3D anisotropic oscillator

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(Date: February 26, 2014)

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,

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

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, ±1, ±2,..... Noting that

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

we get

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

We assume that

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

Then we have

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

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

$$-\frac{\hbar^2}{2\mu}[\frac{1}{\rho}\frac{d}{d\rho}(\rho\frac{dR}{d\rho}) - \frac{m^2}{\rho^2}R] + \frac{1}{2}\mu\omega_1{}^2\rho^2 R = E_{XY}R$$

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 Z}{\partial z^2} + \frac{1}{2}\mu\omega_3{}^2 z^2 Z = E_z Z \qquad \text{(simple harmonics)}$$

with

$$E_z = \hbar\omega_2(n_z + \frac{1}{2}), \qquad E = E_{XY} + E_z$$

Then we get

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

where

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

We put

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

Then

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

In the limit of $\xi \to 0$, 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 $\xi \to \infty$, we get

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

So we have

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

The function satisfies

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

where

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

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

$$C(1) = C(3) = C(5) = ... = 0.....$$

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

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

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

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

The energy eigenvlaue is

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

where $n_r = 0, 1, 2, 3, \ldots$.

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 aniotropic simple harmonics

```
Clear["Global`*"];

F1 = u''[ρ] + (1/ρ) u'[ρ] + (λ - m^2/ρ^2 - ρ^2) u[ρ];

rule1 = {u → (#^m Exp[-#^2/2] f[#] &)};

F1 /. rule1 // FullSimplify

E^(-ρ^2/2) ρ^(-1+m) ((-2 - 2 m + λ) ρ f[ρ] + (1 + 2 m - 2 ρ^2) f′[ρ] + ρ f″[ρ])

F2 = (-2 - 2 m + λ) ρ f[ρ] + (1 + 2 m - 2 ρ^2) f′[ρ] + ρ f″[ρ];

rule2 = {f → (Sum[C[k] #^k, {k, 0, 5}] &)};

eq1 = F2 /. rule2 // Expand;
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eq1
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$$-2\rho C[0]-2m\rho C[0]+\lambda\rho C[0]+C[1]+2mC[1]-4\rho^2C[1]-2m\rho^2C[1]+\lambda\rho^2C[1]+4\rho C[2]+4m\rho C[2]-6\rho^3C[2]-2m\rho^3C[2]+\lambda\rho^3C[2]+9\rho^2C[3]+6m\rho^2C[3]-8\rho^4C[3]-2m\rho^4C[3]+\lambda\rho^4C[3]+16\rho^3C[4]+8m\rho^3C[4]-10\rho^5C[4]-2m\rho^5C[4]+\lambda\rho^5C[4]+25\rho^4C[5]+10m\rho^4C[5]-12\rho^6C[5]-2m\rho^6C[5]+\lambda\rho^6C[5]$$

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

0	$(1+2m)\,C[1]$
1	$(-2-2m+\lambda)\,C[0]+4\,(1+m)\,C[2]$
2	$(-4-2m+\lambda)\,C[1]+3\,(3+2m)\,C[3]$
3	$(-6-2m+\lambda)\,C[2]+8\,(2+m)\,C[4]$
4	$(-8-2m+\lambda)\,C[3]+5\,(5+2m)\,C[5]$

Determination of recursion formula

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

$$\text{eq2} = \left(F2 \,/\, \rho^{-7+2\,k}\right) \;/.\; \text{rule3} \;//\; \text{Simplify};$$

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

3	$(2-4k-2m+\lambda)\,C[2\,(-1+k)]+4\,k\,(k+m)\,C[2\,k]$
4	$(-2-4k-2m+\lambda)\,C[2\,k]+4\,(1+k)\,(1+k+m)\,C[2\,(1+k)]$
5	$(-6-4k-2m+\lambda)\,C[2\,(1+k)]+4\,(2+k)\,(2+k+m)\,C[2\,(2+k)]$
6	$(-10-4k-2m+\lambda)\,C[2\,(2+k)]+4\,(3+k)\,(3+k+m)\,C[2\,(3+k)]$
7	$(-14-4k-2m+\lambda)\,C[2\,(3+k)]$

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

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