Quantum Mechanics (Draft 2010 Nov.)

1. For a 1-dimensional simple harmonic quantum oscillator, $V(x) = \frac{1}{2}m\omega^2 x^2$, it is more convenient to describe the dynamics by dimensionless position parameter $\rho = x/a$ ($a = \sqrt{\frac{\hbar}{m\omega}}$) and dimensionless energy $\epsilon = E/(\frac{1}{2}\hbar\omega)$.

Write down the time-independent Schrodinger equation in terms of ρ derivatives on the eigenfunction $u(\rho)$. Directly show that $u_0(\rho) \sim e^{-\frac{1}{2}\rho^2}$ satisfies your Schrodinger equation. Explain why it is the ground state and give its energy ϵ_0 in the dimensionless unit.

Directly show that $u_1(\rho) \sim \rho e^{-\frac{1}{2}\rho^2}$ satisfies the Schrodinger equation as the first excited state. Also give its energy ϵ_1.

The initial wave function $u(\rho, 0)$ is described by $u(\rho,0) = N(3\sqrt{2}\rho - 4)\exp(-\frac{1}{2}\rho^2)$, with N as the normalization constant.

(i) Find the average energy.

(ii) The momentum operator in the reduced unit is $\wp = -id/d\rho$. Find its mean value $\langle\wp\rangle$ initially.

(iii) We use a dimensionless time parameter $\tau = \frac{1}{2}\omega t$ to study how the wave evolves. Write down the explicit τ dependence of the wave function.

(iv) Find $\langle\wp\rangle$ as a function of time τ.

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2 u(\rho) = \epsilon u(\rho) \ .$$

We can pretend that $\omega = 2$, $2m = 1$, $\hbar = 1$. $\frac{d}{d\rho}u_0(\rho) = -\rho u(\rho)$, $\frac{d^2}{d\rho^2}u_0(\rho) = (\rho^2 - 1)u(\rho)$, so u_0 is a solution with $\epsilon_0 = 1$. u_0 has no node, thus it is a ground state. Similarly u_1, with one node, is the first excited solution for $\epsilon_1 = 3$.

$$u(\rho,0) = N(3\frac{2\rho}{\sqrt{2}} - 4)e^{-\frac{\rho^2}{2}} = N\pi^{\frac{1}{4}}(3u_1(\rho) - 4u_0(\rho)) \ , \quad 1 = N^2\sqrt{\pi}(3^2 + 4^2) \ , \quad N = \frac{1}{5\pi^{\frac{1}{4}}}$$

$$u(\rho,0) = \tfrac{1}{5}(3u_1(\rho) - 4u_0(\rho)) \ , \quad u(\rho,\tau) = \tfrac{1}{5}(3u_1(\rho)e^{-3i\tau} - 4u_0(\rho)e^{-i\tau})$$

The average energy is $\langle\epsilon\rangle = \frac{9}{25} \times 3 + \frac{16}{25} \times 1 = \frac{43}{25}$.

$$u(\rho,\tau) = \frac{1}{5\pi^{\frac{1}{4}}}(3\sqrt{2}\rho e^{-3i\tau} - 4e^{-i\tau})e^{-\frac{\rho^2}{2}} \ , \ u^*(\rho,\tau) = \frac{1}{5\pi^{\frac{1}{4}}}(3\sqrt{2}\rho e^{3i\tau} - 4e^{i\tau})e^{-\frac{\rho^2}{2}}$$

$$-i(d/d\rho)u(\rho,\tau) = -\frac{i}{5\pi^{\frac{1}{4}}}(3\sqrt{2}(1-\rho^2)e^{-3i\tau} + 4\rho e^{-i\tau})e^{-\frac{\rho^2}{2}}$$

$$\langle\wp\rangle_\tau = -\frac{i}{25\pi^{\frac{1}{2}}}\int_{-\infty}^{\infty} 12\sqrt{2}\left(\rho^2 e^{+2i\tau} - e^{-2i\tau} + \rho^2 e^{-2i\tau}\right)e^{-\rho^2}d\rho = \frac{12\sqrt{2}}{25}\sin 2\tau$$

The initial $\langle\wp\rangle_\tau$ is zero, but it changes as a sine function.

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2. In the beginning, a non-relativistic particle of mass $m = \frac{1}{2}$ propagates freely as a wave packet with a mean wave number $q = \frac{4}{27}$. We choose a unit system such that $\hbar = 1$. Find the group velocity and the phase velocity.

Let this wave propagates from the remote left toward a repulsive potential $V(x) = 9(x-\frac{1}{3})^2$ in the region $[-\frac{1}{3}, \frac{1}{3}]$. The potential vanishes otherwise. We can treat the potential as a delta-function potential. Give quantitative reasons why.

Calculate the probabilities of transmission and reflection in the delta potential approximation.

The momentum is $\frac{4}{27}$, the particle velocity (i.e. the group velocity) $\boxed{v_g = \frac{p}{m} = \frac{8}{27}}$. $K = \frac{p^2}{2m} = \frac{16}{729}$. $\omega = \frac{K}{\hbar} = \frac{16}{729}$, the phase velocity is $\boxed{v_{\text{phase}} = \frac{\omega}{k} = \frac{4}{27}}$.

The wavelength of the particle is $2\pi/q = 54\pi/4$, which is much greater than the potential width of a size only 2/3. The height of the potential is also much greater than K. Therefore we can treat the potential as delta function $V(x) = G\delta(x)$. The strength G is given by the integral

$$G = \int_{-\frac{1}{3}}^{\frac{1}{3}} 9(x-\tfrac{1}{3})dx = \tfrac{2}{9}$$

We integrate both sides of Schrodinger equation over a small interval around the origin.

$$\varphi_k(x) = \begin{cases} Ae^{ikx} + B^{-ikx} \ , & \text{for } x < 0 \ , \\ Ce^{ikx} + D^{-ikx} \ , & \text{for } x > 0 \ , \end{cases}$$

The B component represents the reflection and the C piece is the transmission. Although for an incoming wave from the left, we do not need the D component, we keep it for other future purpose temporarily. Continuity of the wave function and its kink in derivatives around the origin gives

$$\begin{array}{c} A + B = C + D \\ \frac{\hbar^2}{2m} ik[(A-B)-(C-D)] + G(C+D) = 0 \end{array} .$$

We can solve A and B in terms of C and D,

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 + \frac{miG}{\hbar^2 k} & +\frac{miG}{\hbar^2 k} \\ -\frac{miG}{\hbar^2 k} & 1 - \frac{miG}{\hbar^2 k} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

Now, we require $D = 0$ for the property of an incoming particle from the left. So

$$T(k) \equiv C/A = \hbar^2 k/(\hbar^2 k + miG) \ , \qquad R(k) \equiv B/A = -miG/(\hbar^2 k + miG) \ .$$

$$|T|^2 = \left| \frac{\frac{4}{27}}{\frac{4}{27} + i\frac{3}{27}} \right|^2 = \frac{16}{25} = 64\%$$

Transmission probability is 64%, and the rest 36% is reflected.

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3. For matrices A, B, C, show that $[AB, C] = A[B, C] + [A, C]B$. Let S_1 (or S_x) be the x-component of the spin vector operator, etc. Using the algebra of angular momentum, $[S_x, S_y] = i\hbar S_z$, and cyclic permutations for a general spin ($S = \frac{1}{2}, 1, \frac{3}{2}, \cdots$), simplify $[S_x^2, S_z]$ and $[S_y^2, S_z]$ in terms of $S_x S_y$ or $S_y S_x$. Then calculate $[\boldsymbol{S}^2, S_z]$. The trace of a

matrix A is defined as Tr $A = \sum_m \langle m|A|m\rangle$ summing over the basis vectors m. Show that Tr $(AB) =$ Tr (BA). Based of some earlier steps, show that Tr $(S_x S_y) = 0$

A dark matter (DM) particle of spin S and mass $M_{\rm DM}$ couples to the fixed target nucleus of spin I by a weak spin-dependent contact interaction

$$\mathcal{V} = g\delta^3(\boldsymbol{r})\boldsymbol{S}\cdot\boldsymbol{I}$$

.

What are possible numbers of $\boldsymbol{S}\cdot\boldsymbol{I}$ in general? Show all these possibilities for the special case $S = \frac{1}{2}$, $I = \frac{9}{2}$.

Justify the following trace relations,

$$\text{Tr }(S_i S_j) = \ C_S\delta_{ij}\ , \qquad \text{similarly} \qquad \text{Tr }(I_i I_j) = C_I\delta_{ij}\ ,$$

Determine coefficients C_S and C_I in terms of general S and I respectively.

Calculate the transition probability

$$\sum |\langle \boldsymbol{k}k, m'_S, m'_I|\mathcal{V}|\boldsymbol{k}, m_S, m_I\rangle|^2$$

from an incoming DM plane wave described by $e^{i\mathbf{k}\cdot\mathbf{r}}$ to the outgoing DM wave $e^{i\mathbf{k}'\cdot\mathbf{r}}$. The sum adds up all spin states m_S and m'_S of the initial and final spin states of the DM particle, as well as m_I and m'_I of nucleus.

After average the initial spins of the DM particle and the nucleus, find the total cross section in the Born approximation. (Hints: The usual potential scattering in the Born approximation is

$$\frac{d\sigma}{d\Omega} = \frac{M^2}{4\pi^2\hbar^4}\left|\int d^3r V(r) e^{i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}}\right|^2 .$$

The above formula has to be generalized to incorporate the spins of S and I.)

$[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB = A[B, C] + [A, C]B.$

$[S_y^2, S_z] = S_y[S_y, S_z] + [S_y, S_z]S_y = iS_yS_x + iS_xS_y.$

$[S_x^2, S_z] = S_x[S_x, S_z] + [S_x, S_z]S_y = -iS_xS_y - iS_xS_y.$

As $[S_z^2, S_z] = 0$, we have $[S_x^2 + S_y^2 + S_z^2, S_z] = 0$, so $[\boldsymbol{S}^2, S_z] = 0.$

Tr $(AB) = \sum_{i,j} A_{ij}B_{ji} = \sum_{i,j} B_{ji}A_{ij} =$ Tr (BA), and Tr$[A, B] = 0$. So $\text{Tr}(S_xS_y) = 0.$

Let J denote the magnitude number of the sum $\boldsymbol{J} = \boldsymbol{S} + \boldsymbol{I}$.

$$\boldsymbol{S}\cdot\boldsymbol{I} = \tfrac{1}{2}[(\boldsymbol{S}+\boldsymbol{I})^2 - \boldsymbol{S}^2 - \boldsymbol{I}^2] = \tfrac{\hbar^2}{2}[J(J+1) - S(S+1) - I(I+1)]\ ,$$

for discrete choices of $J = S + J, S + J - 1, \cdots, |J - S|$.

For the special case $S = \frac{1}{2}$ and $I = \frac{9}{2}$, we have two possibilities,

(a) $J = 5$, $\boldsymbol{S}\cdot\boldsymbol{I} = \frac{9}{4}$,

(b) $J = 4$, $\boldsymbol{S}\cdot\boldsymbol{I} = -\frac{11}{4}$.

The overall tracelessness is checked.

About Tr $(S_iS_j) = \ C_S\delta_{ij}$, we have verified the case $i = x, j = y$. Other unequal $i \neq j$ cases are also true if we permute indices.

Symmetry also implies Tr $(S_xS_x) =$ Tr $(S_yS_y) =$ Tr $(S_zS_z) = C_S$.

$\text{Tr }(S_xS_x) = \frac{1}{3}\text{ Tr }\boldsymbol{S}^2 = \frac{\hbar^2}{3}(2S+1)S(S+1).$

We note that Tr $(\boldsymbol{S}\cdot\boldsymbol{I})^2 = \sum_{i,j} =$ Tr $[(S_i I_i)(S_j I_j)] = \frac{\hbar^4}{9}(2S+1)S(S+1)(2I+1)I(I+1)$.

$$\sum |\langle \boldsymbol{k}k, m_S', m_I'|\mathcal{V}|\boldsymbol{k}, m_S, m_I\rangle|^2 = \frac{g^2\hbar^4}{9}(2S+1)S(S+1)(2I+1)I(I+1)$$

Dividing it by $\frac{1}{2S+1}\frac{1}{2I+1}$ for the average of initial spins, we obtain the unpolarized cross section as

$$\frac{d\sigma}{d\Omega} = \frac{M_{DM}^2}{36\pi^2} g^2 S(S+1)I(I+1) \ .$$

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4. Variation principle.
A quantum particle in a two dimensional potential $V(r) = -V_0 \exp(-r/a)$. Let the trial wave function be $\varphi(r;\beta) = Ce^{-\beta r}$. Determine the normalization C in terms of the attenuation parameter β.

Find the average position and average momentum $\bar{x} = \langle x\rangle$, $\bar{y} = \langle y\rangle$, $\bar{p}_x = \langle p_x\rangle$, $\bar{p}_y = \langle p_y\rangle$.

Determine $\langle \boldsymbol{r}^2\rangle$ and $\langle \boldsymbol{p}^2\rangle$. (Hints: $\int d^2\mathbf{r}\psi^*(\mathbf{r})\nabla^2\psi(\mathbf{r}) = -\int d^2\mathbf{r}|\nabla\psi(\mathbf{r})|^2$.)

What are $\langle x^2\rangle$ and $\langle p_x^2\rangle$?

Calculate the product $\langle(x-\bar{x})^2\rangle\langle(p_x-\bar{p}_x)^2\rangle$, and simplify the result in comparison with the Heisenberg uncertainty.

Find the average kinetic energy and average potential energy.

Now we set $\frac{\hbar}{2m} = 1$, $V_0 = 8$, $a = \frac{1}{2}$. Using the variation principle, estimate the ground state energy. The optimized β turns out to be a simple number.

Normalization is given by

$$C^2\int(2\pi r)e^{-2\beta r}dr = 2\pi C^2\frac{1!}{(2\beta)^2} = \frac{\pi C^2}{2\beta^2} = 1$$

$\boxed{C = \beta\sqrt{\frac{2}{\pi}}}$. By symmetry $\bar{x} = 0$, $\bar{y} = 0$, $\bar{p}_x = 0, \bar{p}_y = 0$.

$$\langle \boldsymbol{r}^2\rangle = C^2\int(2\pi r^3)e^{-2\beta r}dr = 2\pi C^2\frac{3!}{(2\beta)^4} = \frac{3}{2\beta^2}$$

$$\langle \boldsymbol{p}^2\rangle = \hbar^2 C^2\int(2\pi r)\beta^2 e^{-2\beta r}dr = \hbar^2\beta^2 \ .$$

By symmetry, $\langle p_x^2\rangle = \langle p_y^2\rangle = \frac{1}{2}\langle \boldsymbol{p}^2\rangle = \frac{1}{2}\hbar^2\beta^2$. Similarly, $\langle x^2\rangle = \frac{1}{2}\langle \boldsymbol{r}^2\rangle = \frac{3}{4\beta^2}$. Therefore $\langle(x-\bar{x})^2\rangle\langle(p_x-\bar{p}_x)^2\rangle = \frac{3}{8}\hbar^2$, well above the lowest bound $\frac{\hbar^2}{4}$ by Heisenberg's uncertainty principle.

Therefore, the average kinetic energy $\langle K\rangle = \frac{\hbar^2\beta^2}{2m}$, and

$$\langle V\rangle = -C^2\int(2\pi r)V_0 e^{-(2\beta+1/a)r}dr = -V_0\beta^2/(\beta+\tfrac{1}{2a})^2 \ .$$

For the given parameters,

$$\langle E\rangle = \beta^2 - 8\beta^2/(\beta^2+1)^2 \ ,$$

which is minimized at $\beta = 1$ with $(\langle E\rangle)_{\min} = -1$, as a good estimate of the ground state energy.

5. Matrix diagonalization.
The dynamic of a three-state system of configurations $|1\rangle$,$|2\rangle$,$|3\rangle$, is governed by the Hamiltonian $\mathcal{H}_0 = -\sum_{i,j} |i\rangle\langle j|$, which is

$$-|1\rangle\langle 1| - |1\rangle\langle 2| - |1\rangle\langle 3|$$

$$-|2\rangle\langle 1| - |2\rangle\langle 2| - |2\rangle\langle 3|$$

$$-|3\rangle\langle 1| - |3\rangle\langle 2| - |3\rangle\langle 3| \ .$$

Work out the Hamiltonian matrix elements $\langle i|\mathcal{H}_0|j\rangle$, and present the corresponding 3×3 matrix.

Find eigen energies as well as the corresponding eigenstates.

A small perturbation $gV = g|1\rangle\langle 1|$ is applied ($g \ll 1$). Find the 1st order and 2nd order corrections of the ground state energy .

The matrix of Hamiltonian of $\mathcal{H}_0$ is

$$-\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

. It is easy to see the eigen-column-vectors and eigen-values are

$$N_a \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, E_a = -3 \ ; \quad N_b \begin{pmatrix} -2 \\ 1 \\ 1 \end{pmatrix}, E_b = 0 \ ; \quad N_c \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, E_c = 0 \ .$$

The normalizations are $N_a = \frac{1}{\sqrt{3}}$,$N_b = \frac{1}{\sqrt{6}}$, $N_c = \frac{1}{\sqrt{2}}$. As b and c are degenerate in energy, their other superpositions are also acceptable. The ground state and the two excited states are

$$|a\rangle_0 = \tfrac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle)$$

$$|b\rangle_0 = \tfrac{1}{\sqrt{6}}(-2|1\rangle + |2\rangle + |3\rangle)$$

$$|c\rangle_0 = \tfrac{1}{\sqrt{3}}(+|2\rangle - |3\rangle)$$

We find the following matrix elements of the perturbed interaction,

$${}_0\langle a|gV|a\rangle_0 = \tfrac{1}{3}g$$

$${}_0\langle b|gV|a\rangle_0 = \tfrac{1}{\sqrt{18}}(-2g)$$

$${}_0\langle c|gV|a\rangle_0 = 0g$$

The ground energy is corrected by perturbation as

$$E_a = -3 + \tfrac{1}{3}g - \tfrac{2}{27}g^2 + \cdots \ .$$