Creation and Annihilation Operators: "Second Quantization"

Landau & Lifschitz, Quantum Mechanics, section 64

How to cope w/many bosons, fermions
- Laser, lots of photons
- Metal, lots of electrons
- Superfluid, lots of He4 bosons

Change to occupation number basis (Fock Space)

Position Space:

$$\mathcal{H} = \sum_n \underbrace{-\frac{\hbar^2}{2m}\nabla_n^2 + V(\vec{r}_n)}_{\text{Single Particle Operators}} + \sum_{ij} \underbrace{\overbrace{U(\vec{r}_i - \vec{r}_j)}^{\frac{e^2}{|r_i - r_j|}\text{, or vanderWaals}}}_{\text{Two particle operator}}$$

'Second quantization' (grandiose name, nothing new)
- * Designed for few-body interactions
- * Good for interactions between otherwise free particles
- * Links to Greens functions, propagators, density matrices

Change to Fock space = Occupation Number space

Pick a complete, orthonormal <u>single</u> particle basis

$\psi_1(x), \psi_2(x), \ldots$

[Eigenstates of Momentum, energy, position, or...]

Change coordinates from $\Psi(\vec{x}_1, \ldots, \vec{x}_N)$ to $\Phi(N_1, \ldots, N_m)$

Occupation Number Space

$$|\Psi\rangle = \sum_{N_1, N_2, N_3 \ldots} \Phi(N_1, N_2 \ldots) \, |N_1, N_2, \ldots\rangle$$

$$|N_1, N_2, \ldots\rangle = \{\widetilde{Norm}\} \sum_{\tilde{P}} \overbrace{\sigma(\tilde{P})}^{\text{if fermion}} \overbrace{\psi_1(\vec{x}_{\tilde{P}_1}) \psi_1(\vec{x}_{\tilde{P}_2}) \ldots}^{N_1 \text{ times}} \overbrace{\psi_2(\vec{x}_{\tilde{P}_{N_1+1}}) \ldots}^{N_2 \text{ times}}$$

Warning: I permute over particles. Everyone else permutes over single-particle WFs. Relation below.

Fermions: $N_i = \{ {0 \atop 1} \}$ (Pauli exclusion principle: non-interacting)

→ No duplicates

→ Normalization $= \frac{1}{\sqrt{N!}}$

Bosons:

Q: What is Norm if $N_1 = N$, $N_2 = \ldots = 0$?

Q: What about all distinct?

$$\widetilde{Norm} = \frac{1}{\sqrt{N! \, N_1! \, N_2! \ldots}} \quad \text{(JPS notation)}$$

Others permute over 'distinct' relabelings of single-particle states:

$$\sum_P \psi_{P_1}(x_1)\,\psi_{P_2}(x_2)\ldots$$

This is tidier (fewer copies of same state), but less general (doesn't work for WFs that aren't single-particle products).

Q: How many copies are repeated for | N1, N2, ... >?
What is the normalization in the standard notation?

$$\text{Norm} = \sqrt{\frac{N_1!\,N_2!\ldots}{N!}}$$

Back to second quantization. How to write one-body V(x) in occupation number basis?
Note: Actually always want sum_i V(x_i): identical particles have identical interactions.

Diagonal Terms:

$$\langle N_1, N_2, \ldots | V(x_1) | N_1, N_2, \ldots \rangle$$

Q: What is <2,1| V(x1) |2, 1>? <2,1| sum_i V(x_i) |2,1>?

A: Standard notation:

$$\langle x_1, x_2 | 2,1\rangle = \frac{1}{\sqrt{3}}\Big[\psi_1(x_1)\psi_1(x_2)\psi_2(x_3) + \psi_1(x_1)\psi_2(x_2)\psi_1(x_3) + \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)\Big]$$

$$\langle 2,1|V(x_1)|2,1\rangle = \frac{1}{3}\int dx_1\,dx_2\,dx_3 \Big[\psi_1^*(x_1)\underbrace{\psi_1^*(x_2)\psi_2^*(x_3)V(x_1)\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)}_{1 \quad 1}$$

$$+\ \psi_1^*(x_1)\psi_1^*(x_2)\psi_2^*(x_3)\,V(x_1)\,\psi_1(x_1)\psi_2(x_2)\psi_1(x_3)$$

(overlaps marked 0, 0)

$$+\ [7 \text{ more terms}]$$

$$= \frac{1}{3}\underbrace{\int dx_1\,\psi_1^*(x_1)V(x_1)\psi_1^*(x_1)}_{V_{11}} + 0 + 0 + 6\text{ more}$$

Only terms with P1 = P2 contribute...

$$\langle 2,1|V(x_1)|2,1\rangle = \frac{1}{3}(2V_{11}+V_{22})$$

$$\langle 2,1|\sum V(x_i)|2,1\rangle = 2V_{11}+V_{22}$$

$$\langle N_1, N_2, \ldots|\sum V(x_i)|N_1, N_2, \ldots\rangle = \sum N_i V_{ii}$$

Q: What is <2,0| V(x1) |0,2>?

A: Zero. V(x1) can't keep psi_1(x2) psi_2(x2) from giving zero.

Q: What is <2,0| V(x1) |1,1>? [N1 -= 1, N2 += 1]

A: $$\int dx_1 dx_2\, \psi_1^*(x_1)\psi_1^*(x_2)\, V(x_1)\, \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\underbrace{\psi_2(x_2)}_{0} + \psi_1(x_2)\psi_2(x_1)\right]$$

(red: $\int \psi_1^*(x_2)\,\psi_1(x_2) = 1$)

$$= \frac{1}{\sqrt{2}}\int \psi_1^*(x_1)V(x_1)\psi_2(x_1)$$

$$= \frac{1}{\sqrt{2}} V_{12}$$

$$\langle 2,0|\sum V(r_i)|1,1\rangle = \frac{2}{\sqrt{2}}V_{12} = \sqrt{2}\,V_{12}$$

One-body operator allows one number swap. In the end...

$$\langle \ldots N_i, \ldots, N_k - 1, \ldots|\sum V(x_i)|\ldots N_i - 1, \ldots, N_k, \ldots\rangle = \sqrt{N_i N_k}\; V_{ik}$$

Useful annihilation operator:

$$a_k|N_1, \ldots, N_k, \ldots\rangle = \sqrt{N_k}\;|N_1, \ldots, N_k - 1, \ldots\rangle$$

annihilates one particle in state k.

Big matrix in k-sector, only one non-zero entry:

$$\langle N_k - 1|a_k|N_k\rangle = \sqrt{N_k}$$

Hermitian conjugate is creation operator:

$$a_i^+ : \langle N_i | a_i^+ | N_i - 1 \rangle = \langle N_i - 1 | a_i | N_i \rangle^* = \sqrt{N_i}$$

(creates particle in state i)

Uses of creation and annihilation operators:

* Can write one-body operators

$$\sum_i V(x_i) \Rightarrow \sum_{ik} V_{ik} a_i^+ a_k \qquad \sum_i \frac{\hbar^2}{2m} \nabla_i^2 \Rightarrow \sum_p \frac{p^2}{2m} a_p^+ a_p$$

* Can write two-body operators

$$\sum_{ij} U(x_i, x_j) \Rightarrow \frac{1}{2} \sum_{iklm} \langle ik | U | lm \rangle a_i^+ a_k^+ a_l a_m$$

$$\int dx_1 \int dx_2\, \psi_i^*(x_1) \psi_k^*(x_2) \psi_l(x_1) \psi_m(x_2)$$

* Can write Hamiltonians

$$\mathcal{H} = \sum_\alpha \varepsilon_\alpha a_\alpha^+ a_\alpha + \sum_{\alpha,\beta,\gamma,\delta} U_{\alpha\beta\gamma\delta} a_\alpha^+ a_\beta^+ a_\gamma a_\delta$$

(ε_α: Free-particle energy basis)

* Interactions scatter particles from γ, δ to α, β with amplitude $U_{\alpha\beta\gamma\delta}$