1. A rotator whose orientation is specified by the angular coordinates θ and ϕ performs a *hindered rotation* described by the Hamiltonian

$$H = A\mathbf{L}^2 + B\hbar^2 \cos 2\phi$$

with $A >> B$. Calculate the S, P and D energy levels of this system in the first order perturbation theory, and work out unperturbed energy eigenfunctions.

Let $H_0 = A\mathbf{L}^2$ and $H_1 = B\hbar^2 \cos 2\phi$. Eigenstates of H_0 are $Y_{lm}(\theta, \phi)$ with energies $E_l = A\hbar^2 l(l+1)$ and degeneracy $\left(2\bar{l}+1\right)$. $Y_{lm}(\theta,\phi) = P_{lm}(\cos\theta)\, e^{im\phi}$.

$$\begin{aligned}(Y_{lm}, \cos 2\phi Y_{lm'}) &= \int P_{lm}(\cos\theta)\, P_{lm'}(\cos\theta)\, d\cos\theta \int e^{i(m'-m)\phi} \cos 2\phi d\phi \\ &= C\delta_{m,m'\pm 2}\end{aligned}$$

For S state, there is no first order correction. For P states, The hamiltonian matrix is

$$\begin{pmatrix} 0 & 0 & B\hbar^2 a \\ 0 & 0 & 0 \\ B\hbar^2 a & 0 & 0 \end{pmatrix}$$

where $a = \int Y^*_{1-1} Y_{11} d\Omega = -\frac{3}{8\pi}\int_0^\pi \sin^3\theta d\theta \int_0^{2\pi} \cos(2\phi)\, e^{2i\phi} d\phi = -\frac{1}{2}$. Hence the P level splits into three levels.

2. Find the shift in the ground state energy of a 3D harmonic oscillator due to relativistic correction to the kinetic energy.

3. If the general form of a spin-orbit coupling for a particle of mass m and spin $\mathbf{S}$ moving in a central potential $V(r)$ is

$$H_{SO} = \frac{1}{2m^2c^2}\mathbf{S}\cdot\mathbf{L}\frac{1}{r}\frac{dV(r)}{dr},$$

what is the effect of the coupling on the spectrum of 3D harmonic oscillator?

4. By choosing an appropriate trial function, find the energy of the first excited state of harmonic oscillator.

The Hamiltonian: $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

Trial Wave Function: $\psi(x) = xe^{-ax^2}$

$(\psi,\psi) = \int_{-\infty}^{\infty} x^2 e^{-2ax^2} dx = 2\int_0^\infty x^2 e^{-2ax^2}\, dx = \frac{1}{8\left(\sqrt{a}\right)^3} \lim_{x\to\infty}\left(\sqrt{\pi}\sqrt{2}\right) = \frac{1}{8}\sqrt{\frac{2\pi}{a^3}}$

$H\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(xe^{-ax^2}\right) + \frac{1}{2}m\omega^2 x^3 e^{-ax^2} = \frac{\hbar^2 a}{m} xe^{-ax^2}\left(3 - 2ax^2\right) + \frac{1}{2}m\omega^2 x^3 e^{-ax^2}$

$(\psi, H\psi) = 2\int_0^\infty xe^{-ax^2}\left(\frac{\hbar^2 a}{m}xe^{-ax^2}\left(3-2ax^2\right) + \frac{1}{2}m\omega^2 x^3 e^{-ax^2}\right) dx = \frac{3\hbar^2 a}{16m}\sqrt{\frac{2\pi}{a^3}} + \frac{3}{64}\frac{m\omega^2}{a}\sqrt{\frac{2\pi}{a^3}}$

$E = \frac{3\hbar^2 a}{2m} + \frac{3}{8}\frac{m\omega^2}{a}$

$\frac{dE}{da} = \frac{3\hbar^2}{2m} - \frac{3}{8}\frac{m\omega^2}{a^2}$

$a^* = \frac{m\omega}{2\hbar}$

$E^* = \frac{3\hbar^2 a^*}{2m} + \frac{3}{8}\frac{m\omega^2}{a^*} = \frac{3}{2}\hbar\omega$

5. For the Schrödinger equation with a potential $V(x) = g|x|$ $(g > 0)$, use an exponential trial function to estimate the ground state energy. Compare with the estimate from the gaussian trial function.

Let trial function be $\psi(x) = \exp(-\lambda|x|) = \exp(-\lambda x(2\theta(x) - 1))$.

$(\psi, \psi) = 2\int_0^\infty e^{-2\lambda x}dx = \frac{1}{\lambda}$

$\frac{d}{dx}\exp(-\lambda|x|) = \exp(-\lambda|x|)(-\lambda(2\theta(x) - 1))$

$\frac{d^2}{dx^2}\exp(-\lambda|x|) = \exp(-\lambda|x|)(-\lambda(2\theta(x) - 1))^2 + \exp(-\lambda|x|)(-\lambda 2\delta(x))$

$(\psi, H\psi) = \int_{-\infty}^\infty e^{-\lambda x}\left(-\frac{\hbar^2}{2m}(\lambda^2 + (-\lambda 2\delta(x))) + g|x|\right)e^{-\lambda x}dx = -\frac{\hbar^2}{2m}(\lambda - 2\lambda) + \frac{g}{2\lambda^2}$

$E = \frac{\hbar^2\lambda^2}{2m} + \frac{g}{2\lambda}$

$\frac{dE}{d\lambda} = 0 \Rightarrow \lambda^* = \frac{1}{2}2^{2/3}\left(g\frac{m}{\hbar^2}\right)^{1/3}$

$E^* = \frac{3}{4}\sqrt[3]{2}\left(\frac{\hbar^2 g^2}{m}\right)^{1/3} = 0.94494\left(\frac{\hbar^2 g^2}{m}\right)^{1/3}$

6. Use the variational principle to estimate the ground state energy of Hydrogen atom using a trial function $\exp(-\gamma r)$. The Hamiltonian: $H = \frac{p^2}{2m} - \frac{q^2}{r}$

Trial Wave function: $\psi(\mathbf{r}) = e^{-\lambda r}$

$(\psi, \psi) = 4\pi\int_0^\infty e^{-2\lambda r}r^2dr = \frac{\pi}{\lambda^3}$

$H\psi(x) = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}e^{-\lambda r}\right) - \frac{q^2}{r}e^{-\lambda r} = \frac{\lambda\hbar^2}{2m}\left(\frac{2}{r} - \lambda\right)e^{-\lambda r} - \frac{q^2}{r}e^{-\lambda r}$

$(\psi, H\psi) = 4\pi\int_0^\infty e^{-\lambda r}\left(\frac{\lambda\hbar^2}{2m}\left(\frac{2}{r} - \lambda\right)e^{-\lambda r} - \frac{q^2}{r}e^{-\lambda r}\right)r^2dr = \frac{1}{2}\frac{\pi}{\lambda^2 m}\left(-2q^2m + \hbar^2\lambda\right)$

$E = \frac{1}{2}\frac{\lambda}{m}\left(-2q^2m + \hbar^2\lambda\right)$

$\frac{dE}{d\lambda} = \frac{d}{d\lambda}\left(\frac{1}{2}\frac{\lambda}{m}\left(-2q^2m + \hbar^2\lambda\right)\right) = \hbar^2\frac{\lambda}{m} - q^2$

$\lambda^* = \frac{q^2 m}{\hbar^2}$

$E^* = \frac{1}{2}\frac{\lambda^*}{m}\left(-2q^2m + \hbar^2\lambda^*\right) = -\frac{1}{2}\frac{mq^4}{\hbar^2}$

7. Use the variational principle to estimate the ground state energy for the anharmonic oscillator

$$H = \frac{p^2}{2m} + \lambda x^4.$$

Compare with the exact result

$$E_0 = 1.060\lambda^{1/3}\left(\frac{\hbar^2}{2m}\right)^{2/3}$$

Use a gaussian trial function.

The trial function is given by $\psi(x) = e^{-ax^2}$. Then $(.\psi, \psi) = \int_{-\infty}^\infty e^{-2ax^2}dx = \sqrt{\frac{\pi}{2a}}$.

$H\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(e^{-ax^2}\right) + \lambda x^4 e^{-ax^2} = \frac{\hbar^2 a}{m}(1 - 2ax^2)e^{-ax^2} + \lambda x^4 e^{-ax^2}$.

$(\psi, H\psi) = \left(\frac{\hbar^2 a}{2m}\right)\sqrt{\frac{\pi}{2a}} + \frac{3}{16}\frac{\lambda}{a^2}\sqrt{\frac{\pi}{2a}}$

$E = \left(\frac{\hbar^2 a}{2m}\right) + \frac{3}{16}\frac{\lambda}{a^2}$

$a^3_{\min} = \frac{3m\lambda}{4\hbar^2}$

$E_{\min} = \left(\frac{3}{4}\right)^{4/3}2^{2/3}\lambda^{1/3}\left(\frac{\hbar^2}{2m}\right)^{2/3} = 1.082\ \lambda^{1/3}\left(\frac{\hbar^2}{2m}\right)^{2/3}$

8. Use the variational principle to show that a one-dimensional attractive potential will always have a bound state.

   Let $H = p^2/(2m) + V(x)$. Let $V(x) < 0 \; \forall x$ and $\int_{-\infty}^{\infty} V(x)dx = -M$ and is continuous.

   Using a gaussian trial wave-function $(2a/\pi)^{1/4}\exp(-ax^2)$,

   $E = \frac{\hbar^2 a}{2m} + \sqrt{\frac{2a}{\pi}} \int_{-\infty}^{\infty} V(x)e^{-2ax^2}dx$.

   Since the integral approaches $-M$ as $a \to 0$, it is always possible to choose a such that the E is negative. This implies that the ground state energy is always negative and hence is bounded. It is not necessary to assume that the potential is integrable.

9. Using a gaussian trial function, $e^{-\lambda x^2}$ for a potential well represented by

$$H = \frac{p^2}{2m} - V_0 e^{-\alpha x^2}$$

   where V_0 and $\alpha > 0$.

10. Find the ground state energy of double oscillator described by potential

$$V(x) = \frac{1}{2}m\omega^2(|x| - a)^2$$

   (*Hint*: See section 8.5 in Quantum Mechanics by Merzbacher.)