

3D anisotropic oscillator
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1. Introduction

The potential energy in a particular anisotropic harmonic oscillator with cylindrical symmetry is given by

$$V = \frac{1}{2}(\mu\omega_1^2 \rho^2 + \mu\omega_3^2 z^2),$$

with $\omega_3 \neq \omega_1$

- (a) Determine the energy eigenvalues and the degeneracies of the three lowest energy levels by using Cartesian coordinates.
- (b) Solve the energy eigenvalue equation in cylindrical co-ordinates and check your results in comparison with those of (a).

2. Cylindrical co-ordinate

We use the cylindrical co-ordinate,

$$\nabla^2 \psi = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2}$$

We now consider the Schrödinger equation for the anisotropic 3D simple harmonics,

$$-\frac{\hbar^2}{2\mu} \nabla^2 \psi + \frac{1}{2}(\mu\omega_1^2 \rho^2 + \mu\omega_3^2 z^2) \psi = E \psi$$

From the invariance of the Hamiltonian under the rotation around the z axis, we have

$$[\hat{H}, \hat{L}_z] = 0$$

Thus ψ is the eigenket of $\hat{L}_z$ with the eigen value $m\hbar$,

$$L_z \psi = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \psi = m\hbar \psi$$

where m is integer; $m = 0, \pm 1, \pm 2, \dots$. Noting that

$$\frac{\partial^2 \psi}{\partial \phi^2} = -m^2 \psi$$

we get

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \psi}{\partial \rho} \right) - \frac{m^2}{\rho^2} \psi \right] + \frac{1}{2} \mu \omega_1^2 \rho^2 \psi + \left(-\frac{\hbar^2}{2\mu} \frac{\partial^2 \psi}{\partial z^2} + \frac{1}{2} \mu \omega_3^2 z^2 \psi \right) = E \psi$$

We assume that

$$\psi = R(\rho) \Phi(\phi) Z(z)$$

Then we have

$$\left\{ -\frac{\hbar^2}{2\mu} \left[\frac{1}{\rho} \frac{d}{d\rho} \left(\rho \frac{dR}{d\rho} \right) - \frac{m^2}{\rho^2} R \right] + \frac{1}{2} \mu \omega_1^2 \rho^2 R \right\} \Phi Z + \left(-\frac{\hbar^2}{2\mu} \frac{\partial^2 Z}{\partial z^2} + \frac{1}{2} \mu \omega_3^2 z^2 Z \right) R \Phi = E R \Phi Z$$

Dividing the above equation by $\psi = R(\rho) \Phi(\phi) Z(z)$, we get two independent differential equations

$$\begin{aligned} & -\frac{\hbar^2}{2\mu} \left[\frac{1}{\rho} \frac{d}{d\rho} \left(\rho \frac{dR}{d\rho} \right) - \frac{m^2}{\rho^2} R \right] + \frac{1}{2} \mu \omega_1^2 \rho^2 R = E_{xy} R \\ & -\frac{\hbar^2}{2\mu} \frac{\partial^2 Z}{\partial z^2} + \frac{1}{2} \mu \omega_3^2 z^2 Z = E_z Z \quad (\text{simple harmonics}) \end{aligned}$$

with

$$E_z = \hbar \omega_2 \left(n_z + \frac{1}{2} \right), \quad E = E_{xy} + E_z$$

Then we get

$$\frac{d^2 R}{d^2 \rho} + \frac{1}{\rho} \frac{dR}{d\rho} - \left(\frac{m^2}{\rho^2} R + \frac{\mu^2 \omega_1^2}{\hbar^2} \rho^2 \right) R + k^2 R = 0$$

where

$$\frac{2\mu E_{XY}}{\hbar^2} = k^2, \quad \lambda = \frac{2E_{XY}}{\hbar\omega_1} = \frac{\hbar k^2}{\mu\omega_1}$$

We put

$$\xi = \sqrt{\frac{\mu\omega_1}{\hbar}}\rho$$

Then

$$\frac{d^2 R}{d\xi^2} + \frac{1}{\xi} \frac{dR}{d\xi} - \left(\frac{m^2}{\xi^2} R + \xi^2\right) R + \lambda R = 0$$

In the limit of $\xi \rightarrow 0$, we assume that $R = \xi^s$

$$s(s-1) + s - m^2 = 0$$

$$s = \pm m.$$

When $m > 0$, we need to choose $R = \xi^m$. When $m < 0$, we need to choose $R = \xi^{-m}$. Thus we use

$$R = \xi^{|m|}.$$

In the limit of $\xi \rightarrow \infty$, we get

$$\frac{d^2 R}{d\xi^2} - \xi^2 R = 0$$

So we have

$$R = \exp\left(-\frac{\xi^2}{2}\right)$$

The function satisfies

$$R = \xi^{|m|} \exp\left(-\frac{\xi^2}{2}\right) f(\xi)$$

where

$$f''(\xi) + \left(\frac{2|m|+1}{\xi} - 2\xi\right) f'(\xi) + [\lambda - (2|m|+2)] f(\xi) = 0$$

We solve this differential equation by using the series expansion. Suppose that $f(\xi)$ is given by

$$f(\xi) = \sum_{k=0}^{\infty} C(k) \xi^k$$

Then we have the recursion relations as

$$\begin{aligned} (1+2m)C(1) &= 0 \\ (-2-2m+\lambda)C(0) + 4(1+m)C(2) &= 0 \\ (-4-2m+\lambda)C(1) + 3(3+2m)C(3) &= 0 \end{aligned}$$

Then we have

$$C(1) = C(3) = C(5) = \dots = 0 \dots$$

Thus $f(\xi)$ should be an even function of ξ . So we assume this time that

$$f(\xi) = \sum_{k=0}^{\infty} C(2k) \xi^{2k}$$

Then the recursion relation is obtained as

$$C(2k+2) = \frac{(-\lambda + 2 + 4k + 2|m|)}{4(1+k)(1+k+|m|)} C(2k)$$

Suppose that for $k = n_r$, the value of λ is given by

$$\lambda = \frac{2E_{xy}}{\hbar\omega_1} = 2 + 4n_r + 2|m|.$$

Then we have

$$C(2n_r + 2) = C(2n_r + 4) = \dots = 0.$$

The series terminates, indicating that $f(\xi)$ will be a polynomial with the co-efficients

$$C(0), C(2), C(4), C(6), \dots, C(2n_r).$$

The energy eigenvalue is

$$E_{xy} = (1 + 2n_r + |m|)\hbar\omega_1,$$

where $n_r = 0, 1, 2, 3, \dots$

Then the energy eigenvalue is

$$E = E_{xy} + E_z = (1 + 2n_r + |m|)\hbar\omega_1 + (n_z + \frac{1}{2})\hbar\omega_3.$$

3. Mathematica

Series expansion: 3D anisotropic simple harmonics

```
Clear["Global`*"];
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$$\mathbf{F1} = \mathbf{u}'''[\rho] + \left(\frac{1}{\rho}\right) \mathbf{u}'[\rho] + \left(\lambda - \frac{m^2}{\rho^2} - \rho^2\right) \mathbf{u}[\rho];$$

$$\text{rule1} = \left\{ \mathbf{u} \rightarrow \left(\#^m \text{Exp}\left[-\frac{\#^2}{2}\right] \mathbf{f}[\#] \right) \right\};$$

```
 $\mathbf{F1} /. \text{rule1} // \text{FullSimplify}$ 
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$$e^{-\frac{\rho^2}{2}} \rho^{-1+m} \left((-2 - 2m + \lambda) \rho \mathbf{f}[\rho] + (1 + 2m - 2\rho^2) \mathbf{f}'[\rho] + \rho \mathbf{f}''[\rho] \right)$$

$$\mathbf{F2} = (-2 - 2m + \lambda) \rho \mathbf{f}[\rho] + (1 + 2m - 2\rho^2) \mathbf{f}'[\rho] + \rho \mathbf{f}''[\rho];$$

$$\text{rule2} = \left\{ \mathbf{f} \rightarrow \left(\sum_{k=0}^5 \mathbf{C}[\mathbf{k}] \#^k \right) \right\};$$

```
eq1 =  $\mathbf{F2} /. \text{rule2} // \text{Expand};$ 
```

eq1

$$\begin{aligned}
 & -2 \rho C[0] - 2 m \rho C[0] + \lambda \rho C[0] + C[1] + 2 m C[1] - 4 \rho^2 C[1] - \\
 & 2 m \rho^2 C[1] + \lambda \rho^2 C[1] + 4 \rho C[2] + 4 m \rho C[2] - 6 \rho^3 C[2] - 2 m \rho^3 C[2] + \\
 & \lambda \rho^3 C[2] + 9 \rho^2 C[3] + 6 m \rho^2 C[3] - 8 \rho^4 C[3] - 2 m \rho^4 C[3] + \lambda \rho^4 C[3] + \\
 & 16 \rho^3 C[4] + 8 m \rho^3 C[4] - 10 \rho^5 C[4] - 2 m \rho^5 C[4] + \lambda \rho^5 C[4] + \\
 & 25 \rho^4 C[5] + 10 m \rho^4 C[5] - 12 \rho^6 C[5] - 2 m \rho^6 C[5] + \lambda \rho^6 C[5]
 \end{aligned}$$

```
list1 = Table[{n, Coefficient[eq1, ρ, n]}, {n, 0, 4}] // Simplify;
list1 // TableForm
```

```

0      (1 + 2 m) C[1]
1      (-2 - 2 m + λ) C[0] + 4 (1 + m) C[2]
2      (-4 - 2 m + λ) C[1] + 3 (3 + 2 m) C[3]
3      (-6 - 2 m + λ) C[2] + 8 (2 + m) C[4]
4      (-8 - 2 m + λ) C[3] + 5 (5 + 2 m) C[5]
```

Determination of recursion formula

$$\text{rule3} = \left\{ f \rightarrow \left(\sum_{n=k-3}^{k+3} C[2n] \rho^{2n} \right) \right\};$$

```
eq2 = (F2 / ρ-7+2k) /. rule3 // Simplify;
```

```
list2 = Table[{n, Coefficient[eq2, ρ, 2 n]}, {n, 3, 7}] // Simplify;
list2 // TableForm
```

```

3      (2 - 4 k - 2 m + λ) C[2 (-1 + k)] + 4 k (k + m) C[2 k]
4      (-2 - 4 k - 2 m + λ) C[2 k] + 4 (1 + k) (1 + k + m) C[2 (1 + k)]
5      (-6 - 4 k - 2 m + λ) C[2 (1 + k)] + 4 (2 + k) (2 + k + m) C[2 (2 + k)]
6      (-10 - 4 k - 2 m + λ) C[2 (2 + k)] + 4 (3 + k) (3 + k + m) C[2 (3 + k)]
7      (-14 - 4 k - 2 m + λ) C[2 (3 + k)]
```

```
Solve[list2[[2, 2]] == 0, C[2 (1 + k)]]
```

$$\left\{ \left\{ C[2 (1 + k)] \rightarrow \frac{(2 + 4 k + 2 m - \lambda) C[2 k]}{4 (1 + k) (1 + k + m)} \right\} \right\}$$