

Tutorial 5 Solutions

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YES

② This is a 3 dimensional problem with V independent of θ and ϕ .

Radial equation

$$-\frac{\hbar^2}{2m} \left(R'' + \frac{2}{r} R' \right) + \frac{l(l+1)\hbar^2}{2mr^2} R = ER$$

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YES

$$V = \frac{k_x x^2}{2} + \frac{k_y y^2}{2} + \frac{k_z z^2}{2}$$

$$= \frac{k_x}{2} (x^2 + y^2 + z^2) \quad [\text{Given } k_x = k_y = k_z]$$

$$V = \frac{k_x}{2} r^2 \quad [r^2 = x^2 + y^2 + z^2]$$

V is a function of r only.

$$-\frac{\hbar^2}{2m} \left(R'' + \frac{2}{r} R' \right) + \frac{l(l+1)\hbar^2}{2mr^2} R + \frac{k_x}{2} r^2 R = ER$$

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$r = \text{constant}$ is called the rigid rotor problem.

$$\hat{H} = \frac{-\hbar^2}{2\mu} \nabla^2$$

Since r is a constant, terms involving derivatives of r are omitted.

$$\Rightarrow \hat{H} = \frac{\hat{L}^2}{2\mu d^2}$$

$d \rightarrow$ distance between the 2 particles

$$\hat{H} \psi = E \psi$$

$$\frac{\hat{L}^2}{2\mu d^2} R(r) Y_l^m(\theta, \phi) = E R(r) Y_l^m(\theta, \phi)$$

$$l(l+1)\hbar^2 Y_l^m(\theta, \phi) = E Y_l^m(\theta, \phi)$$

$$E = \frac{J(J+1)\hbar^2}{2\mu d^2}$$

$$J = 0, 1, 2, \dots$$

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[It is a convention to use J instead of l in rigid rotor problem]

The rotational motion of a diatomic molecule can be modeled using rigid rotor. Here μ is the reduced mass of the diatomic molecule and d is the bond distance. The approximation we make here is that the molecule doesn't vibrate i.e., d is a constant.

When $J=0$, $E=0$. Does this violate uncertainty principle?

No

When $J=0$, angular momentum is zero and hence $\Delta L=0$. But we do not have angle information because there is no potential energy in the system.

But in case of harmonic oscillator $E=0$ is not allowed because $E=0$ would mean that $\Delta p=0$ and $\Delta x=0$.

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In particle in a infinite well, the particle never escapes the well and it is always bound. Similarly in harmonic oscillator, the particle is bound to $V = \frac{1}{2}kx^2$ till $x \rightarrow \infty$. But in case of hydrogen atom the particle is bound to the nucleus only for some value of r and then it essentially becomes a free particle (ionization).