Thursday, April 11, 2013

2^{nd} Quantization for many-body physics

We consider the eigenstates of an operator Θ: $\Theta|\psi_i\rangle = \theta_i|\psi_i\rangle$

~~We define the Fock states for this Operator~~

we define the Fock states, or occupation number states, for this operator as

$$|0, \ldots, n_i=1, \ldots, 0\rangle \equiv |\psi_i\rangle$$

the general Fock state $|n_1, n_2, \ldots, n_N\rangle$ means that there are n_1 particles in state $|\psi_1\rangle$
n_2 particles in state $|\psi_2\rangle$
$\vdots$

the Fock states with different occupation numbers are considered orthonormal.

The state $|0\rangle = |0, 0, \ldots, 0\rangle \neq 0$ is referred to as the vacuum state

In analogy, with the creation and annihilation operators for excitations of the harmonic oscillator (i.e. particles are the excitations of some abstract "harmonic oscillator"), we define the ~~field~~ operators $a_j^{\dagger}$ and a_j:

$$a_j^{+}|0\rangle = |0, 0, \ldots, n_j = 1, \ldots 0\rangle \equiv |\psi_j\rangle$$

$$a_j\,|0, 0, \ldots, n_j = 1, \ldots 0\rangle = |0\rangle \quad = \delta_{ij}|0\rangle$$

and $a_j|0\rangle = 0$ and $a_i|0, \ldots, n_j = 1, \ldots 0\rangle = 0$ if $i \neq j$

The quantum statistics of the (identical) particles ~~are~~ are embedded in the "commutation" relations for a_j and a_j^{+}:

recall: $\{A, B\} = AB + BA$

Bosons (commutators)

$$[a_i^{+}, a_j^{+}] = 0$$

$$[a_i, a_j] = 0$$

$$[a_i, a_j^{+}] = \delta_{ij}$$

Fermions (anti-commutators)

$$\{a_i^{+}, a_j^{+}\} = 0$$

$$\{a_i, a_j\} = 0$$

$$\{a_i, a_j^{+}\} = \delta_{ij}$$

Define the number operator: $N_i = a_i^{+} a$

$$N_i|\ldots, n_i, \ldots\rangle = n_i|\ldots, n_i, \ldots\rangle$$

$$a_i|\ldots, n_i, \ldots\rangle = \sqrt{n_i}\,|\ldots, n_i - 1, \ldots\rangle$$

$$a_i^{+}|\ldots, n_i, \ldots\rangle = \sqrt{n_i + 1}\,|\ldots, n_i + 1, \ldots\rangle$$

Example: 2 identical particles in 2 distinct states ψ_a and ψ_b

bosons

$$a_a^{+} a_b^{+}|0\rangle = |1, 1\rangle \neq |\psi_a\rangle|\psi_b\rangle$$

$$= a_b^{+} a_a^{+}|0\rangle = |1, 1\rangle \equiv \frac{1}{\sqrt{2}}\left(|\psi_a\rangle|\psi_b\rangle + |\psi_b\rangle|\psi_a\rangle\right)$$

note: $(a_a^{+})^2 = a_a^{+}|1, 0\rangle = \sqrt{2}\,|2, 0\rangle$

fermions

$$a_a^{+} a_b^{+}|0\rangle = a_a^{+}|0, 1\rangle = |1, 1\rangle$$

$$= -a_b^{+} a_a^{+}|0\rangle = -a_b^{+}|1, 0\rangle = \cancel{-|1, 1\rangle}$$

a_b^{+} operator cannot act directly on $|1, 0\rangle$

note: $a_a^{+} a_a^{+}|0\rangle = a_a^{+}|1, 0\rangle = 0$

$\{a_a^{+}, a_a^{+}\} = 0$ ~~⇒ Pauli exclusion~~

Pauli Exclusion principle is enforced automatically.

(fermions) $a_i |n_1, n_2, \ldots, n_i, \ldots\rangle = \begin{cases} (-1)^s |n_1, n_2, \ldots n_i = 0, \ldots\rangle & \text{if } n_i = 1 \\ 0 & \text{if } n_i = 0 \end{cases}$

$= a_i (a_1^+ a_2^+ a_6^+ \ldots |0\rangle)$

$$a_i^+ |n_1, n_2, \ldots, n_i, \ldots\rangle = \begin{cases} 0 & \text{if } n_i = 1 \\ (-1)^s |n_1, n_2, \ldots, n_i = 1, \ldots\rangle & \text{if } n_i = 0 \end{cases}$$

where $s = n_1 + n_2 + \cdots + n_{i-1}$ | $N_i = a_i^+ a_i \rightarrow$ eigenvalues 0, 1.

<u>Constructing operators in 2nd quantized notation</u>

We expect the multiparticle operator for "additive"

~~We expect~~ $\langle n_1, n_2, \ldots | \Theta | n_1, n_2, \ldots \rangle = n_1 \Theta_1 + n_2 \Theta_2 + \ldots$

This can be done with $\Theta = \sum_i \Theta_i N_i = \sum_i \Theta_i a_i^+ a_i$

<u>Changing basis in 2nd quantized notation</u> (i.e. what if you needed to work with several operators?)

Consider an alternate ~~basis~~ eigenbasis (for the Φ operator): $|\phi_i\rangle$, then:

$$|\psi_i\rangle = \sum_j |\phi_j\rangle\langle\phi_j|\psi_i\rangle$$

(creation operator for $|\phi_j\rangle$)

$$\Longleftrightarrow \quad a_i^+|0\rangle = \sum_j \langle\phi_j|\psi_i\rangle b_j^+|0\rangle, \text{ where } b_j^+|0\rangle \equiv |\phi_j\rangle$$

this suggests $\begin{cases} a_i^+ = \sum_j \langle\phi_j|\psi_i\rangle b_j^+ \\ a_i = \sum_j \langle\phi_j|\psi_i\rangle^* b_j = \sum_j \langle\psi_i|\phi_j\rangle b_j \end{cases}$

Example: change of basis for an operator

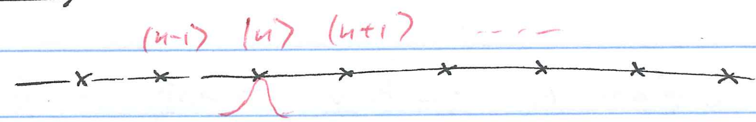
$$\Theta = \sum_i \theta_i a_i^\dagger a_i = \sum_i \theta_i \left(\sum_j \langle \phi_j | \psi_i \rangle b_j^\dagger\right)\left(\sum_\ell \langle \psi_i | \phi_\ell \rangle b_\ell\right)$$

$$= \sum_{j,\ell} b_j^\dagger b_\ell \langle \phi_j | \underbrace{\left(\sum_i \theta_i |\psi_i\rangle\langle\psi_i|\right)}_{\Theta} | \phi_\ell \rangle$$

$$= \sum_{j,\ell} b_j^\dagger b_\ell \underbrace{\langle \phi_j | \Theta | \phi_\ell \rangle}$$

Θ matrix elements in the $|\phi_i\rangle$ basis

Tight binding model in 2nd quantized notation



Recall

$$H = \begin{array}{c} \\ \langle n-1| \\ \langle n| \\ \langle n+1| \\ \vdots \end{array}\begin{array}{c} \begin{array}{ccccc} & |n-1) & |n) & |n+1) & \cdots \end{array} \\ \begin{bmatrix} \ddots & & & & \\ & E_0 & -A & & 0 \\ & -A & E_0 & -A & \\ & & -A & E_0 & -A \\ & 0 & & -A & E_0 \\ & & & & \ddots \end{bmatrix} \end{array}$$

$$\rightarrow \quad H = E_0 \sum_i N_i - A \sum_i \left(a_{i-1}^\dagger a_i + a_{i+1}^\dagger a_i\right)$$

$a_i^\dagger a_{i+1}$

$$= E_0 \sum_i N_i - A \sum_i \left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i\right)$$

this term is just an energy offset if total particle number is constant

How do we add on-site interactions between particles?

$U>0$ repulsive

$U<0$ attractive

for bosons:

$$H_{int} = \frac{U_{\uparrow\downarrow}}{2} \sum_i N_{i\uparrow} N_{i\downarrow} + \frac{U_{\uparrow\uparrow}}{2} \sum_i N_{i\uparrow}(N_{i\uparrow}-1) + \frac{U_{\downarrow\downarrow}}{2} \sum_i N_{i\downarrow}(N_{i\downarrow}-1)$$

for fermions:

$$H_{int} = U \sum_i N_{i,\uparrow} N_{i,\downarrow} = U \sum_i a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow}$$

$$H_{total} = E_0 \sum_{i,\sigma} N_{i,\sigma} - A \sum_{i,\sigma} \left(a_{i,\sigma}^\dagger a_{i+1,\sigma} + a_{i+1,\sigma}^\dagger a_{i,\sigma}\right) + U \sum_i a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow}$$

2D version (on square grid): Boson ~~Hanc~~ version → solved

Fermion version → un solved (analytically & numerically)

(Fermi-Hubbard model)

(ground state is unknown, but may describe high-T_c super conductors)

Stopped here

PHOTONS: Quantization of the E-M field (PDQ)

In the absence of {charges, currents}, Maxwell's equations are

$$\begin{cases} \vec{\nabla}\cdot\vec{E} = 0 \\ \vec{\nabla}\times\vec{E} = -\dfrac{\partial \vec{B}}{\partial t} \\ \vec{\nabla}\cdot\vec{B} = 0 \\ \vec{\nabla}\times\vec{B} = \dfrac{1}{c^2}\dfrac{\partial \vec{E}}{\partial t} \end{cases}$$

In the Coulomb gauge, $\vec{\nabla}\cdot\vec{A} = 0 \Rightarrow \nabla^2 V = 0$

→ set $V = 0$

In this case: $\begin{cases} \vec{E} = -\dfrac{1}{c}\dfrac{\partial \vec{A}}{\partial t} \\ \vec{B} = \vec{\nabla}\times\vec{A} \end{cases}$ and $\vec{A}$ satisfies a wave equation: $\nabla^2 A - \dfrac{1}{c^2}\dfrac{\partial^2 A}{\partial t^2} = 0$

$\omega = ck$

$$\Rightarrow \text{Solutions: } \vec{A}_{k,s}(\vec{r},t) = \underbrace{A_{k,s}\, e^{i(\vec{k}\cdot\vec{r}-\omega t)}\, \hat{e}_{k,s} + A^*_{k,s}\, e^{-i(\vec{k}\cdot\vec{r}-\omega t)}\, \hat{e}_{k,s}}_{\text{real}}$$

to be specified

The general solution is: $\vec{A}(\vec{r},t) = \sum_{k,s} \vec{A}_{k,s}$ ← sum over discrete modes in box universe of volume V.

↳ $\vec{E} = -\dfrac{1}{c}\dfrac{\partial \vec{A}}{\partial t}$, $\vec{B} = \vec{\nabla}\times\vec{A}$

The energy and ~~Hamilto~~ "thus" Hamiltonian are given by

$$H_{\text{classical}} \equiv E = \frac{1}{2}\int_V d^3r \left\{ \varepsilon_0 \vec{E}^2 + \frac{1}{\mu_0}\vec{B}^2 \right\}$$