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Lecture 37 - 3D Simple Harmonic Oscillator

1. 3D Simple Harmonic Oscillator
2. $\ell = 0$ case
3. Vector Operators

1. The 3D Simple Harmonic Oscillator

Let $k = m = \hbar = 1$

Start by solving in usual Cartesian basis:

$$\mathcal{H} = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2)$$

$$= \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_z$$

↑ treat as three independent 1D oscillators that all commute

$$\mathcal{H}_\alpha = \left(\frac{p_\alpha^2 + X_\alpha^2}{2}\right) \;;\; X_{\alpha = x,y,z} = X, Y, Z$$

$[\mathcal{H}_\alpha, \mathcal{H}_\beta] = 0$ as usual

We can use the creation & number operators

$a_\alpha^\dagger = \frac{(X_\alpha - i p_\alpha)}{\sqrt{2}}$, $n_\alpha = a_\alpha^\dagger a_\alpha$

$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}$ to simultaneously diagonalize $\mathcal{H}_\alpha$

$[n_\alpha, n_\beta] = 0 \Rightarrow n_x$ are commuting Hermitian operators, so they are also simultaneously diagonalizable

Relating to energies and # of states -

$$\mathcal{H} = \underbrace{N_{tot}} + 3/2$$

$N_{tot} = \hat{n}_x + \hat{n}_y + \hat{n}_z$; where $n_x, n_y, n_z \geq 0$ are eigenstates of $\mathcal{H}$ with eigenvalues $E = (n_x + n_y + n_z) + 3/2$

of (n_x, n_y, n_z) with $N_{tot} = n_x + n_y + n_z \Rightarrow$ # of states (degeneracy)

→ How many ways can we add up 3 integers (n_x, n_y, n_z) to get N_{tot}?
Use combinatorics!

states (degeneracy) = coefficient of $\lambda^{N_{tot}}$ in $\underbrace{\left(\sum_{n_x} \lambda^{n_x}\right)}_{(1-\lambda)^{-1}\text{, a geometric series}}\left(\sum_{n_y} \lambda^{n_y}\right)\left(\sum_{n_z} \lambda^{n_z}\right)$

Generating function trick:

└ aka the partition function

→ expand in λ

$$\left(\sum_{n_x} \lambda^{n_x}\right)\left(\sum_{n_y} \lambda^{n_y}\right)\left(\sum_{n_z} \lambda^{n_z}\right) = \sum_{n_x n_y n_z} \lambda^{n_x + n_y + n_z / N_{tot}}$$

→

delta function allows us to write this in terms of N_{tot}

$$= \sum_{N_{tot}} \sum_{n_x n_y n_z} \underbrace{\delta(n_x + n_y + n_z, N_{tot})}_{\text{the degeneracy}} \lambda^{N_{tot}}$$

$$= \sum_{N_{tot}=0}^{\infty} (\text{deg.}) \lambda^{N_{tot}}$$

coefficients of $\lambda^{N_{tot}}$ are the degeneracies of N_{tot}

$$= (1-\lambda)^{-3}$$

→ binomial theorem

$$= \sum_{N_{tot}} (-1)^{N_{tot}} \frac{(-3)(-3-1)\overbrace{\ldots(-3-N_{tot}+1)}}{N_{tot}!} \lambda^{N_{tot}}$$

binomial expansion:

$$(1+x)^n = 1 + nx + \underbrace{\frac{n(n-1)}{2!}}_{=\binom{n}{2}} x^2 + \frac{n(n-1)(n-2)}{3!} x^3 + \ldots$$

$$\frac{(N_{tot}+2)(N_{tot}+1)\cancel{N_{tot}\ldots 3}}{\cancel{N_{tot}}(\cancel{N_{tot}-1})\ldots 2\cdot 1}$$

all other terms cancel out

$$= \frac{(N_{tot}+2)(N_{tot}+1)}{2},$$

the degeneracy coefficients of $\lambda^{N_{tot}}$

$E-3/2$	n_x	n_y	n_z
0	0	0	0
1	1	0	0
1	0	1	0
1	0	0	1
2		etc.	
⋮			

#degeneracies

$\frac{1}{2}(N_{tot}+1)(N_{tot}+2)$ states

@ $E = N_{tot} + 3/2$

best described by SU(3)

SU(3) invariance of 3D SHO

$$\mathcal{H} = \hat{N}_{tot} + 3/2 \, ; \quad \hat{N}_{tot} = \sum_{\alpha = x,y,z} \underbrace{a^\dagger_\alpha a_\alpha}$$

where $[a_\alpha, a^\dagger_\beta] = \delta_{\alpha\beta}$

Consider a linear transformation:

$$\hat{a}^\dagger_\alpha = \sum_{\alpha'} U_{\alpha\alpha'} a^\dagger_{\alpha'} \quad (\mathrm{I})$$

$$\rightarrow [\hat{a}^\dagger_\alpha, a_\beta] = \sum_{\alpha'\beta'} U_{\alpha\alpha'} U^*_{\beta\beta'} \underbrace{[a^\dagger_{\alpha'}, a_{\beta'}]}_{\delta_{\beta'\alpha'}}$$

$$= \sum_{\alpha'} U_{\alpha\alpha'} (U^\dagger)_{\alpha'\beta} = (UU^\dagger)_{\alpha\beta}$$

If U is unitary, (i.e., $U \in U(3)$)

$$[\hat{a}^\dagger_\alpha, \hat{a}_\beta] = \delta_{\alpha\beta}$$

└ $\hat{a}^\dagger_\alpha$ obeys the same commutation relations as $a^\dagger_\alpha$

furthermore,

$$\sum_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha = \sum_{\alpha'\beta'\alpha} U_{\alpha\alpha'} U^*_{\alpha\beta'} a^\dagger_{\alpha'} a_{\beta'}$$

$$= \sum_{\beta'\alpha'} \underbrace{\sum_\alpha (U^\dagger)_{\beta'\alpha} U_{\alpha\alpha'}}_{(U^\dagger U)_{\beta'\alpha'} = \delta_{\beta'\alpha'}} a^\dagger_{\alpha'} a_{\beta'}$$

$$= \sum_{\beta'} a^\dagger_{\beta'} a_{\beta'} = N_{tot}$$

$\Rightarrow$ $U(3)$ transformation (I) leaves N_{tot}, and therefore $\mathcal{H}$, invariant

How does $\vec{L}$ (angular momentum) fit in here?

$$\langle x\, y\, z | n_x\, n_y\, n_z \rangle = \underbrace{\langle x | n_x \rangle}_{\psi_{1D,n_x}(x)} \overbrace{\langle y | n_y \rangle}^{\psi_{1D,n_y}(y)} \underbrace{\langle z | n_z \rangle}_{\psi_{1D,n_z}(z)}$$

3-dimensional SHO represented as the product of 1D vector subspaces (wavefunctions in real space) where $\psi^{SHO}_{1D,n}(x)$ are the eigenstates of the 1D SHO

$[\mathcal{H}, L_\alpha] = 0 \rightarrow$ There should be simultaneous set of eigenstates of the Cartesian basis; $\mathcal{H}$, L^2, and L_z

↑ where L_α are the angular momentum operators for the 3D SHO

($\mathcal{H}$ commutes with L^2, L_z, etc.)

but $L_z |n_x\, n_y\, n_z\rangle \propto |n_x\, n_y\, n_z\rangle$

└ same eigenstates ↗

The set of eigenstates are labeled by $|N_{tot}, \ell, m\rangle$ such that

$$\mathcal{H} |N_{tot}, \ell, m\rangle = \underbrace{(N_{tot} + 3/2)}_{E} |N_{tot}, \ell, m\rangle$$

$L^2|N_{tot},\ell,m> = \ell(\ell+1)\hbar^2|N_{tot},\ell,m>$

$L_z|N_{tot},\ell,m> = m\hbar|N_{tot},\ell,m>$

*What are $|N_{tot},\ell,m>$ in relation to $|n_x,n_y,n_z>$?

$\rightarrow |N_{tot},L^2,L_z> \equiv \sum_{n_x n_y n_z} |n_x,n_y,N_{tot}-n_x-n_y> \underbrace{<n_x,n_y,N_{tot}-n_x-n_y|N_{tot},L^2,L_z>}_{1}$

- for $N_{tot}=0$:

(the ground state)

$|n_x=0,n_y=0,n_z=0> = |N_{tot}=0, \underbrace{L^2=L_z=0}>$

because the ground state is non-degenerate; deg. $=\frac{1}{2}(1)(2)=1$

- for $N_{tot}=1$:

deg. $=\frac{1}{2}(2)(3)=3$

$N_{tot}=0$, the ground state

$|n_x=1,n_y=0,n_z=\overset{\downarrow}{0}> = a_x^\dagger|0>$

$\rightarrow$ 3 states are $a^\dagger_{\alpha=x,y,z}|0>$

- for $N_{tot}=2$:

deg. $=\frac{1}{2}(3)(4)=6$

$a_\alpha^{\dagger 2}|0> \rightarrow \underbrace{a_x^\dagger a_y^\dagger|0>}$

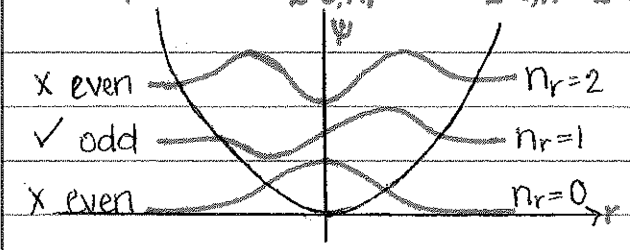
6 states (3 states each)

2. $\underline{\ell=0} \rightarrow L^2=L_z=0$

The 3D S.H.O. simplifies to the 1D S.H.O. for the $\ell=0$ case

where the $\ell=0$ states satisfy:

$[-\partial_r^2+\frac{1}{2}r^2]U_{\ell=0,n_r}(r) = E_{\ell=0,n}U_{\ell=0,n_r}(r)$



Boundary Condition:

Only odd wavefunctions

$U_n(r)=-U_n(-r)$

Bound state energies

handles only the radial component of the wavefunction

$E_n=n_r+\frac{1}{2} \rightarrow E=\cancel{1/2}, 3/2, \cancel{5/2}, 7/2, \ldots$ have $\ell=0$ states

even n_r-values do not satisfy the boundary condition

$$E_n = \overbrace{(2\tilde{n}_r + 1)}^{n_r} + 1/2$$

└ forces to spatially odd solutions

In terms of N_{tot}:

↑ handles all eigenstates of the wavefunction (where n_x, n_y, and n_z do NOT commute with n_r)

$$\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_z, \quad \mathcal{H}_i = a_i^\dagger a_i + \frac{1}{2}$$

$$\rightarrow E = (n_x + \tfrac{1}{2}) + (n_y + \tfrac{1}{2}) + (n_z + \tfrac{1}{2})$$

$$= \underbrace{N_{tot}}_{2\tilde{n}_r} + 3/2$$

$2\tilde{n}_r$ -- forces to an even # of states → only even solutions for N_{tot} are allowed for $\ell = 0$

$N_{tot} = 0$

$E = 3/2$; $\ell = 0$ state

$N_{tot} = 1$

$E = 5/2$; NO $\ell = 0$ state

$N_{tot} = 2$

$E = 7/2$; $\ell = 0$ state

Even-numbered N_{tot} values each have exactly one state at $\ell = 0$ out of the $\frac{1}{2}(N_{tot}+1)(N_{tot}+2)$ states with energy $E(N_{tot}) = N_{tot} + 3/2$

$U_n(r) = \psi_{1D,n}(r)$

└ n^{th} SHO in 1D

* deg. $= \frac{1}{2}(3)(4) = 6$ → there must be 5 other states (other ℓ-values) for $N_{tot} = 2$

Constructing $\ell = 0$ states

$N_{tot} = 0 = n_x + n_y + n_z$ is non-degenerate

i.e., $n_x = n_y = n_z = 0$ ⇒ the state must be the $\ell = 0$ state

$|N_{tot} = 0 = \ell = m\rangle = |n_x = n_y = n_z = 0\rangle \equiv |0\rangle$

* more generally, $\ell = 0$ states are rotationally invariant

Claim:

The states $A^p|0\rangle$, where $A = \sum_\alpha a_\alpha^{\dagger 2}$, are $\ell = 0$ states

└ a scalar operator (to be defined later this lecture)

Proof:

$\mathcal{D}(R) A \mathcal{D}^\dagger(R) = A$

where $[L_\alpha, A] = 0$

→

$$\mathcal{D}(R)A^p|0\rangle = \underbrace{(\mathcal{D}(R)A\mathcal{D}^\dagger(R))}_{A}{}^p\underbrace{\mathcal{D}(R)|0\rangle}_{|0\rangle\text{ - ground state; rotationally invariant}}$$

$$= A^p|0\rangle$$

Rotational invariance $\Longleftrightarrow$ $A^p|0\rangle$ is an $\ell=0$ state

$$A^p|0\rangle = \left(\sum_\alpha a_\alpha^{\dagger 2}\right)^p|0\rangle$$

$$= \sum_{n_x+n_y+n_z=p} \underbrace{\begin{pmatrix} p \\ n_x\ n_y\ n_z \end{pmatrix}}_{\text{combinatorics}} a_x^{\dagger 2n_x} a_y^{\dagger 2n_y} a_z^{\dagger 2n_z}|0\rangle$$

$$= \sum_{n_x+n_y+n_z=p} \frac{p!}{n_x!n_y!n_z!}\sqrt{(2n_x)!(2n_y)!(2n_z)!}\,|2n_x, 2n_y, 2n_z\rangle$$

$$\propto |N_{tot}=2(n_x+n_y+n_z)=2p, \ell=0, m=0\rangle$$

(since there is only one $\ell=0$ state for each even N_{tot})

Simplest (non-zero) case: $p=1$

$$|N_{tot}=2, \ell=0, m=0\rangle \propto A|0\rangle$$

$$\propto \left(\sum_\alpha a_\alpha^{\dagger 2}\right)|0\rangle$$

$$= 2^{3/2}\underbrace{(a_x^{\dagger 2} + a_y^{\dagger 2} + a_z^{\dagger 2})}_{\text{uniform superposition required}}|0\rangle$$

normalization constant

$\rightarrow |n_x, n_y, n_z\rangle$ rotation $\rightarrow$

$$= \frac{1}{\sqrt{3}}(|n_x=2, n_y=0, n_z=0\rangle + |n_x=0, n_y=2, n_z=0\rangle + |n_x=0, n_y=0, n_z=2\rangle)$$

$\llcorner$ must be superposition of $n_\alpha=2$ states, not $n_\alpha=1, n_\beta=1$ states

$$\langle r, \theta, \varphi|N_{tot}=2, \ell=0\rangle = \frac{1}{\sqrt{4\pi}}\frac{1}{r}\psi^{SHO}_{10, n_r=3}(r)$$ — General solution SHO

Why is a uniform superposition required?

3. Vector Operators

If you apply $\mathcal{D}(R)$ to a vector operator, it rotates like a standard vector

$\rightarrow$ that is, the expectation value of a vector operator in quantum mechanics transforms like a classical vector under rotation

$$|\alpha\rangle \rightarrow \mathcal{D}(R)|\alpha\rangle$$

$$\underbrace{\langle\alpha|V_i|\alpha\rangle}_{\text{general vector operator}} \rightarrow \langle\alpha|\mathcal{D}^\dagger(R)V_i\mathcal{D}(R)|\alpha\rangle = \underbrace{\sum_j \overset{\text{rotation matrix}}{R_{ij}}\langle\alpha|V_j|\alpha\rangle}_{\text{true for any arbitrary ket }|\alpha\rangle}$$

Position/momentum (x_α, p_α), etc., are vector operators

→ The creation operators $a_\alpha^\dagger$ are also vector operators

$a_\alpha^\dagger = \frac{1}{\sqrt{2}}(\underbrace{X_\alpha} - ip_\alpha)$

$X_\alpha \equiv$ Vector operator

$\mathcal{D}(R) X_\alpha \mathcal{D}^\dagger(R) = \sum_\beta R_{\alpha\beta} X_\beta$

$\mathcal{D}(R) a_\alpha^\dagger \mathcal{D}^\dagger(R) = \sum_\beta R_{\alpha\beta} a_\beta^\dagger$

⇒ If the creation operator behaves like a vector, then the ground state must be a uniform superposition in x, y, and z because the $\ell = 0$ ground state must be rotationally invariant

can sandwich because $\mathcal{D}(R)$ is unitary

$$\mathcal{D}(R)\sum_\alpha a_\alpha^\dagger a_\alpha \mathcal{D}^\dagger(R) = \sum_\alpha \underbrace{\mathcal{D}(R) a_\alpha^\dagger \mathcal{D}^\dagger(R)}_{R_{\alpha\beta} a_\beta^\dagger} \mathcal{D}(R) a_\alpha \mathcal{D}^\dagger(R)$$

$$= \sum_{\alpha\beta\beta'} R_{\alpha\beta} a_\beta^\dagger R_{\alpha\beta'} a_{\beta'}$$

$$\sum_\alpha R_{\alpha\beta} R_{\alpha\beta'} = \sum_\alpha (R^T)_{\beta'\alpha} R_{\alpha\beta}$$

$$= \underbrace{(R^T R)}_{\mathbb{1}}{}_{\beta'\beta} = \delta_{\beta'\beta} \quad (R \in SO(3))$$

$$= \sum_\beta a_\beta^\dagger a_\beta = \sum_\alpha a_\alpha^\dagger a_\alpha$$

Scalar operators are rotationally invariant operators.

Claim: $a^{\dagger 2}$ is a scalar operator

Proof:

$$\mathcal{D}(R)\sum_\alpha a_\alpha^{\dagger 2} \mathcal{D}^\dagger(R) = \sum_\alpha \mathcal{D}(R) a_\alpha^\dagger \mathcal{D}^\dagger(R) \mathcal{D}(R) a_\alpha^\dagger \mathcal{D}^\dagger(R)$$

→ express $\mathcal{D}(R)$ in terms of rotation matrices, $\mathcal{D}(R) V_\alpha \mathcal{D}^\dagger(R) = \sum_\beta R_{\alpha\beta} V_\beta$ ↓

$$= \sum_{\beta\beta'\alpha} R_{\alpha\beta} R_{\alpha\beta'} a_\beta^\dagger a_{\beta'}^\dagger = \sum_{\beta\beta'} \underbrace{\left(\sum_\alpha R^T_{\beta'\alpha} R_{\alpha\beta}\right)}_{R \text{ is an orthogonal rotation; } R^T R = \mathbb{1}} a_\beta^\dagger a_{\beta'}^\dagger$$

$$= \sum_{\beta\beta'} \delta_{\beta\beta'} a_\beta^\dagger a_{\beta'}^\dagger$$

$$= \sum_\beta a_\beta^{\dagger 2} = \sum_\alpha a_\alpha^{\dagger 2}$$

$\sum_\alpha a_\alpha^{\dagger 2}$ is a scalar (rotationally invariant) operator

If $A = \sum_\alpha a_\alpha^{\dagger 2}$, then $\mathcal{D}(R) A \mathcal{D}^\dagger(R) = A$

⟺ $[\mathcal{D}(R), A] = 0$; $[L_\alpha, A] = 0 = [A, L^2]$

$$\mathcal{D}(R)|N_{tot} = 2, \ell = 0\rangle = C\mathcal{D}(R)\left(\sum_\alpha a_\alpha^{\dagger 2}\right)|0\rangle$$

→ insert $\mathcal{D}^\dagger(R)\mathcal{D}(R)$ $(= \mathbb{1})$

$$= C\,\underbrace{\mathcal{D}(R)\left(\sum_\alpha a_\alpha^{\dagger 2}\right)\mathcal{D}^\dagger(R)}_{\sum_\alpha a_\alpha^{\dagger 2}}\underbrace{\mathcal{D}(R)|0\rangle}_{|0\rangle}$$

$= |N_{tot} = 2, \ell = 0\rangle$ Rotationally invariant!

Parity of (ℓ, m) states

$$[A, \hat{N}_{tot}] = \underbrace{-2A}_{\text{i.e., A increases } N_{tot} \text{ by } 2}$$

$$\hat{N}_{tot} A |N_{tot}\rangle = A(\hat{N}_{tot} + 2)|N_{tot}\rangle$$
$$= (\hat{N}_{tot} + 2) A |N_{tot}\rangle$$
$$\Rightarrow A|N_{tot}\rangle \propto |N_{tot} + 2\rangle$$

$$L^2 A |N_{tot}, \ell, m\rangle = A L^2 |N_{tot}, \ell, m\rangle$$
$$= (\ell+1)\ell\hbar^2 A |N_{tot}, \ell, m\rangle$$

$$L_z A |N_{tot}, \ell, m\rangle = m\hbar A |N_{tot}, \ell, m\rangle$$
$$\Rightarrow A^p |N_{tot}, \ell, m\rangle \propto |N_{tot} + 2p, \ell, m\rangle$$

If there is some ℓ state at some N_{tot} then there is one set of (ℓ, m) states for each $N'_{tot} > N_{tot}$ that have the same parity as N'_{tot}

i.e., $N'_{tot} - N_{tot} = 2p \geq 0$