Second Quantization Lecture

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \qquad [\hat{p},\hat{x}] = -i\hbar, \ \hat{p} = -i\hbar\frac{d}{dx}$$

$$= \frac{m\omega^2}{2}\left(\frac{1}{m^2\omega^2}\hat{p}^2 + \hat{x}^2\right)$$

$$= \frac{m\omega^2}{2}\left(\hat{x} - i\frac{1}{m\omega}\hat{p}\right)\left(\hat{x} + i\frac{1}{m\omega}\hat{p}\right) - \frac{m\omega^2}{2}i\frac{1}{m\omega}\overbrace{\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)}^{i\hbar}$$

$$= \frac{m\omega^2}{2}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) + \frac{\hbar\omega}{2}$$

$$= \hbar\omega \cdot \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) + \frac{\hbar\omega}{2}$$

$$= \hbar\omega\, a^+ a + \frac{\hbar\omega}{2}$$

$$= \hbar\omega\left(a^+ a + \frac{1}{2}\right)$$

Define: (note: no hat)

$$a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{i}{m\omega}p\right)$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p\right)$$

Then (comment about commutators)

$$[a, a^+] = aa^+ - a^+a = 1 \qquad [a^+, a^+] = 1 \qquad [a, a] = 1$$

* Commutator practice

Inspired by form of energy, $\hat{H}|0\rangle = \frac{\hbar\omega}{2}|0\rangle$, how a acts on $|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$

$$a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}\cdot -i\hbar\frac{d}{dx}\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\cdot\left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right)e^{-\frac{m\omega x^2}{2\hbar}}$$

$$e^{-\frac{m\omega x^2}{2\hbar}}\cdot\left(x + \frac{\hbar}{m\omega}\cdot -\frac{m\omega}{\hbar}x\right)$$

$$0$$

Now examine, $a^+|0\rangle$, from before

$$a^+|0\rangle = \sqrt{\frac{m\omega}{2\hbar}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \left(x - \frac{\hbar}{m\omega} \cdot - \frac{m\omega}{\hbar} x\right)$$

$$= \qquad\qquad\qquad\qquad \cdot 2x$$

$$= \sqrt{\frac{m\omega}{2\hbar}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot 2x \cdot e^{-\frac{m\omega x^2}{2\hbar}}$$

ie first excited state

Commutator practice

Practice with commutators: using $[a, a^+] = aa^+ - a^+a = 1$

$$[a^+a, a] = a^+aa - aa^+a$$

$$= a^+aa - (1 + a^+a)a$$

$$= -a$$

Note: shuffle a^+ to the left, as how appears in H

$$[a^+a, a^+] = a^+aa^+ - a^+a^+a$$

$$= a^+(1 + a^+a) - a^+a^+a$$

$$= a^+$$

Now ask if $|\alpha\rangle$ is eigenstate of a^+a with eigenvalue α, then what is $a|\alpha\rangle$

$$a^\dagger a a \left|\alpha\right\rangle = \left(-a + a a^\dagger a\right)\left|\alpha\right\rangle$$

$$= (\alpha - 1) \, a \left|\alpha\right\rangle$$

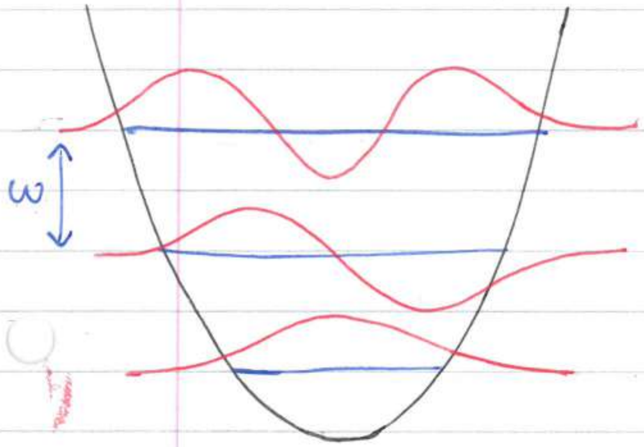
$$a^\dagger a \left[a\left|\alpha\right\rangle\right] = (\alpha-1)\left[a\left|\alpha\right\rangle\right]$$ unless $a\left|\alpha\right\rangle = 0$

ie eigenstate with value $\alpha - 1$

Now check $a^\dagger\left|\alpha\right\rangle$

$$a^\dagger a a^\dagger \left|\alpha\right\rangle = \left(a^\dagger + a^\dagger a^\dagger a\right)\left|\alpha\right\rangle$$

$$= (\alpha + 1) \, a^\dagger \left|\alpha\right\rangle$$ ie eigenstate with value $\alpha + 1$



$|2\rangle = a^{\dagger 2}|0\rangle$ $\quad a^\dagger a|2\rangle = 2|2\rangle$ $\quad E = \frac{5\hbar\omega}{2}$

$|1\rangle = a^\dagger|0\rangle$ $\quad a^\dagger a|1\rangle = 1|1\rangle$ $\quad E = \frac{3\hbar\omega}{2}$

$|0\rangle = |0\rangle$ $\quad a^\dagger a|0\rangle = 0|0\rangle$ $\quad E = \frac{\hbar\omega}{2}$

$\left|0\right\rangle$ represents vacuum ie no particles

$a^{\dagger n}\left|0\right\rangle$ represent n-particle state ie $a^\dagger$ creates a particle

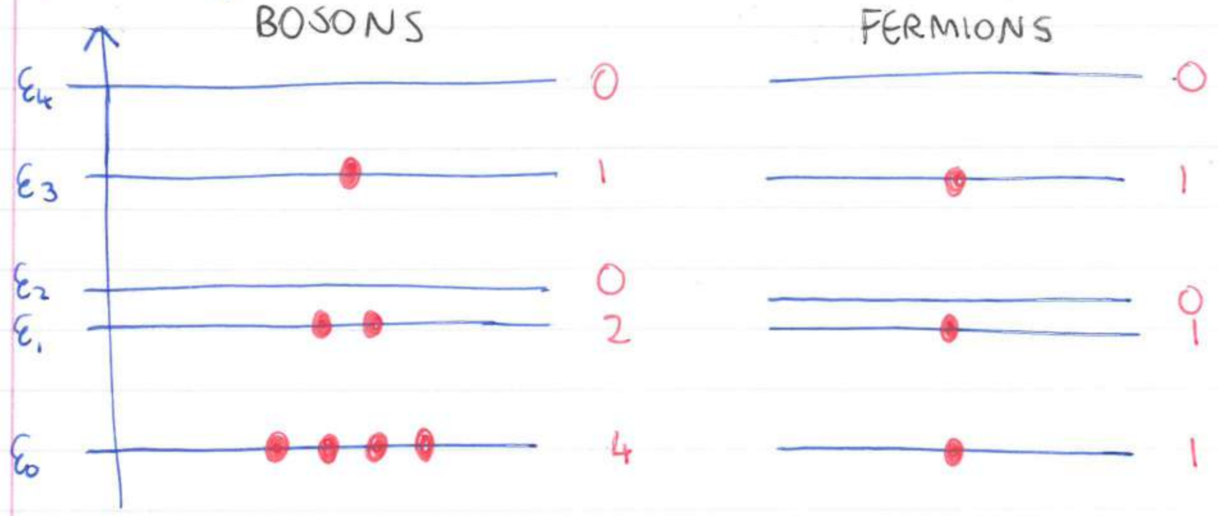
a annihilates a particle

] useful in making wavefn

$a^\dagger a\left|n\right\rangle = n\left|n\right\rangle$ counts number of particles so useful in construction of the Hamiltonian

(note destroy and create, giving out n.

Now construct bosonic wavefunction, energy levels not equally spaced eg bandstructure



$$|\Psi\rangle = (a_0^+)^4 (a_1^+)^2 (a_3^+) |\Omega\rangle$$

each like harmonic oscillator with equally spaced energy levels

Now try the same for fermions

$$\{c_i^+, c_j\} = \delta_{ij} = c_i^+ c_j + c_j c_i^+$$

$\{c_i^+, c_j^+\} = 0$ Note: $(c_i^+)^2 = 0$ so cannot create two

$$\{c_i, c_j\} = 0$$

$|\Psi\rangle = c_0^+ c_1^+ c_3^+ |\Omega\rangle$ vs singlet $\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)\right)$

Fill fermion antisymmetry in here

3e atom → Slater determinant seen in computational course

Benefits:

- Avoid complex Slater determinant $\Psi(x_1, x_2, x_3) = \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \psi_3(x_3) \\ \psi_2(x_1) & \psi_2(x_2) & \psi_3(x_3) \\ \psi_3(x_1) & \psi_3(x_2) & \psi_3(x_3) \end{vmatrix}$
- Encompass symmetry in problem
- Easier Hamiltonian that counts particles
- Name "second quantization": first: wavefn from classical continuum - energy / normalisation
  second: quantized states as a^+, a