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Fall 2014 QM Comp

(spherical finite square well)

1. Scattering of a particle from a 3D radial Potential

A particle of mass m and Energy $E = \frac{\hbar^2 k^2}{2m}$ scatters off a 3 dimensional radial potential

$$V(r) = -V_0 \qquad a > r$$
$$= 0 \qquad r \geq a$$

a) Why does the $l=0$ partial wave dominate the scattering near threshold (zero energy)?

From Sakurai chp 6.6 we recall that the effective potential includes the centrifugal term

(6.6.1) $$V_{eff} = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

From a classical perspective, at low energies the centrifugal part of the potential is harder to overcome for low energy incoming waves → the potential is basically masked for incoming solutions which are dominated by the (uninteresting) centrifugal portion, they can't penetrate to the weak and localized $V(r)$ potential.

Quantum mechanically we recall the integral equation for the partial wave

(6.6.2) $$\frac{e^{i\delta_l}\sin(\delta_l)}{k} = -\frac{2m}{\hbar^2}\int_0^\infty j_l(kr)\,V(r)\,A_l(r)\,r^2 dr$$

Where $A_l(r) \sim j_l(kr)$, and if the $V(r)$ range is less than $1/k$ distance scale then the right side varies as

* $$\frac{e^{i\delta_l}\sin(\delta_l)}{k} \propto k^{2l}$$ for low energy scattering of localized $V(r)$

and the left side is approximated/varies as

$$\frac{e^{i\delta_\ell}\sin(\delta_\ell)}{k} \approx \frac{1\cdot\delta_\ell}{k} \approx \frac{\delta_\ell}{k} \quad \text{for small } \delta_\ell$$

(6.6.3) then $\delta_\ell \propto k^{2\ell+1}$

And the partial wave amplitude is given as

(6.4.28, 38, 39) $$f_\ell(k) = -\frac{\pi T_\ell(E)}{k} = \frac{S_\ell - 1}{2ik} = \frac{e^{i\delta_\ell}\sin(\delta_\ell)}{k}$$

And the full scattering amplitude is the sum over partial waves

(6.4.40) $$f(\theta) = \sum_{\ell=0} (2\ell+1)\, f_\ell(k)\, P_\ell(\cos\theta)$$

So inputing our result for low E or k we get

$$f(\theta) \approx \sum_{\ell=0} (2\ell+1)\frac{\delta_\ell}{k} P_\ell(\cos\theta) \propto \sum_{\ell=0} (2\ell+1)\, k^{2\ell}\, P_\ell(\cos\theta)$$

So for small energies where $k \approx 0$ the $\ell = 0$ term dominates and only s wave scattering is very important. $\boxed{\text{QED}}$

1.b) Derive an expression for the S-wave phase shift $\delta_{l=0}$ by matching the $l=0$ waves at $r=a$.

from Sakurai's discussion of phase shifts we know

(6.4.48) $$\langle \vec{x} | \psi^+ \rangle = \psi^+(\vec{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0} i^l (2l+1) A_l(r) P_l(\cos\theta) \quad r > a$$

6.4.49) $$\text{with } A_l(r) = C_l^{(1)} h_l^{(1)}(kr) + C_l^{(2)} h_l^{(2)}(kr)$$

6.4.52) $$A_l(r) = e^{i\delta_l}[\cos(\delta_l) j_l(kr) - \sin(\delta_l) n_l(kr)]$$

$$\& \quad \langle \vec{x} | \psi^+ \rangle = \psi^+(\vec{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0} i^l (2l+1) U_l(r) P_l(\cos\theta) \quad r < a$$

(6.4.56) ⓐ $$U_l(r) = r A_l(r)$$

6.4.57) $$U_l \big|_{r=0} = 0$$

6.4.55 & integrate up from $r=0$ to $r=a$ $$\left\{ \frac{d^2 U_l}{dr^2} + \left(k^2 - \frac{2m V(r)}{\hbar^2} - \frac{l(l+1)}{r^2}\right) U_l = 0 \right.$$

6.6.2) ⓑ or use $$e^{i\delta_l} \frac{\sin(\delta_l)}{k} = \frac{-2m}{\hbar^2} \int_0^\infty j_l(kr) V(r) A_l(r) r^2 dr$$

*

just assume sinusoidal & shifted solutions and use reality condition at origin to exclude cos

$$A_{l=0} \propto \psi(\vec{r})$$

$$\text{With } A_{l=0} \cong \frac{A \cdot \sin(k_1 r)}{r} \quad r < a \qquad k_1^2 = k^2 + k_0^2$$

$$\left(\frac{2m}{\hbar^2}(E+V_0) \cdot r\right) \qquad \frac{\hbar^2 k_0^2}{2m} = V_0$$

$$A_{l=0} \simeq \frac{B \cdot \sin(kr + \delta_0)}{r} \quad r > a$$

∴ matching log derivatives at a gives

$$k_1 \cot(k_1 r) = k \cot(kr + \delta_0)$$

$$\therefore \quad \boxed{\cot(\delta_0) = \frac{k \sin(ka) + k_1 \cot(k_1 a) \cos(ka)}{k \cos(ka) - k_1 \cot(k_1 a) \sin(ka)}}$$

1, c) What is the threshold cross-section?

$$\sigma(k) = 4\pi \sum_{\ell} (2\ell+1) \left| \frac{\sin^2 \delta_\ell}{k^2} \right| \qquad \text{from } f_\ell(k) \approx \frac{\sin(\delta_\ell) e^{i\delta_\ell}}{k}$$

$$\approx 4\pi \frac{\delta_0^2(k)}{k^2}$$

$$\frac{\delta_0}{k} \approx \frac{1}{k \cot(\delta_0)} \text{ from part (b) } = a - \frac{\tan(k_0 a)}{k_0}$$

$$\text{so } \sigma(k=0) = 4\pi \left(a - \frac{\tan(k_0 a)}{k_0} \right)^2$$

✓

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2. Particle with EDM moving in an electrostatic potential

Consider a particle of mass m and zero charge but an electric dipole moment $\vec{d} = d\vec{s}$, with $\vec{s}$ the spin of the particle. Assume that the particle moves in a spherically symmetric electro-static potential $\phi(r)$ with $\vec{r} = (x, y, z)$

a) Write down the corresponding Hamiltonian for this particle.

$$H = -\frac{\hbar^2}{2m}\vec{\nabla}^2 - d\vec{s}\cdot\left(-\vec{\nabla}\phi(r)\right) = \frac{\hat{P}^2}{2m} - \vec{E}\cdot\vec{d} \quad , \vec{E} = -\vec{\nabla}\phi(r)$$

$$V_{int} = -\vec{d}\cdot\vec{E} = +d\vec{s}\cdot\vec{\nabla}\phi(r)$$

b) Is this Hamiltonian invariant under:

$$\vec{s}\cdot[\vec{J}, \vec{\nabla}\phi(r)] + [\vec{J}, \vec{s}]\cdot\vec{\nabla}\phi(r) = \vec{s}\cdot[\vec{J}, \vec{r}] = 0 ;$$

a) Space Rotations : $[\vec{J}, p^2] = 0$, $[\vec{J}, \vec{s}\cdot\vec{\nabla}\phi(r)] =$

$\pi^\dagger \vec{s}\pi = +\vec{s}$; s is odd · odd = even → no

b) Parity : $\pi^\dagger P \pi = -P$, $\therefore$ p^2 is even, $\pi^\dagger x \pi = -x$, $\therefore$ $\vec{\nabla}$ is odd → $\pi^\dagger H \pi \neq H$

c) Time reversal : $\theta p \theta^{-1} = -p$, $\therefore$ p^2 is even, $\theta x \theta^{-1}$, $\therefore$ $\vec{\nabla}$ is even

$S \propto J \propto \hat{x} \times \hat{p} \propto$ → odd × even = odd $\therefore$ H is not inv

↳ no to P & T, yes $\vec{J}$

Now assume that the particle has spin 1/2 and is confined to move between two parallel planes at $x = \pm L/2$ of a capacitor with an electric potential $\phi(\vec{r}) = Ez$. → $\vec{\nabla}\phi = \hat{z}E$

c) Find the energies and wave functions of this particle

$$H = -\frac{\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) + d\, S_z E$$

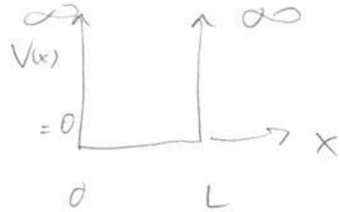
Boundary conditions leave wave functions free for y + z, so we get plane waves $Y(y) = \frac{1}{(2\pi)^{3/2}} e^{\frac{i p_y y}{\hbar}}$, $Z(z) = \frac{1}{(2\pi)^{3/2}} e^{\frac{i p_z z}{\hbar}}$

Then $X(x) = \sqrt{\frac{2}{L}}\left(\cos\left(\frac{n\pi}{L}x\right) + \sin\left(\frac{n\pi}{L}x\right)\right)$ $\quad E_x \;\; \frac{n_x^2 \hbar^2}{2m\pi^2\hbar^2}$ $\quad E_y = E_z = \frac{P}{2m}$; $E_z = \frac{P_z^2}{2m} \pm$

[illegible] $\pm dE\frac{\hbar}{2}$

d) Consider the lowest energy state with momentum $p_y = 0$, $p_z = p$. Write the corresponding wave function & its rotation by $\vec{\theta} = \frac{\pi}{4}\hat{x}$

3. Consider a 1D system of two indistinguishable particles of mass m confined to an infinitely deep square potential well



a) Write down the general structure of the two-particle spatial wave function $\Psi(x_1, x_2)$ and find the energy spectrum, assuming the particles do not interact.

this one is obvious.

Spring 2015 Comp

QM

1. A particle in a perturbed harmonic potential

A particle of mass m in two dimensions is confined by an isotropic harmonic oscillator potential of frequency ω, while subject to a weak and anisotropic perturbation of strength $\alpha \ll 1$. The total hamiltonian describing the motion of the particle is

$$H = H_0 + V = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2} m\omega^2 (x^2+y^2) + \alpha m\omega^2 xy$$

a) What are the energies and degeneracies of the three lowest lying unperturbed states?

$$E_{00} = \hbar\omega\left(\tfrac{1}{2}+\tfrac{1}{2}+0+0\right) = \hbar\omega \quad , \quad E_{01} = \hbar\omega\left(\tfrac{1}{2}+\tfrac{1}{2}+0+1\right) = E_{10} = 2\hbar\omega$$

So the ground state is the $n_x = 0$, $n_y = 0$, $E_{00} = \frac{1}{2}\hbar\omega$ state and the first excited state is the doubly degenerate case where n_x or $n_y = 1$ and the other is $= 0$.

b) Use perturbation theory to correct the energies to first order in α.

$$\Delta E_{00} = \langle 00|V|00\rangle = \alpha m\omega^2 {}_x\langle 0|x|0\rangle_x \; {}_y\langle 0|y|0\rangle_y$$

where $\langle 0|x|0\rangle = \left(0\middle|\sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)\middle|0\right) = 0$

So $\Delta E_{00} = 0$

Next, ΔE_{01} is not obtainable in this way since the first excited state is degenerate and therefore comprised of a mixture of its constituent states → we use degenerate perturbation theory, by force or with the

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$$x = \sqrt{\frac{\hbar}{2m\omega}}(a^{+}+a) \qquad a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(a^{+}-a) \qquad a^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)$$

1.b) ctd. We try to diagonalize within the subspace of the first excited state

$$\Delta E \rightarrow \langle 01/10 | V | 01/10 \rangle$$

$$\begin{array}{ccc} & & \\ & = \alpha m\omega^2 \begin{pmatrix} \cancel{\langle 0|x|0\rangle}_{0}\langle 1|y|1\rangle & {}_{0}\cancel{\langle 1|x|0\rangle}\langle 0|y|1\rangle \\ \langle 0|x|1\rangle\langle 0|y|1\rangle & \cancel{\langle 1|x|1\rangle}\langle 0|y|0\rangle \end{pmatrix} & \begin{array}{c} |01\rangle_{xy} \\ |10\rangle_{xy} \end{array} \\ & \begin{array}{cc} {}_{xy}\langle 01| & \qquad {}_{xy}\langle 10| \end{array} & \end{array}$$

Where now ${}_{x}\langle 0|x|1\rangle_{x} = {}_{x}\langle 1|x|0\rangle_{x} = {}_{y}\langle 0|y|1\rangle_{y} = {}_{y}\langle 1|y|0\rangle_{y}$

$$= \sqrt{\frac{\hbar}{2m\omega}} \langle 1| a^{+}+a |0\rangle = \sqrt{\frac{\hbar}{2m\omega}}$$

$$= \alpha m\omega^2 \left(\sqrt{\frac{\hbar}{2m\omega}}\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

So the eigenvalues are $\pm \frac{\alpha m\omega^2 \hbar}{2m\omega} = \boxed{\pm \frac{\alpha\omega\hbar}{2} = \Delta E_{10}}$

and the eigenvectors are

$$\frac{\alpha\omega\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a_{1,2} \\ b_{1,2} \end{pmatrix} = \pm \frac{\alpha\omega\hbar}{2}\begin{pmatrix} a_{1,2} \\ b_{1,2} \end{pmatrix}$$

iff $b_1 = a_1 = \frac{1}{\sqrt{2}}$

$b_2 = -a_2 = \frac{1}{\sqrt{2}}$

eigenvectors $\boxed{\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad \& \quad \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}}$

c) Find the exact spectrum of H.

We achieve this via a change of variables.

$$a = \frac{1}{\sqrt{2}}(x+y) \quad \& \quad b = \frac{1}{\sqrt{2}}(x-y)$$

s.t. $a^2 + b^2 = \frac{1}{2}(x+y)^2 + \frac{1}{2}(x-y)^2 = \frac{1}{2}(x^2 + x^2 + y^2 + y^2 + 2xy - 2xy) = x^2 + y^2$

& $a^2 = \frac{1}{2}(x^2 + y^2 + 2xy)$

$b^2 = \frac{1}{2}(x^2 + y^2 - 2xy)$

$\therefore \alpha m\omega^2 xy = \alpha m\omega^2 \frac{1}{2}(a^2 - b^2)$

$\therefore \frac{1}{2}m\omega^2(x^2+y^2) = \frac{1}{2}m\omega^2(a^2+b^2)$

$\therefore \frac{p_x^2}{2m} + \frac{p_y^2}{2m} = \frac{p_a^2 + p_b^2}{2m}$

So $H = \frac{p_a^2 + p_b^2}{2m} + \frac{1}{2}m\omega^2\left((1+\alpha)a^2 + (1-\alpha)b^2\right)$

So $\omega_a = \sqrt{1+\alpha}\cdot\omega$ & $\omega_b = \sqrt{1-\alpha}\cdot\omega$

$$\therefore E_{n_a n_b} = \hbar\omega_a\left(\frac{1}{2} + n_a\right) + \hbar\omega_b\left(\frac{1}{2} + n_b\right)$$

d) Check that the perturbative results in part b) are recovered

$$E_{00} = \hbar\omega\sqrt{1+\alpha}\cdot\frac{1}{2} + \hbar\omega\sqrt{1-\alpha}\cdot\frac{1}{2}$$
$$= \hbar\omega\cdot\frac{1}{2}\left(1+\cancel{\tfrac{1}{2}\alpha} + 1 - \cancel{\tfrac{1}{2}\alpha}\right) = \hbar\omega \quad ✓$$

$$E_{10} = \hbar\omega\sqrt{1+\alpha}\cdot\frac{3}{2} + \hbar\omega\sqrt{1-\alpha}\cdot\frac{1}{2}$$
$$= \hbar\omega\cdot\frac{1}{2}\left(3+\tfrac{3}{2}\alpha + 1 - \tfrac{1}{2}\alpha\right) = \hbar\omega\left(2+\tfrac{1}{2}\alpha\right) \quad ✓$$

$$E_{01} = \hbar\omega\sqrt{1+\alpha}\cdot\frac{1}{2} + \hbar\omega\sqrt{1-\alpha}\cdot\frac{3}{2}$$
$$= \hbar\omega\cdot\frac{1}{2}\left(1+\tfrac{1}{2}\alpha + 3 - \tfrac{3}{2}\alpha\right) = \hbar\omega\left(2-\tfrac{1}{2}\alpha\right) \quad ✓$$

So the results match.

e) Assume that 2 identical electrons are subject to the same anisotropic Hamiltonian. Write down the explicit wave-functions and degeneracies of the two lowest energy states.

We are dealing with fermions, which must be overall antisymmetric. Both electrons can be in x or in y, so we have to put both electrons in both energy states.

For the ground state E_{00}, $n_a = 0$ & $n_b = 0$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\;\; x \qquad\quad y$

$E_{00} = \hbar\omega$, $d = 1$

$$\boxed{\Psi = \underbrace{\psi_0(x)\,\psi_0(y)}_{\text{symm}} \cdot \underbrace{\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)}_{\text{anti-sym}}}$$

$E_{10} = 2\hbar\omega - \frac{1}{2}\alpha\hbar\omega$, $d = 4$

4 states

$$\Psi = \frac{1}{\sqrt{2}}\left(\psi_0(x)\,\psi_1(y) + \psi_1(x)\,\psi_0(y)\right) \cdot \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$\Psi = \frac{1}{\sqrt{2}} \;\text{''}\; - \;\text{''} \cdot \left\{|\uparrow\uparrow\rangle,\ |\downarrow\downarrow\rangle \text{ or } \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)\right.$$

2. Consider a one-dimensional non-relativistic particle of mass m and kinetic energy E scattering off the potential barrier $U(x)$ composed of two static δ's.

$$U(x) = \beta_1 \left(\delta(x) + \delta(x-a) \right)$$

a) Can the particle tunnel through this barrier with out reflection? Explain your answer.

b) If so, at what value(s) of the kinetic energy does this happen?

— See comp solution for eloquent explanation

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Now, consider a three-dimensional non-relativistic particle of mass m and kinetic energy E scattering off the potential $U(\vec{r})$ composed of two static δ's.

$$U(\vec{r}) = \beta_3 \left(\delta^{(3)}(\vec{r} - \vec{r}_1) + \delta^{(3)}(\vec{r} - \vec{r}_2) \right)$$

Suppose that for each of the δ's the S-wave scattering length $a < 0$.

c) Write explicitly the S-wave bound wave function near each of the centers. Check that each does not support a bound state for $a < 0$,

d) Can the potential $U(\vec{r})$ with two centers support a bound state? If so under what conditions? explain. — see solu

$\chi = r \cdot \Psi_1$

Hint: for a hard core potential of radius R, the S-wave scattering length a is defined as $d \ln \chi(R) / dR = -1/a$ with $\chi(R)$ the S-wave reduced wave-funct

$$a = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\,\hat{p} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} \pm \frac{i}{m\omega}\hat{p}\right)$$
$$a^{+} = \text{" \quad '' } - \text{ '' \quad ''}$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a^{+}+a) \quad p = i\sqrt{\frac{\hbar m\omega}{2}}\,(a^{+}-a)$$

3. Harmonic Oscillator subject to a transient external force

Consider a one-dimensional quantum-harmonic oscillator with mass m and resonance frequency ω. The oscillator initially $(t\to-\infty)$ is in its ground state, It is then subjected to a transient classical force, $F(t)$, with $F(t\to\pm\infty)=0$.

a) Write down the Hamiltonian $\hat{H}$ of the forced oscillator described above in terms of the usual ladder operators $\hat{a}$ + $\hat{a}^{+}$, and solve their equations of motion in the heisenberg picture. Show that the hamiltonian for $t\to\pm\infty$ takes the form $\hat{H} = \hbar\omega\,(\hat{a}^{+}_{\pm\infty}\hat{a}_{\pm\infty} + \frac{1}{2})$, where $\hat{a}^{+}_{\infty} = \hat{a}^{+}_{-\infty} - \alpha^{*}$ and $\hat{a}_{\infty} = \hat{a}_{-\infty} + \alpha$, and determine the complex term α.

$$\hat{V}(t) = \int dx\, F(t) \overset{CM\ QM}{=} \hat{x}\cdot F(t) = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}+\hat{a}^{+})\cdot F(t)$$

$$H_0 = \hbar\omega\left(\hat{a}^{+}\hat{a} + \tfrac{1}{2}\right)$$

Heisenberg equation of motion

$$\frac{d}{dt}\hat{A} = \frac{i}{\hbar}[\hat{H},\hat{A}] = \frac{1}{i\hbar}[\hat{A},\hat{H}]$$

so $$\frac{d}{dt}\hat{a}(t) = \frac{1}{i\hbar}[\hat{a}(t),\hat{H}(t)]$$

and we recall that $[\hat{A},\hat{H}] = \dfrac{dH}{dA^{+}}$

$$\frac{d}{dt}\hat{a}(t) = \frac{1}{i\hbar}\frac{d}{d\hat{a}^{+}}\left(\hbar\omega\left(\hat{a}^{+}\hat{a}+\tfrac{1}{2}\right) + F(t)\sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}^{+}+\hat{a})\right)$$

$$= \frac{1}{i\hbar}\left[\hbar\omega\,\hat{a} + F(t)\sqrt{\frac{\hbar}{2m\omega}}\cdot 1\right]$$

$$\dot{\hat{a}}(t) = -i\omega\,\hat{a}(t) - i\frac{F(t)}{\sqrt{2m\omega\hbar}}$$

then assuming $\hat{a}(t) = \hat{a}(\omega)\,e^{-i\omega t}$ we get

$$\dot{\hat{a}}(t) + i\omega\,\hat{a}(t) = -i\,\frac{F(t)}{\sqrt{2m\omega\hbar}}$$

fourier transform

$$(i\omega + i\omega)\,\hat{a}(\omega) = -i\,\frac{F(\omega)}{\sqrt{2m\omega\hbar}} \rightarrow \hat{a}(\omega) = \frac{-i\,\hat{F}(\omega)}{2\sqrt{2m\omega\hbar}}$$

$$\hat{a}(t) = \hat{a}(-\infty) - \underbrace{\int_{-\infty}^{t} i\,\frac{F(t')\,e^{-i\omega t'}}{2\sqrt{2m\omega\hbar}}\,dt'}_{=\alpha}$$

b) etc.

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Fall 2015 comp QM

1. Spin 1/2 resonance and neutron interferometry

An electron of charge e + mass m_e is subject to a uniform magnetic field $B_0 \hat{z}$ and has its spin along the positive z axis. At $t=0$ an additional time dependent magnetic field is switched on in the transverse plane with:

$$B_\perp \left(\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y} \right)$$

a) Write down the schrödinger equation for this time dependent problem and solve it.

Our particle is at rest, so $p^2/2m = 0$, then

$$H = H_0 + V(t) = -\vec{\mu}\cdot B_0\hat{z} - \vec{\mu}\cdot B_\perp \left(\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y}\right)$$

where $\vec{\mu} = \frac{eg}{2m}\vec{S}$ with $g \simeq 2$ + $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

$$H = -\frac{e}{m}\cdot\frac{\hbar}{2}\sigma_z B_0 - \frac{e}{m}\frac{\hbar}{2}\left(\sigma_x \cos(\omega t) + \sigma_y \sin(\omega t)\right)$$

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

$$H = -\frac{e}{m}\frac{\hbar}{2}\left[B_0\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + B_\perp\begin{pmatrix} 0 & \cos(\omega t) - i\sin(\omega t) \\ \cos(\omega t) + i\sin(\omega t) & 0 \end{pmatrix}\right]$$

So the energies for the unperturbed H_0 are obviously

$\pm \frac{e}{m}\frac{\hbar}{2}B_0$ for the $\begin{pmatrix} 0 \\ 1 \end{pmatrix}_z$ + $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ spinors respectively.

Then we use this z-spinor basis to solve the time dependent problem exactly, using the interaction picture where

$$V_I = e^{iH_0t/\hbar} V e^{-iH_0t/\hbar}$$

then the TDSE becomes

$$i\hbar \frac{\partial}{\partial t} |\psi(t,t_0)\rangle_I = V_I |\psi(t,t_0)\rangle_I$$

$$i\hbar \frac{\partial}{\partial t} \underbrace{\langle n|\psi\rangle_I}_{c_n} = \langle n|V_I|\psi\rangle_I$$

$$= \sum_m \langle n|V_I|m\rangle \underbrace{\langle m|\psi\rangle_I}_{c_m}$$

$$\langle n| e^{iH_0t/\hbar} V e^{-iH_0t/\hbar} |m\rangle = e^{i\underbrace{(E_n-E_m)t/\hbar}} V_{nm}$$

$$\frac{E_n-E_m}{\hbar} = \omega_{nm}$$

$$i\hbar \frac{\partial}{\partial t} c_n = \sum_m e^{i\omega_{nm}t} V_{nm} c_m$$

$$\boxed{i\hbar \frac{\partial}{\partial t} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} V_{00} & V_{10} e^{i\omega_{01}t} \\ V_{10} e^{i\omega_{10}} & V_{11} \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}}$$

The interaction picture Schrödinger equation → rabi oscillations.

Now, $V(t) = -\frac{e\hbar}{2m} B_1 \begin{pmatrix} 0 & \cos(\omega t) - i\sin(\omega t) \\ \cos(\omega t) + i\sin(\omega t) & 0 \end{pmatrix} = -\frac{e\hbar B_1}{2m} \begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix}$

and it is already in the V_{nm} basis and form.

$$i\hbar \begin{pmatrix} \dot{c}_0 \\ \dot{c}_1 \end{pmatrix} = \gamma \begin{pmatrix} 0 & e^{-i(\omega-\omega_{01})t} \\ e^{i(\omega-\omega_{01})t} & 0 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \qquad \gamma = -\frac{e\hbar}{2m} B_1$$

$$i\hbar \dot{C}_0 = \gamma e^{-i(\omega-\omega_{01})t} C_1 \quad + \quad i\hbar \dot{C}_1 = \gamma e^{i(\omega-\omega_{01})t} C_0$$

So we have a coupled DE to solve. lets assume a new solution of the form

$$C_0 = e^{-i(\omega-\omega_0)t/2}\, a, \quad C_1 = e^{+i(\omega-\omega_0)t/2}\, b$$

$C_0(0) = 1 \therefore a(0) = 1 \qquad C_1(0) = 0 \therefore b(0) = 0$

Then

$$\left(-\frac{i(\omega-\omega_0)}{2}\cdot a + \dot{a}\right) \cancel{e^{-i(\omega-\omega_0)t/2}} \cdot i\hbar = \gamma \cancel{e^{-i(\omega-\omega_0)t}} \cdot \cancel{e^{+i(\omega-\omega_0)t/2}} \cdot b$$

$$\frac{\gamma}{i\hbar} b = -\frac{i(\omega-\omega_0)}{2} a + \dot{a}$$

$$\left(\frac{i(\omega-\omega_0)}{2}\cdot b + \dot{b}\right) e^{+i(\omega-\omega_0)t/2} \cdot i\hbar = \gamma e^{i(\omega-\omega_0)t} \cdot e^{-i(\omega-\omega_0)t/2} \cdot a$$

$$\frac{\gamma}{i\hbar} a = \frac{i(\omega-\omega_0)}{2} b + \dot{b} \rightarrow \frac{\gamma}{i\hbar}\dot{a} = \frac{i(\omega-\omega_0)}{2}\dot{b} + \ddot{b}$$

$$\frac{\gamma}{i\hbar} b = \frac{-i(\omega-\omega_0)}{2\,\gamma/i\hbar} \cdot \left(\frac{i(\omega-\omega_0)}{2} b + \dot{b}\right) + \frac{i(\omega-\omega_0)}{2\,\gamma/i\hbar}\dot{b} + \frac{\ddot{b}}{\gamma/i\hbar}$$

$$+\frac{\gamma^2 b}{\hbar^2} + \frac{(\omega-\omega_0)^2}{4} b - \cancel{\frac{i(\omega-\omega_0)}{2}\dot{b}} + \cancel{\frac{i(\omega-\omega_0)}{2}\dot{b}} + \ddot{b} = 0$$

$$\therefore \ddot{b} + \left(\frac{+\gamma^2}{\hbar^2} + \frac{(\omega-\omega_0)^2}{4}\right) b = 0 \qquad \& \; b(0) = 0$$

$$b(t) = A\cos(\omega' t) + B\sin(\omega' t) \qquad \& \; A = 0,$$

$$b(t) = B\sin(\omega' t) \qquad \omega' = \sqrt{\frac{(\omega-\omega_0)^2}{4} + \gamma^2/\hbar^2}$$

Similarly then $\frac{\gamma}{i\hbar} a(t) = \frac{i(\omega-\omega_0)}{2} \cdot B\sin(\omega' t) + B\omega'\cos(\ldots$

and $a(0) = 1$ so $\frac{\gamma}{i\hbar} = B\omega'$

$B = \frac{\gamma}{\ldots}$,

So $a(t) = -\frac{\cancel{\hbar}(\omega-\omega_0)}{2\cancel{\gamma}}\cdot\frac{\cancel{\gamma}}{i\hbar\omega'}\sin(\omega' t) + \frac{i\cancel{\hbar}}{\cancel{\gamma}}\frac{\cancel{\gamma}}{i\cancel{\hbar}\omega'}\cos(\omega' t)$

$$\boxed{\begin{aligned} a(t) &= \frac{i(\omega-\omega_0)}{2\omega'}\sin(\omega' t) + \frac{\cos(\omega' t)}{\omega'} \\ b(t) &= \frac{\gamma}{i\hbar\omega'}\sin(\omega' t) \end{aligned}}$$

$$C_0(t) = e^{-i(\omega-\omega_0)t/2}\,a(t),\quad C_1(t) = e^{i(\omega-\omega_0)t/2}\,b(t) \quad \boxed{\text{QED}}$$

$$\gamma = -\frac{e\hbar}{2m}B_\perp,\quad \omega' = \sqrt{\frac{(\omega-\omega_0)^2}{4}+\frac{\gamma^2}{\hbar^2}} = \sqrt{\frac{(\omega-\omega_0)^2}{4}+\frac{e^2B_\perp^2}{4m^2}}$$

$$\omega_0 = \omega_{01} = \frac{E_0-E_1}{\hbar}$$

QED

b) What is the probability in time to find the electron with its spin along the negative z-axis, and for what frequency is the spin flip max?

$$|C_1(t)|^2 = P_1(t) = \frac{\gamma^2}{\hbar^2\omega'^2}\sin^2(\omega' t)$$

Amplitude is maxed for ω'^2 smallest, $\therefore \boxed{\omega \simeq \omega_{01}}$ $\boxed{\text{QED}}$

$$\omega \sim \omega_0 = \frac{E_0-E_1}{\hbar} = \frac{2}{\hbar}\cdot\frac{eB_0\hbar}{2m_e} = \boxed{\frac{eB_0}{m_e}}$$

max for $\sin^2(\omega' t) = 1$ which is

time $\omega' t = n\pi$ or $\cancel{0}$ unattainable

$$t^2\left(\frac{(\omega-\omega_0)^2}{4}+\frac{\gamma^2}{\hbar^2}\right) = \frac{n^2\pi^2}{4}$$

$$\boxed{(\omega-\omega_0)^2 = \frac{\cancel{4}n^2\pi^2}{\cancel{4}t^2} - \frac{4\gamma^2}{\hbar^2}}$$

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a + b are correct → see Rabi oscillations solution in the book.

c) Neutron spin flipper are based on this magnetic set up. Denoting by t_n the time that a neutron is in the field, find the minimum value of t_n for a maximum spin flip to occur. Explicitly write down the neutron state at this time. The neutron magnetic moment is μ_n.

as in b) $$\max P_1(t) = \frac{\gamma^2}{\hbar^2 \omega'^2} \sin^2(\omega' t)$$

$$\therefore \quad \omega' t = 1 \cdot \pi/2$$

$$t^2 \left(\frac{(\omega-\omega_0)^2}{4} + \frac{\gamma^2}{\hbar^2} \right) = \frac{\pi^2}{4}$$

& $\omega = \omega_0$ maximizes so

$$t^2 = \frac{\pi^2}{4} \cdot \frac{\hbar^2}{\gamma^2} \rightarrow t = \frac{\pi}{2} \cdot \frac{\hbar}{\gamma}$$

$$\gamma = \frac{-e\hbar}{2m} B_\perp \text{ for } e^- \rightarrow \frac{\hbar \mu_n B_\perp}{2}$$

$$t_{max} = \frac{\pi \hbar \cdot 2}{2 \hbar \mu_n B_\perp} = \boxed{\frac{\pi}{\mu_n B_\perp} = t_{max}}$$

at t_{max} the neutron spin state is

$$|\psi(t_{max})\rangle = \underbrace{-i}_{} e^{-iE_1 \cdot t_{max}} |1\rangle = -i e^{-i\frac{\omega_0}{\omega_\perp}} |\downarrow\rangle = -i e^{-i\frac{\pi B_0}{2 B_\perp}} |\downarrow\rangle$$

from prefactors on $C_1(t) \propto b(t)$ solution!

Spring 2016 Comp QM

3. Approximations for a quartic potential

Consider a particle with mass m in a one-dimensional quartic potential $V = \beta x^4$ where β is a positive constant.

a) Use dimensional analysis to determine how the eigenstate energies depend on β. Hint: use the Schrödinger equation in terms of dimensionless variables

$$\left(-\frac{1}{2}\frac{d^2}{d\bar{x}^2} + \bar{x}^4\right)\psi = \varepsilon\psi$$

We know $$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \beta x^4\right)\psi = E\psi$$

$$\frac{\hbar^2}{m}\frac{1}{L^2} = \beta L^4 \rightarrow L = \left(\frac{\hbar^2}{\beta m}\right)^{1/6}$$

So we define $\bar{x} = \frac{x}{L}$ & $\varepsilon = \frac{E \cdot mL^2}{\hbar^2}$

$$\therefore -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\bar{x}^2}\frac{1}{L^2} + \beta\bar{x}^4L^4 = \frac{\varepsilon\hbar^2}{mL^2}$$

$$-\frac{1}{2}\frac{\partial^2}{\partial\bar{x}^2} + \cancel{\frac{m\beta}{\hbar^2}}\bar{x}^4 \cdot \cancel{\frac{\hbar^2}{\beta m}} = \frac{\varepsilon \cancel{m}}{\cancel{m}}$$

$$\boxed{\left(-\frac{1}{2}\frac{\partial^2}{\partial\bar{x}^2} + \bar{x}^4\right)\psi = \varepsilon\psi}$$ ✓

$$\therefore E \propto \frac{\hbar^2}{mL^2} \propto \frac{\hbar^2}{m}\left(\frac{\beta m}{\hbar^2}\right)^{2/6}$$

$$\boxed{E \propto \beta^{1/3}}$$

$V < E \therefore E - V > 0$

b) Calculate the eigenstate energies E_n, $n \in \mathbb{N}$, in the WKB approximation. Compare the WKB spectrum of this quartic anharmonic oscillator with the spectrum of the harmonic oscillator and the particle in a box

$$\oint p\,dx = \overset{h}{\overset{\shortparallel}{2\pi\hbar}}\left(n+\tfrac{1}{2}\right)$$ and we go from $V(x) = E$'s roots

$$V(x) = \beta x^4 = E \quad \text{for} \quad x_0 = \pm\left(\frac{E}{\beta}\right)^{1/4}$$

$$p = \sqrt{2m(E-V)} = \left(2m\left(E - \beta x^4\right)\right)^{1/2}$$

$$2\int_{-x_0}^{+x_0}\left[2m\left(E-\beta x^4\right)\right]^{1/2}dx = 2\sqrt{2m}\sqrt{\beta}\int_{-x_0}^{x_0}\left(\frac{E}{\beta}-x^4\right)^{1/2}dx = 2\pi\hbar(n+$$

$$u = \frac{x}{E^{1/4}}\cdot\beta^{1/4} \quad du = \left(\frac{\beta}{E}\right)^{1/4}dx \quad x_0 = \pm\left(\frac{E}{\beta}\right)^{1/4}.\ u_0 = \pm 1$$

$$2\sqrt{2}\sqrt{m}\sqrt{\beta}\cdot\left(\frac{E}{\beta}\right)^{1/2}\cdot\left(\frac{E}{\beta}\right)^{1/4}\underbrace{\int_{-1}^{1}\left(1-u^4\right)du}_{\sim 1 = \gamma} = 2\pi\hbar\left(n+\tfrac{1}{2}\right)$$

$$\gamma\cdot\cancel{2}\cdot\sqrt{2m\beta}\cdot\left(\frac{E}{\beta}\right)^{3/4} = \cancel{2}\pi\hbar\left(n+\tfrac{1}{2}\right)$$

$$E^{3/4} = \beta^{1/4}\cdot\pi\,\frac{1}{\gamma}\,\frac{1}{\sqrt{2m}}\,\hbar\left(n+\tfrac{1}{2}\right)$$

$$E_n = \beta^{1/3}\cdot\left[\frac{\pi\hbar}{\gamma\sqrt{2m}}\left(n+\tfrac{1}{2}\right)\right]^{4/3} \quad \checkmark$$

$E_n \propto n^{4/3}$ and this is faster than $\propto n$ SHO and slower than $\propto n^2$ box.

c) for which values of n is the WKB method most accurate?

$$n \to \text{large}$$

d) Approximate the energy E_0 of the ground state of the βx^4 anharmonic oscillator by applying the variational method with Gaussian wave function

$$\Psi_0 = C e^{-x^2/\lambda^2}$$ where λ is a real parameter.

First → the normalization of Ψ_0 is

$$\int_{-\infty}^{\infty} |\Psi_0|^2 \, dx = 1 \quad \therefore \quad C_0^2 \int_{-\infty}^{\infty} e^{-2x^2/\lambda^2} dx = C_0^2 \cdot \sqrt{\frac{\pi}{2/\lambda^2}}$$

$$1 = C_0^2 \, \lambda \sqrt{\frac{\pi}{2}}$$

$$\therefore \quad C_0 = \left(\frac{2}{\pi}\right)^{1/4} \frac{1}{\sqrt{\lambda}}$$

Then
$$\mathcal{E}_{guess} = \langle \Psi_0 | H | \Psi_0 \rangle$$
$$= \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{\lambda} \cdot \int_{-\infty}^{\infty} dx \, e^{-x^2/\lambda^2} \cdot \left(-\frac{1}{2}\frac{d^2}{dx^2} + x^4\right) e^{-x^2/\lambda^2}$$

where
$$e^{-x^2/\lambda^2} \frac{d^2}{dx^2} e^{-x^2/\lambda^2} = \cancel{\frac{d}{dx}\left(\frac{d}{dx} e^{-x^2/\lambda^2} \cdot e^{-x^2/\lambda^2}\right)} - \left(\frac{d}{dx} e^{-x^2/\lambda^2}\right)$$

no support at $\pm\infty$

$$= -\left(\frac{d}{dx} e^{-x^2/\lambda^2}\right)^2$$

$$= -\left(-\frac{2x}{\lambda^2} e^{-x^2/\lambda^2}\right)^2 = -\frac{4x^2}{\lambda^4} e^{-2x^2/\lambda^2}$$

$$\mathcal{E}_{guess} = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{\lambda} \cdot \int_{-\infty}^{\infty} dx \left[\frac{2x^2}{\lambda^4} e^{-2x^2/\lambda^2} + x^4 e^{-x^2/\lambda^2}\right]$$

$$\therefore \quad \mathcal{E}_{guess} = \sqrt{\frac{2}{\pi}}\,\frac{1}{\lambda}\cdot\left(\frac{2}{\lambda^4}\cdot\sqrt{\frac{\pi}{2/\lambda^2}}\cdot\frac{1}{2\cdot 2/\lambda^2} + \sqrt{\frac{\pi}{1/\lambda^2}}\cdot\frac{3}{4(1/\lambda^2)^2}\right)$$

$$= \sqrt{\frac{2}{\pi}}\,\frac{1}{\lambda}\left(\frac{\sqrt{2\pi}}{\lambda^3}\cdot\frac{\lambda^2}{4} + \lambda\sqrt{\pi}\,\frac{3}{4}\,\lambda^4\right)$$

$$\mathcal{E}_{guess} = \frac{1}{2\lambda^2} + \frac{3}{4}\sqrt{2}\,\lambda^4$$

$$\frac{\partial \mathcal{E}}{\partial \lambda^2} = 0 = -\frac{1}{2\lambda^4} + \frac{3\sqrt{2}}{2}\lambda^2 \quad \therefore \lambda^6 = \frac{1}{3\sqrt{2}} \qquad \lambda^2 = \left(\frac{1}{18}\right)^{1/6}$$

$$\mathcal{E} = \text{a mess.} = \frac{18^{1/6}}{2} + \frac{18^{1/2}}{4}\cdot 18^{-2/6} = \underset{KE}{\frac{18^{1/6}}{2}} + \underset{PE}{\frac{18^{+1/6}}{4}} \quad 2KE = 4PE!$$

e) do these results satisfy the virial therem? Explain.
do the variational method or wkb method provide upper/lower bounds on the ground state energy?

→ wkb → none.
variational → upper

Virial theorem $2\langle KE\rangle = \left\langle x\frac{\partial V}{\partial x}\right\rangle$

then $\partial_x \beta x^4 = 4\cdot\beta x^3$ so $x\frac{\partial V}{\partial x} = 4\cdot V$

so $2\langle KE\rangle = 4\langle PE\rangle$ according to theorem

& $\mathcal{E} = \underset{KE}{\frac{18^{1/6}}{2}} + \underset{PE}{\frac{18^{1/6}}{4}}$ ✓ its good.

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f) Write down a wave function that can be used for the variational method to obtain an approximate value of the energy E_1 of the first excited state of the quartic HO.

→ it needs to be orthogonal to e^{-x^2/λ^2}, so lets try

$$\Psi_1 = C_1 \, x \cdot e^{-x^2/\lambda^2}$$

first higher hermite polynomial ∝ first excited state of SHO.