41. Find the energy eigenstates, energy eigenvalues, and degeneracies of the 3-D isotropic harmonic oscillator, with Hamiltonian

\[
H = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 R^2 = \sum_{\alpha=1}^{3} \left( \frac{P_{\alpha}^2}{2m} + \frac{1}{2} m \omega^2 X_{\alpha}^2 \right) = \sum_{\alpha=1}^{3} H_{\alpha}.
\]

**Solution:** \( H \) can be written

\[
H = \sum_{\alpha=1}^{3} \left( \frac{P_{\alpha}^2}{2m} + \frac{1}{2} m \omega^2 X_{\alpha}^2 \right) = \sum_{\alpha=1}^{3} H_{\alpha}
\]

where \( H_{\alpha} = \frac{P_{\alpha}^2}{2m} + \frac{1}{2} m \omega^2 X_{\alpha}^2 \), with \( \alpha = 1, 2, 3 \) is the Hamiltonian for a single 1D oscillator. We treat the state space as a direct product \( S_{3D} = S_x \otimes S_y \otimes S_z \), and solve the problem for \( H_{\alpha} \) in each factor space to find eigenstates

\[
H_{\alpha}|n_{\alpha}\rangle = (n_{\alpha} + \frac{1}{2}) \hbar \omega |n_{\alpha}\rangle \quad \phi_{n_{\alpha}}(q_{\alpha}) = \frac{\pi^{-1/4}}{2^{n_{\alpha}/2} \sqrt{n_{\alpha}!}} e^{-q_{\alpha}^2/2} H_{n_{\alpha}}(q_{\alpha}) \quad q_{\alpha} = x_{\alpha} \sqrt{\hbar \omega/\hbar}
\]

where \( n_{\alpha} = 0, 1, 2, \ldots \). Thus, in the combined space, the eigenstates are direct product eigenstates

\[
H|n_x, n_y, n_z\rangle = \varepsilon_{n_x, n_y, n_z} |n_x, n_y, n_z\rangle
\]

with energies

\[
\varepsilon_{n_x, n_y, n_z} = \left( n_x + n_y + n_z + \frac{3}{2} \right) \hbar \omega = \left( n + \frac{3}{2} \right) \hbar \omega \equiv \varepsilon_n
\]

where \( n = n_x + n_y + n_z \). Note that the ground state of the 3-dimensional oscillator has an energy \( \varepsilon_0 = 3 \hbar \omega/2 \).

These eigenstates have wave functions

\[
\phi_{n_x, n_y, n_z}(q_x, q_y, q_z) = \frac{\pi^{-3/4}}{\sqrt{2^n n_x! n_y! n_z!}} e^{-q_x^2/2} H_{n_x}(q_x) H_{n_y}(q_y) H_{n_z}(q_z).
\]

The degeneracy \( g_n \) of energy \( \varepsilon_n = (n + 3/2) \hbar \omega \) is equal to the number of ways of representing the integer \( n \) as a sum of three positive integers. For each value that \( n_x \) can take between 0 and \( n \), inclusive, there are \( h(n_x) = n - n_x + 1 \) ways that \( n_y \) and \( n_z \) can add up to give \( n - n_x \) (i.e., we can have \( n_y = 0 \) and \( n_z = n - n_x \), and then increment \( n_y \) and decrement \( n_z \) one step at a time until \( n_y = n - n_x \) and \( n_z = 0 \)). Thus, we have

\[
g_n = \sum_{n_x=0}^{n} h(n_x) = \sum_{n_x=0}^{n} [n - n_x + 1] = \sum_{n_x=0}^{n} n - \sum_{n_x=0}^{n} n_x + \sum_{n_x=0}^{n} 1
\]

The first sum gives \( n(n+1) \); the last gives \( n + 1 \). The middle term gives \( n(n+1)/2 \). Adding these gives

\[
g_n = \frac{(n + 1)(n + 2)}{2}.
\]
42. A particle of mass $m$ moves in a 3 dimensional cubic box (i.e., square well) having one corner at the origin and edges of length $L$ that lie along the positive $x$, $y$, and $z$-axes in the first quadrant (the potential vanishes inside the box, and is infinite outside the box). Show that direct product states $|n_x, n_y, n_z\rangle$ formed from appropriate one-dimensional square well problems satisfy the energy eigenvalue equation, and the correct boundary conditions. Find the energy eigenvalues and energy eigenfunctions in the position representation. Find the degeneracy of the four lowest energy states.

For a 1D square well lying on the interval $x \in [0, L]$ of the $x$-axis, the energy eigenfunctions and eigenenergies are given by the relations

$$\phi_{n_x}(x) = \langle x|n_x\rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n_x \pi x}{L}\right)$$

for $x$ in the interval, and vanish outside the interval. Thus, treating the state space as a direct product $S_{3D} = S_x \otimes S_y \otimes S_z$, we find that the states $|n_x, n_y, n_z\rangle$ with $n_x, n_y, n_z \in \{1, 2, 3, \ldots\}$ and which have wave functions that vanish outside the cubic box, and within it take the form

$$\phi_{n_x, n_y, n_z}(x, y, z) = \langle x, y, z|n_x, n_y, n_z\rangle = \langle x|n_x\rangle\langle y|n_y\rangle\langle z|n_z\rangle = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z)$$

are eigenstates with energy eigenvalues

$$\varepsilon_{n_x, n_y, n_z} = \frac{h^2 n_x^2 \pi^2}{2mL^2} = n_x^2 E_0$$

where $n^2 = n_x^2 + n_y^2 + n_z^2$

and

$$E_0 = \frac{\hbar^2 \pi^2}{2mL^2}$$

The four lowest energy states associated with values of $(n_x, n_y, n_z)$ indicated are shown below

(a) the nondegenerate ground state,

$$(n_x, n_y, n_z) = (1, 1, 1) \quad \varepsilon_0 = 3E_0 \quad g_0 = 1$$

(b) the 3-fold degenerate first excited state

$$(n_x, n_y, n_z) = (2, 1, 1), (1, 2, 1), (1, 1, 2) \quad \varepsilon_1 = 6E_0 \quad g_1 = 3$$

(c) the 3-fold degenerate second excited state

$$(n_x, n_y, n_z) = (2, 2, 1), (2, 1, 2), (1, 2, 2) \quad \varepsilon_2 = 9E_0 \quad g_2 = 3$$

(d) the 3-fold degenerate third excited state

$$(n_x, n_y, n_z) = (3, 1, 1), (1, 3, 1), (1, 1, 3) \quad \varepsilon_3 = 11E_0 \quad g_3 = 3$$
43. A particle in 1D is confined by a potential

\[ V(x) = \beta |x| \]

where \( \beta \) is a positive constant. Estimate the ground state energy of this system using a trial wave function of the form \( \psi(x) = Ae^{-\alpha x^2} \).

**Solution:** We first need to normalize the wave function, which requires that

\[ 1 = |A|^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2} \, dx = |A|^2 \sqrt{\frac{\pi}{2\alpha}} \quad A = (2\alpha/\pi)^{1/4} \]

The mean kinetic energy for this state is

\[ \langle T \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \frac{d\psi}{dx} \cdot \frac{d\psi}{dx} \, dx = \frac{\hbar^2}{2m} \sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} \frac{d}{dx} \left( e^{-\alpha x^2} \right) \, dx \]

\[ = \frac{\hbar^2}{2m} \sqrt{\frac{2\alpha}{\pi}} \cdot 2 \int_{0}^{\infty} \left( 2\alpha x e^{-\alpha x^2} \right) \, dx = \frac{\hbar^2 \alpha}{2m} \]

The mean potential energy is

\[ \langle V \rangle = \int_{-\infty}^{\infty} \beta x |\psi(x)|^2 \, dx = \sqrt{\frac{2\alpha}{\pi}} \beta \cdot 2 \int_{0}^{\infty} x e^{-2\alpha x^2} \, dx = \frac{\beta}{\sqrt{2\pi \alpha}} \]

so

\[ \langle H(\alpha) \rangle = \frac{\hbar^2 \alpha}{2m} + \frac{\beta}{\sqrt{2\pi \alpha}}. \]

Setting \( \partial \langle H(\alpha) \rangle / \partial \alpha = 0 \) we obtain the condition

\[ \frac{\hbar^2}{2m} = \frac{\beta}{2 \sqrt{2\pi \alpha}} \frac{1}{\alpha^{3/2}} \]

so that

\[ \alpha = \left( \frac{2\beta m}{\eta \hbar^2} \right)^{2/3} \quad \eta = \sqrt{8\pi}. \]

Multiplying by \( \alpha \) the condition above that led to this value we find that

\[ \langle T \rangle = \frac{\hbar^2 \alpha}{2m} = \frac{\beta}{2 \sqrt{2\pi \alpha}} = \frac{1}{2} \langle V \rangle \]

so \( \langle V \rangle = 2\langle T \rangle \), and our estimate of the ground state energy becomes

\[ E_{\text{car}}^0 = \frac{\hbar^2 \alpha}{2m} + \frac{\beta}{2 \sqrt{2\pi \alpha}} + \frac{\hbar^2 \alpha}{2m} + 2 \frac{\hbar^2 \alpha}{2m} = \frac{3 \hbar^2 \alpha}{2m} \]

\[ = \frac{3\hbar^2}{2m} \left( \frac{2\beta m}{\eta \hbar^2} \right)^{2/3} \sim 0.81 \left( \frac{\hbar^2 \beta^2}{m} \right)^{1/3} \]
44. Consider an electron bound to a nucleus of charge +e, with Hamiltonian

\[ H = \frac{p^2}{2m} - \frac{e^2}{r}. \]

Use the variational method to estimate the energy of the electronic ground state. Use as a trial ground state wavefunction the exponential \( \psi_{1s}(r) = Ae^{-\alpha r} \), varying the width parameter \( \alpha \).

**Solution:** We first need to normalize the state, which requires that

\[ 1 = \int d^3r \, |\psi|^2 = 4\pi |A|^2 \int_0^\infty r^2 e^{-2\alpha r} dr = |A|^2 \frac{\pi}{\alpha^3} \]

which gives \( A = \sqrt{\alpha^3/\pi} \). For this spherically symmetric state the mean kinetic energy can be written

\begin{align*}
\langle T \rangle &= \frac{\hbar^2}{2m} \int d^3r \, |\frac{\partial \psi}{\partial r}|^2 = \frac{\hbar^2}{2m} \frac{\alpha^3}{\pi} (4\pi) \int_0^\infty dr \, r^2 \left( \frac{\partial}{\partial r} e^{-\alpha r} \right)^2 \\
&= \frac{\hbar^2 \alpha^3}{2m} \frac{\alpha^3}{\pi} (4\pi) \int_0^\infty r^2 e^{-2\alpha r} dr = \frac{\hbar^2 \alpha^2}{2m}
\end{align*}

while the mean potential energy takes the form

\[ \langle V \rangle = -e^2 \int d^3r \, \frac{|\psi|^2}{r} = -e^2 \frac{\alpha^3}{\pi} (4\pi) \int_0^\infty r \, e^{-2\alpha r} dr = -e^2 \alpha. \]

Thus the total energy is

\[ \langle H \rangle = \frac{\hbar^2 \alpha^2}{2m} - e^2 \alpha. \]

Minimizing this with respect to \( \alpha \) we find that

\[ \frac{\hbar^2 \alpha}{m} = e^2 \quad \Rightarrow \quad \alpha = \frac{me^2}{\hbar^2} = a_0^{-1} \]

where \( a_0 = \hbar^2/me^2 \) is the Bohr radius. For this value of \( \alpha \), the mean energy is

\begin{align*}
\langle H \rangle &= \frac{\hbar^2 \alpha^2}{2m} - e^2 \alpha = \frac{1}{2} e^2 \alpha - e^2 \alpha = -\frac{1}{2} e^2 \alpha \\
&= -\frac{1}{2} \frac{me^4}{\hbar^2} \sim -13.6eV
\end{align*}

which is the exact result, since the variational method picked out the exact ground state. Replacing \( e^2 \) with \( Ze^2 \) gives the result for hydrogenic atoms with larger values of the nuclear charge.