

$$= \langle n_x^{(0)} n_y^{(0)} n_z^{(0)} | H_1 | n_x^{(0)} n_y^{(0)} n_z^{(0)} \rangle$$

$$= \frac{\hbar}{2m\omega} \langle n_x^{(0)} n_y^{(0)} n_z^{(0)} | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | n_x^{(0)} n_y^{(0)} n_z^{(0)} \rangle$$

$$= \frac{\hbar}{2m\omega} \Big\{ \overset{\sqrt{n_x}\sqrt{n_y}}{\uparrow} \delta_{n_x, n_x-1}\, \delta_{n_y, n_y-1} + \overset{\sqrt{n_x}\sqrt{n_y+1}}{\uparrow} \delta_{n_x, n_{x-1}}\, \delta_{n_y, n_y+1} + \overset{\sqrt{n_x+1}\sqrt{n_y}}{\uparrow} \delta_{n_x, n_x+1}\, \delta_{n_y, n_y-1}$$
$$+ \overset{\sqrt{n_x+1}\sqrt{n_y+1}}{\uparrow} \delta_{n_x, n_x+1}\, \delta_{n_y, n_y+1} \Big\}$$

$$= \frac{\hbar}{2m\omega} \Big\{ 1 \langle 010 | 010 \rangle + 1 \langle 100 | 100 \rangle \Big\}$$

$$= \frac{\hbar}{m\omega}$$

$$E_2 = E_2^{(0)} + E_2^{(1)} = \frac{5}{2}\hbar\omega + \frac{\lambda\hbar}{m\omega}$$

PROBLEM 5: Variational Method

In the x-basis, the Hamiltonian for a hydrogen atom is

$$\begin{aligned} H &= \frac{P^2}{2m} - \frac{e^2}{r} \\ &= -\frac{\hbar^2}{2m}\nabla^2 - \frac{e}{r}. \end{aligned}$$

Let us choose

$$\psi_\alpha(r) = e^{-\alpha r^2}, \quad \alpha > 0$$

as a trial wave function for the ground state.

(a) [2 points] Find $\langle\psi_\alpha|\psi_\alpha\rangle$. (**N.B.** This wave function is not normalized.)

(b) [4 points] Find the expectation value of the Hamiltonian $\langle H\rangle$.

(c) [4 points] Determine the best bound on the energy for the ground state of this system using the variational method and the trial wave function given above. // question

P5

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e}{r}$$

$$\psi_\alpha(r) = e^{-\alpha r^2}, \quad \alpha > 0$$

a]

$$\langle\psi_\alpha|\psi_\alpha\rangle = \int_{-\infty}^{+\infty} \langle\psi_\alpha|r\rangle\langle r|\psi_\alpha\rangle \, dr$$

??

$$= \int_{-\infty}^{+\infty} e^{-2\alpha r^2} dr = \int_{-\infty}^{+\infty} e^{-2\alpha(x^2+y^2+z^2)} dx\,dy\,dz$$

$$= \left(\sqrt{\frac{\pi}{2\alpha}}\right)^3 \checkmark$$

or, $\int_{-\infty}^{+\infty} |r\rangle\langle r| dr = 1$?

$\sim \int |r,\theta,\phi\rangle\langle r,\theta,\phi| \, dr\, d\Omega = 1$ } equivalent

$$\langle\psi_\alpha|\psi_\alpha\rangle = \int \psi^*(r,\theta,\phi)\,\psi(r,\theta,\phi)\, r^2\, dr\, \sin\theta\, d\theta\, d\phi$$

$$= 4\pi \int r^2 e^{-2\alpha r^2} dr$$

b. $\langle H\rangle = \int_{-\infty}^{+\infty} \psi_\alpha^*(r)\; H\, \psi_\alpha(r)\, dr$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \psi^*_\alpha(r)\,\nabla^2\psi_\alpha(r)\,dr - \int_{-\infty}^{+\infty} \psi^*_\alpha(r)\,\frac{e}{r}\,\psi_\alpha(r)\,dr$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} e^{-\alpha r^2}\frac{d^2}{dr^2}\,e^{-\alpha r^2}dr - \underbrace{e\int_{-\infty}^{+\infty} \frac{1}{r}\, e^{-2\alpha r^2}\,dr}$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} e^{-\alpha r^2}\frac{d}{dr}\left(-\alpha\cdot 2r\, e^{-\alpha r^2}\right)dr - \sim$$

$$= \frac{\hbar^2\alpha}{2m}\int_{-\infty}^{+\infty} e^{-\alpha r^2}\left(2e^{-\alpha r^2} - 2\alpha r^2 e^{-\alpha r^2}\right)dr - \sim$$

$$= \frac{2\hbar^2\alpha}{2m}\int_{-\infty}^{+\infty} e^{-2\alpha r^2}\,dr - \frac{\hbar^2\alpha^2}{\cancel{2}m}\int_{-\infty}^{+\infty} r^2 e^{-2\alpha r^2}\,dr - e\int_{-\infty}^{+\infty}\frac{1}{r}\, e^{-2\alpha r^2}\,dr$$

cannot

$$= \frac{\cancel{2}\hbar^2\alpha}{m}\left(\frac{\pi}{2\alpha}\right)^{3/2} - \frac{\hbar^2\alpha^2}{m}\left(\frac{1}{4a}\sqrt{\frac{\pi}{2a}}\right)^3 - e\int_{-\infty}^{+\infty}\frac{1}{r}\, e^{-2\alpha r^2}\,dr$$

do that

$$\int_{-\infty}^{+\infty} \frac{1}{r} e^{-2\alpha r^2} dr$$

$\int u\,dv = uv - \int v\,du$

$du = e^{-2\alpha r^2} dr$

$u =$

$$= \int_0^r \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \frac{1}{r} e^{-2\alpha r^2} r^2 dr \sin\theta d\theta d\phi$$

$-2\alpha r^2$

$2\alpha r^2 = x$

$\Rightarrow 4\alpha r dr = dx$

$\Rightarrow r dr = \frac{1}{4\alpha} dx$

$r = 0, x = 0$

$r = \infty \Rightarrow x = \infty$

$$= 4\pi \int_0^{\infty} r e^{-2\alpha r^2} dr$$

$$= 4\pi \frac{1}{4\alpha} \int_0^{\infty} e^{-x} dx$$

$$= \frac{\pi}{\alpha} \left[-e^{-x} \right]_0^{\infty}$$

$$= \frac{\pi}{\alpha}$$

$$\langle H \rangle = \frac{\hbar^2 \alpha}{m} \left(\frac{\pi}{2\alpha} \right)^{3/2} - \frac{\hbar^2 \alpha^2}{m} \left(\frac{1}{4\alpha} \right)^3 \left(\frac{\pi}{2\alpha} \right)^{3/2} - \frac{e\pi}{\alpha}$$

$$= \frac{\hbar^2 \alpha}{m} \left(\frac{\pi}{2\alpha} \right)^{3/2} \left[1 - \alpha \left(\frac{1}{4\alpha} \right)^3 \right] - \frac{e\pi}{\alpha} = 0$$

$$= \frac{\hbar^2 \pi^{3/2} \alpha^{-\frac{1}{2}}}{m\, 2\sqrt{2}} \left[1 - \frac{1}{64} \alpha^{-2} \right] - \frac{e\pi}{\alpha} = 0$$

$$= \underbrace{\frac{\hbar^2 \pi^{3/2}}{2\sqrt{2}\, m}}_{\beta} \left[\alpha^{-\frac{1}{2}} - \frac{1}{64} \alpha^{-5/2} \right] - \frac{e\pi}{\alpha} = 0$$

$$\frac{d\langle H \rangle}{d\alpha} = \beta \left[-\frac{1}{2} \alpha^{-3/2} + \frac{5}{2} \times \frac{1}{64} \alpha^{-7/2} \right] + e\pi \alpha^{-2} = 0$$

PROBLEM 6: Radioactive Decay

In this problem you will calculate the transmission and reflection coefficients for a simple potential step. Then you will use this result to estimate the tunneling probability through an arbitrary potential. This evaluated tunneling probability is called the Gamow Factor. Finally, you will use the Gamow Factor to explain radioactive decay by calculating the decay probability for an α-particle being emitted from a radioactive nuclei and the mean lifetime for that process.

(a) [4 points] **Potential Step:** Calculate the transmission and reflection coefficients for a particle with total energy E interacting with a potential barrier that is a simple potential step ($V_0 > 0$):

$E > V_0$ & $E < V_0$?

$$V(x) = \begin{cases} 0, & \text{if } x < 0 \\ V_0, & \text{if } 0 < x < a \\ 0, & \text{if } x > a. \end{cases}$$

(b) [3 points] **Arbitrary Potential:** A particle of total energy E interacts with an arbitrary potential barrier $V = V(x)$. The classical turning points are $x = x_1$ and $x = x_2$. Assume the potential curve $V(x)$ is sufficiently smooth, then divide the interval $[x_1, x_2]$ into intervals of length Δx_i, large compared with the relative $\boxed{\text{penetration depth}}$ $d_i = \hbar\left[8m(v(x_i) - E)\right]^{-1/2}$ of a particle in the rectangular barriers. Find an expression for the transmission coefficient T (the Gamow Factor) in this approximate way for the barrier $V = V(x)$, knowing that

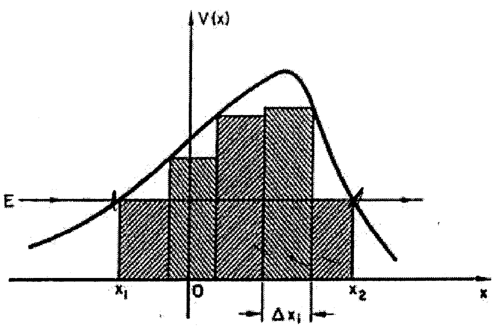
$$T = \int_{x_1}^{x_2} T_i \approx e^{\left[-\frac{1}{\hbar}\sqrt{8m(V(x_i)-E)}\right]} dx =$$

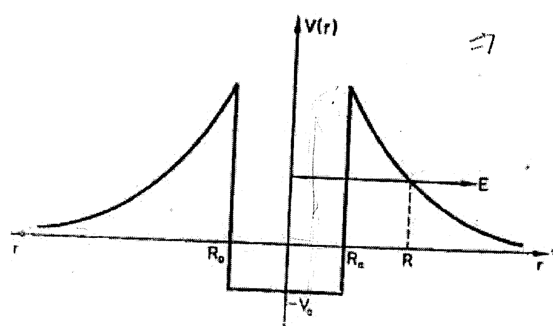
$8mV(x_i) - E = u$

$\Rightarrow 8m \frac{dV}{dx} = du$

$\Rightarrow$

for the *ith* rectangular barrier.





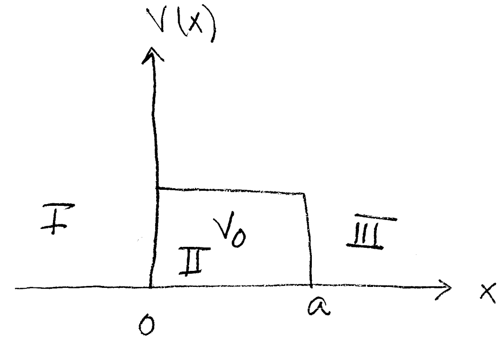
(c) [3 points] **α-emission of radioactive nuclei:** Now show that α-particles with energies of a few MeV can leave potential wells with depths of tens of MeV. Use a simplified model potential, *i.e.* let $V(r) = -V_0$ if $r < R_0$, and $V(r) = \frac{e_1 e_2}{r}$ if $r > R_0$. Now calculate Gamow's factor for this barrier, *i.e.* the decay probability for emission of α-particles of energy E through the barrier. Express the result in terms of the final velocity of the α-particle, and estimate the mean lifetime of an α-emitting nucleus.

✓S-10 P.1 ×F-09 P.1 F-09 P.5 S-10. P3 F8. P11

F8. P4 S10. P1 S7. P1 S7. P2 ✓S7. P5

✓F7. P2 ✓F6. P1 F6. P2 S6. P2

P6



a) In this case, consider $E < V_0$

• Region I

$$\frac{d^2\psi_I(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi_I(x) = 0$$

$$K_1^2 = \frac{2mE}{\hbar^2}$$

$$\Rightarrow \quad \psi_I(x) = Ae^{iK_1x} + Be^{-iK_1x}$$

$e^{iKx} \rightarrow$ represents going right

$e^{-iKx} \rightarrow$ represents going left since it can scattered back

• Region II

$$\frac{d^2\psi_{II}(x)}{dx^2} - \frac{2mV_0}{\hbar^2}\psi_{II}(x) = E\,\psi_{II}(x)$$

Since $V_0 > E$

$$K_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$\Rightarrow \quad \frac{d^2\psi_{II}(x)}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2}\psi_{II}(x)$$

$$\Rightarrow \lambda = \pm K_2$$

$$\Rightarrow \quad \psi_{II}(x) = Ce^{-K_2x} + De^{K_2x}$$

• Region III

$$K^2 = \frac{2mE}{\hbar^2}$$

$$\frac{d^2\psi_{III}(x)}{dx^2} + \frac{2mE}{\hbar}\psi_{III}(x) = 0$$

$$\Rightarrow \lambda = \pm iK$$

$$\Rightarrow \psi_{III}(x) = Ee^{-iK_1x} + Fe^{+iK_1x}$$

but $x \rightarrow \infty$ $e^{iK_1} \rightarrow \infty$ so $F = 0$

$$\psi_{III}(x) = E e^{-ik_1 x}$$

* Boundary conditions

~ at $x = 0$

$$\psi_I(0) = \psi_{II}(0)$$

$$\Rightarrow \quad A + B = C + D \quad \ldots (1)$$

$$\frac{d\psi_I}{dx}\bigg|_{x=0} = \frac{d\psi_{II}}{dx}\bigg|_{x=0}$$

$$\Rightarrow \left[ik_1 A e^{ik_1 x} - ik_1 B e^{-ik_1 x}\right]_{x=0} = \left[-k_2 C e^{-k_2 x} + k_2 D e^{+k_2 x}\right]_{x=0}$$

$$\Rightarrow \quad ik_1 A - ik_1 B = -k_2 (C - D)$$

$$\Rightarrow \quad A - B = i\frac{k_2}{k_1}(C - D) \quad \ldots (2)$$

~ at $x = a$

$$\psi_{II}(a) = \psi_{III}(a)$$

$$\Rightarrow \quad C e^{-k_2 a} + D e^{k_2 a} = E e^{-ik_1 a} \quad (3)$$

$$\frac{d\psi_{II}}{dx}\bigg|_{x=a} = \frac{d\psi_{III}}{dx}\bigg|_{x=a}$$

$$\Rightarrow \quad -k_2 C e^{-k_2 a} + k_2 D e^{k_2 a} = -ik_3 E e^{-ik_1 a}$$

$$\Rightarrow \quad C e^{-k_2 a} - D e^{k_2 a} = \frac{ik_1}{k_2} E e^{-ik_1 a} \quad (4)$$

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{J_{ref}}{J_{inc}}\right|^2$$

$$T = \left|\frac{E}{D}\right|^2 = \left|\frac{J_{trans}}{J_{inc}}\right|^2$$

(1) − (2)

$$2D = (A+B) + \frac{iK_1}{K_2}(A-B) = \left(1+\frac{iK_1}{K_2}\right)A + \left(1-\frac{iK_1}{K_2}\right)B \quad (5)$$

(3) − (4)

$$2D\, e^{K_2 a} = \left(1-\frac{iK_1}{K_2}\right) E\, e^{-iK_1 a} \quad (6)$$

(5) & (6) ⇒

$$A\left(1+\frac{iK_1}{K_2}\right)e^{K_2 a} + B\left(1-\frac{iK_1}{K_2}\right)e^{K_2 a} = \left(1-\frac{iK_1}{K_2}\right)e^{-iK_1 a}\, E$$

$$\Rightarrow \quad \frac{B}{A}\left(1-\frac{iK_1}{K_2}\right)e^{K_2 a} + \left(1+\frac{iK_1}{K_2}\right)e^{K_2 a} = \left(1-\frac{iK_1}{K_2}\right)e^{-iK_1 a}\,\underline{E} \quad (7)$$

(1) + (2)

$$2C = (A+B) - \frac{iK_1}{K_2}(A-B) = \left(1-\frac{iK_1}{K_2}\right)A + \left(1+\frac{iK_1}{K_2}\right)B \quad (8)$$

(3) + (4)

$$2C\, e^{-K_2 a} = \left(1+\frac{iK_1}{K_2}\right) E\, e^{-iK_1 a} \quad (9)$$

(8) & (9)

$$A\left(1-\frac{iK_1}{K_2}\right)e^{-K_2 a} + B\left(1+\frac{iK_1}{K_2}\right)e^{-K_2 a} = E\left(1+\frac{iK_1}{K_2}\right)e^{-iK_1 a}$$

$$\Rightarrow \frac{B}{A}\left(1+\frac{ik_1}{k_2}\right)e^{-k_2 a} + \left(1-\frac{ik_1}{k_2}\right)e^{-k_2 a} = E\left(1+\frac{ik_1}{k_2}\right)e^{-ik_1 a} \quad (10)$$

(7) & (10)

$$\frac{B}{A}e^{-k_2 a} + \frac{1-\frac{ik_1}{k_2}}{1+\frac{ik_1}{k_2}}e^{-k_2 a} = \frac{B}{A}e^{k_2 a} + \frac{1+\frac{ik_1}{k_2}}{1-\frac{ik_1}{k_2}}e^{k_2 a}$$

$$\Rightarrow \frac{B}{A}\left(e^{-k_2 a} - e^{k_2 a}\right) = \frac{1+\frac{ik_1}{k_2}}{1-\frac{ik_1}{k_2}}e^{k_2 a} - \frac{1-\frac{ik_1}{k_2}}{1+\frac{ik_1}{k_2}}e^{-k_2 a}$$

$$= \frac{(1+ik_1/k_2)^2}{1+\frac{k_1^2}{k_2^2}}e^{k_2 a} - \frac{\left(1-\frac{ik_1}{k_2}\right)^2}{1+\frac{k_1^2}{k_2^2}}e^{-k_2 a}$$

$$= \frac{1+\frac{k_1^2}{k_2^2}+2i\frac{k_1}{k_2}}{1+\frac{k_1^2}{k_2^2}}e^{k_2 a} - \frac{1+\frac{k_1^2}{k_2^2}-2i\frac{k_1}{k_2}}{1+\frac{k_1^2}{k_2^2}}e^{-k_2 a}$$

$$= e^{k_2 a} - e^{-k_2 a} + i\frac{2k_1/k_2}{1+\frac{k_1^2}{k_2^2}}\left(e^{k_2 a}+e^{-k_2 a}\right)$$

$$\Rightarrow \frac{B}{A} = -1 - i\frac{2k_1 k_2}{k_1^2+k_2^2}\frac{e^{k_2 a}+e^{-k_2 a}}{\left(e^{k_2 a}-e^{-k_2 a}\right)}$$

$$R = |B/A|^2 = 1 + \frac{4k_1^2 k_2^2}{(k_1^2+k_2^2)^2}\frac{\cosh^2 k_2 a}{\sinh^2 k_2 a}$$

$R + T = 1$

$$\Rightarrow T = \frac{4k_1^2 k_2^2}{(k_1^2+k_2^2)^2}\left(\frac{\cosh^2 k_2 a}{\sinh^2 k_2 a}\right)$$