# 5402 Problem Set 3

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## Question I.

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**Anharmonic oscillator**

Consider a three dimensional anharmonic oscillator with non spherically symmetric potential

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2 + \frac{\lambda}{4!}(x^2 + y^2 + \alpha z^2)^2$$

where $\mathbf{x} = (x, y, z)$. The constant $\alpha$ can be either smaller or greater than 1.

**(a)** What irreducible tensor operators are present in the decomposition of the potential? You do not need to perform any detailed calculation. Use the known irreducible tensor properties of $z^2$ and $x^2 + y^2$, and the rules of addition of angular momentum.

Then harmonic term is taken care of by $T_0^0$, and the anharmonic term is handled by a rank 2 $T_2^q$. The form is of $Y_2^0$ if the constant $\alpha = -2$.

Now set up a variational calculation of the vacuum energy. Since the potential is not rotationally symmetric, the ground state will not carry a definite angular momentum. Nevertheless, for simplicity let us consider two variational ansatze, each one of which has a definite angular momentum:

**(b)** $\Psi_0(\mathbf{x}) = N_0 \exp\{-\Omega\mathbf{x}^2\}$

and

**(c)** $\Psi_2(\mathbf{x}) = N_1 Y_1^0(\theta) \exp\{-\beta r^2\}$

where $N_i$ are normalization constants, $\Omega$ and $\beta$ are variational parameters.

For each variational wave function calculate the expectation value of the Hamiltonian and determine the best variational frequencies $\Omega_0$ and $\beta_0$. Which one of the variational functions does a better job?

Calculating the expectation values of the Hamiltonian in these states we have

$$\langle\psi|H|\psi\rangle = \int \psi^* H\psi$$

We can set up the integral for (b) as

$$\int \psi^* H\psi = \int (N_0 e^{-\Omega\mathbf{x}^2})^* \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2 + \frac{\lambda}{4!}(x^2 + y^2 + \alpha z^2)^2 N_0 e^{-\Omega\mathbf{x}^2}$$

and for (c) as

$$\int \psi^* H\psi = \int (N_1 Y_1^0(\theta) e^{-\beta r^2})^* \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2 + \frac{\lambda}{4!}(x^2 + y^2 + \alpha z^2)^2 N_1 Y_1^0(\theta) e^{-\beta r^2}$$

We can then solve these using Mathematica. The next step is to solve the normalization condition $\langle\psi|\psi\rangle$, then take the variational equation and minimize.

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$$

Then if we take the derivative with respect to the variational parameters $\Omega$ or $\beta$ and minimize we solve the variational method for the ground state.

**(d)** Consider now a superposition of the two best variational wave functions:

$$\Psi_a(\mathbf{x}) = aN_0 \exp\{-\Omega\mathbf{x}^2\} + \sqrt{1-a^2}N_1 Y_1^0(\theta)\exp\{-\beta r^2\}$$

Now consider $a$ as a an additional variational parameter. Can varying with respect to $a$ further improve the variational value of the ground state energy? (Hint: ask yourself if the Hamiltonian has nonvanishing matrix elements between $\Psi_0$ and $\Psi_1$)

We can solve the variational problem again

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$$

and minimize by taking the derivative with respect to the variational parameter $a$. This should be able to further improve the variational value of the ground state energy (an additional parameter will not hurt the approximation).

## Question II.

Shankar 16.1.4

For the oscillator choose

$$\begin{aligned} \psi &= (x-a)^2(x+a)^2 & |x| \leq a \\ &= 0 & |x| > a \end{aligned}$$

Calculate $E(a)$, minimize it and compare to $\hbar\omega/2$

The Hamiltonian for a harmonic oscillator is given by

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2x^2$$

We have

$$\begin{aligned}
E(\psi) &= \int_{-a}^{a} (x^2 - a^2)^2 H (x^2 - a^2)^2 \, \mathrm{d}x \\
&= \frac{3\hbar^2}{2a^2 m} + \frac{1}{22} m\omega^2 a^2 \\
\delta E &= [-\frac{3\hbar^2}{a^3} + \frac{1}{11} m\omega^2 a]\delta a \\
&= 0 \\
a &= \left(\frac{33\hbar^2}{m^2\omega^2}\right)^{1/4} \\
E_{min} &= \hbar\omega \left[\frac{1}{2}\sqrt{\frac{3}{11}} + \frac{1}{2}\sqrt{\frac{3}{11}}\right] \\
&= \sqrt{\frac{3}{11}}\hbar\omega \\
&\geq E_0 \\
&\approx .52\hbar\omega
\end{aligned}$$

**Question III.**

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Shankar 16.1.5

Solve the variational problem for the $l = 1$ states of the electron in a potential $V = -e^2/r$. In your trial function incorporate (i) correct behavior as $r \to 0$, appropriate to $l = 1$, (ii) correct number of nodes to minimize energy, (iii) correct behavior of wave function as $r \to \infty$ in a Coulomb potential (i.e., exponential instead of Gaussian damping). Does it matter what $m$ you choose for $Y_l^m$? Comment on the relation of the energy bound you obtain to the exact answer.

For the $l = 1$ states we have

$$\begin{aligned}
\psi &= Y_1^m(\theta, \phi) R(z) \\
&= Y_1^m(\theta, \phi) \frac{U(z)}{z}
\end{aligned}$$

where $U(z)$ is independent of $m$.

$$\left(-\frac{\hbar}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2} - \frac{e^2}{2} + \frac{l(l+1)\hbar^2}{2mz^2}\right) U = EU$$

$$\begin{aligned}
H_{eff} &= -\frac{\hbar^2}{2m}\delta - \frac{e^2}{2} + \frac{hbar^2}{mz^2} \\
U_{z\to 0} &\sim z^{l+1} \\
&= z^2 \\
U_{z\to\infty} &\sim z^2 e^{-\alpha z/2} \\
\int_0^\infty U^2 \,\mathrm{d}z &= \int_0^\infty z^4 e^{-\alpha z}\,\mathrm{d}z \\
&= \frac{1}{\alpha^5}\int_0^\infty x^4 e^{-x}\,\mathrm{d}x \\
&= \frac{24}{\alpha^5}
\end{aligned}$$

We can now find the expectation value $\langle U|H_{eff}|U\rangle$ as

$$\begin{aligned}
\langle U|H_{eff}|U\rangle &= -e^2\int_o^\infty e^{\alpha z} z^3\,\mathrm{d}z + \frac{\hbar^2}{m\alpha^3}\int_0^\infty e^{-\alpha z} z^2\,\mathrm{d}z + \frac{\hbar^2}{2m}\int_0^\infty (U'(z))^2\,\mathrm{d}z \\
&= \frac{-e^2}{\alpha^4}\Gamma(4) + \frac{\hbar^2}{m\alpha^3}\Gamma(3) + \frac{\hbar^2}{2m}\int_0^\infty (U'(z))^2\,\mathrm{d}z \\
&= \frac{-e^2}{\alpha^4}\Gamma(4) + \frac{\hbar^2}{m\alpha^3}\Gamma(3) + \frac{\hbar^2}{m\alpha^3}
\end{aligned}$$

For the exact result

$$\begin{aligned}
\langle E\rangle &= \left(\frac{-e^2}{\alpha^4}\Gamma(4) + \frac{\hbar^2}{m\alpha^3}\Gamma(3) + \frac{\hbar^2}{m\alpha^3}\right)\frac{\alpha^5}{24} \\
&= \frac{\hbar^2\alpha^2}{8m} - \frac{e^2\alpha}{4} \\
\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}\alpha} &= 0 \\
\alpha &= \frac{me^2}{\hbar^2} \\
\langle E\rangle &= -\frac{me^4}{8\hbar^2}
\end{aligned}$$

## Question IV.

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Shankar 16.2.5

In 1974 two new particles called the $\psi$ and $\psi'$ were discovered, with rest energies 3.1 and 3.7 GeV, respectively (1 GeV = $10^9$ eV). These are believed to be nonrelativistic bound states of a "charmed" quark of mass $m = 1.5$ Gev$/c^2$ (i.e., $mc^2 = 1.5$ GeV) and an antiquark of the same mass, in a linear potential $V(r) = V_0 + kr$. By assuming that these are the $n = 0$ and $n = 1$ bound states of zero orbital angular momentum, calculate $V_0$ using the WKB formula. What do you predict for the rest mass of $\psi''$, the $n = 2$ state? (The measured value is $\simeq$4.2 GeV/$c^2$.) [Hints: (1) Work with GeV instead of eV. (2) There is no need to determine $k$ explicitly.]

For this potential the WKB approximation for the $n$th level is given by

$$(n + \frac{3}{4})\hbar\pi = \int_0^{r_n} \sqrt{2\mu(E_n - V_0 - kr)}\,\mathrm{d}r$$

where $mu = m/2$ is the reduced mass. The 3/4 shift is from the $l = 0$ case, and $r_n = (E_n - V_0)/k$ is the classical turning point. We then have

$$\begin{aligned}(n + \frac{3}{4})\hbar\pi &= \sqrt{mk}\int_0^{r_n} \sqrt{r_n - r)}\,\mathrm{d}r \\ &= \frac{2}{3}\sqrt{mk}r_n^{3/2}\end{aligned}$$

which gives

$$\begin{aligned}E_n &= V_0 + \left(n + \frac{3}{4}\right)^{2/3}\alpha \\ \alpha &\equiv \left(\frac{9k^2\hbar^2\pi^2}{4m}\right)^{1/3}\end{aligned}$$

Plugging in gives us $V_0 = 2.3$ GeV, and for the $n = 2$ case we have 4.2 GeV, as given in the problem

## Question V.

Shankar 16.2.7

Find the allowed levels of the harmonic oscillator by the WKB method.

The harmonic oscillator Hamiltonian is given by

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

WKB leads us to

$$\begin{aligned}(n + \frac{1}{2})\hbar\pi &= \int_{-x_{max}}^{x_{max}} p\,\mathrm{d}d \\ &= \int_{-x_{max}}^{x_{max}} \sqrt{2m(E - \frac{1}{2}m\omega^2 x^2)}\,\mathrm{d}x \\ &= 2\sqrt{2mE}\int_0^{x_{max}} \sqrt{1 - \frac{1}{2E}m\omega^2 x^2}\,\mathrm{d}x \\ &= 2\sqrt{2mE}\int_0^{x_{max}} \sqrt{1 - \frac{x^2}{x_{max}^2}}\,\mathrm{d}x \\ &= \frac{\pi}{2}\sqrt{2mE}x_{max}\end{aligned}$$

Which yields

$$E = \frac{1}{2}m\omega^2x^2$$

$$x_{max} = \sqrt{\frac{2E}{m}}\frac{1}{\omega}$$

$$E = \hbar\omega(n + \frac{1}{2})$$