

J13Q.3 (Solution by Jim Wu)

Two distinguishable but equal-mass particles move and interact in three dimensions $\vec{r}_i = (x_i, y_i, z_i)$ with the Hamiltonian

$$H = -\frac{\hbar^2}{2m}(|\nabla_1|^2 + |\nabla_2|^2) + \frac{k}{2}(|\vec{r}_1|^2 + |\vec{r}_2|^2) + g(x_1x_2 + y_1y_2 - 2z_1z_2)$$

Solve for the ground state wave function $\psi_0(\vec{r}_1, \vec{r}_2)$ when it exists, and say for what range of g it does exist (assume both m and k are positive).

Solution:

Let's work using center of mass and relative coordinates:

$$\begin{aligned}\mathbf{R} &= \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \\ \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2 \\ \mathbf{P} &= \mathbf{p}_1 + \mathbf{p}_2 \\ \mathbf{p} &= \frac{\mathbf{p}_1 - \mathbf{p}_2}{2}\end{aligned}$$

and let's call $\mathbf{R} = (X, Y, Z)$ and $\mathbf{r} = (x, y, z)$. After some algebra manipulations, we find that

$$\begin{aligned}\mathbf{r}_1^2 + \mathbf{r}_2^2 &= 2\mathbf{R}^2 + \frac{1}{2}\mathbf{r}^2 \\ \mathbf{p}_1^2 + \mathbf{p}_2^2 &= \frac{1}{2}\mathbf{P}^2 + 2\mathbf{p}^2 \\ x_1x_2 &= X^2 - \frac{x^2}{4} \\ y_1y_2 &= Y^2 - \frac{y^2}{4} \\ z_1z_2 &= Z^2 - \frac{z^2}{4}\end{aligned}$$

Substituting this back into the Hamiltonian and using the total mass $M = m + m = 2m$ and reduced mass $\mu = \frac{m^2}{m+m} = \frac{m}{2}$, we get

$$\begin{aligned}H &= \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + \frac{k}{2} \left(2\mathbf{R}^2 + \frac{1}{2}\mathbf{r}^2 \right) + g \left[\left(X^2 - \frac{x^2}{4} \right) + \left(Y^2 - \frac{y^2}{4} \right) - 2 \left(Z^2 - \frac{z^2}{4} \right) \right] \\ &= \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + \frac{1}{2}(2k + 2g)X^2 + \frac{1}{2}(2k + 2g)Y^2 + \frac{1}{2}(2k - 4g)Z^2 \\ &\quad + \frac{1}{2} \left(\frac{k-g}{2} \right) x^2 + \frac{1}{2} \left(\frac{k-g}{2} \right) y^2 + \frac{1}{2} \left(\frac{k+2g}{2} \right) z^2\end{aligned}$$

To simplify the expression a bit, let

$$\begin{aligned}M\omega_X = M\omega_Y &= 2(k+g) & M\omega_Z &= 2(k-2g) \\ \mu\omega_x = \mu\omega_y &= \frac{k-g}{2} & \mu\omega_z &= \frac{k+2g}{2}\end{aligned}$$

and so

$$H = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + \frac{1}{2}M\omega_X^2 X^2 + \frac{1}{2}M\omega_Y^2 Y^2 + \frac{1}{2}M\omega_Z^2 Z^2 + \frac{1}{2}\mu\omega_x^2 x^2 + \frac{1}{2}\mu\omega_y^2 y^2 + \frac{1}{2}\mu\omega_z^2 z^2$$

Note this is just a Hamiltonian of six simple harmonic oscillators, but we need all the coefficients of the parabolic potentials to be positive. So, a bound state exists when $-\frac{k}{2} < g < \frac{k}{2}$. The ground state wave function is given by

$$|n_X, n_Y, n_Z, n_x, n_y, n_z\rangle = |0, 0, 0, 0, 0, 0\rangle$$

Recalling that the ground state of the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ is $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$, the ground state wave function of our Hamiltonian in position space is

$$\begin{aligned} \psi_0(\mathbf{r}_1, \mathbf{r}_2) = & \left[\left(\frac{M\omega_X}{\pi\hbar}\right)^{1/4} e^{-\frac{M\omega_X}{2\hbar}X^2} \right] \times \left[\left(\frac{M\omega_Y}{\pi\hbar}\right)^{1/4} e^{-\frac{M\omega_Y}{2\hbar}Y^2} \right] \times \left[\left(\frac{M\omega_Z}{\pi\hbar}\right)^{1/4} e^{-\frac{M\omega_Z}{2\hbar}Z^2} \right] \\ & \times \left[\left(\frac{\mu\omega_x}{\pi\hbar}\right)^{1/4} e^{-\frac{\mu\omega_x}{2\hbar}x^2} \right] \times \left[\left(\frac{\mu\omega_y}{\pi\hbar}\right)^{1/4} e^{-\frac{\mu\omega_y}{2\hbar}y^2} \right] \times \left[\left(\frac{\mu\omega_z}{\pi\hbar}\right)^{1/4} e^{-\frac{\mu\omega_z}{2\hbar}z^2} \right] \end{aligned}$$

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