Lecture V: Second Quantised Representation of Operators

So far we have developed an operator-based formulation of many-particle states. However, for this representation to be useful, we have to understand how the action of first quantised operators on many-particle states can be formulated within the framework of the second quantisation. To do so, it is natural to look for a formulation in the diagonal basis and recall the action of the particle number operator. To begin, let us consider...

▷ One-body operators, i.e. operators which address only one particle at a time

$$\hat{\mathcal{O}}_1 = \sum_{n=1}^{N} \hat{o}_n, \qquad \text{e.g. k.e. } \hat{T} = \sum_{n=1}^{N} \frac{\hat{p}_n^2}{2m}$$

- Suppose $\hat{o}$ diagonal in orthonormal basis $|\lambda\rangle$ *e.g.* $\hat{o} = \hat{p}^2/2m$ *with* $|p\rangle$ *and* $o_p = p^2/2m$
  i.e. $\hat{o} = \sum_{\lambda=0}^{\infty} |\lambda\rangle o_\lambda \langle\lambda|, \qquad o_\lambda = \langle\lambda|\hat{o}|\lambda\rangle$

$$\begin{aligned}\langle\lambda_1', \cdots \lambda_N'|\hat{\mathcal{O}}_1|\lambda_1, \cdots \lambda_N\rangle &= \left(\sum_{i=1}^{N} o_{\lambda_i}\right)\langle\lambda_1', \cdots \lambda_N'|\lambda_1, \cdots \lambda_N\rangle \\ &= \langle\lambda_1', \cdots \lambda_N'|\sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda|\lambda_1, \cdots \lambda_N\rangle,\end{aligned}$$

Since this holds for any basis state, $\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} o_\lambda a_\lambda^\dagger a_\lambda$

i.e. in diagonal representation, simply count number of particles in state λ *and multipy by corresponding eigenvalue of one-body operator*

Transforming to general basis (recall $a_\lambda = \sum_\nu \langle\lambda|\nu\rangle a_\nu$)

$$\boxed{\hat{\mathcal{O}}_1 = \sum_{\lambda\mu\nu} \langle\mu|\lambda\rangle o_\lambda \langle\lambda|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu}$$

i.e. $\hat{\mathcal{O}}_1$ scatters particle from state ν to μ with probability amplitude $\langle\mu|\hat{o}|\nu\rangle$

▷ Examples of one-body operators:

1. Total number operator: $\hat{N} = \int dx\ a^\dagger(x)a(x) = \sum_k a_k^\dagger a_k$
2. Electron spin operator: $\hat{\mathbf{S}} = \sum_{\alpha\beta} a_\alpha^\dagger \mathbf{S}_{\alpha\beta} a_\beta, \qquad \mathbf{S}_{\alpha\beta} = \langle\alpha|\hat{\mathbf{S}}|\beta\rangle = \frac{1}{2}\sigma_{\alpha\beta}$
   where $\alpha = \uparrow, \downarrow$, and σ are Pauli spin matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mapsto \hat{S}^z = \frac{1}{2}(n_\uparrow - n_\downarrow), \qquad \sigma_+ = \sigma_x + i\sigma_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mapsto \hat{S}^+ = a_\uparrow^\dagger a_\downarrow$$

3. Free particle Hamiltonian

$$\sum_p \frac{p^2}{2m} a_p^\dagger a_p \stackrel{\text{Exercise}}{=} \int_0^L dx\ a^\dagger(x) \frac{(-\hbar^2 \partial_x^2)}{2m} a(x)$$

i.e. $$\boxed{\hat{H} = \hat{T} + \hat{V} = \int_0^L dx\ a^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] a(x)}$$

where $\hat{p} = -i\hbar\partial_x$

▷ Two-body operators, i.e. operators which engage two-particles

E.g. symmetric pairwise interaction: $V(x,x') \equiv V(x',x)$ (such as Coulomb) acting between two-particle states

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ |x,x'\rangle V(x,x')\langle x,x'|$$

When acting on many-particle states,

$$\hat{V}|x_1, x_2, \cdots x_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle$$

How can one express $\hat{V}$ in second quantised form?

might guess that

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ a^\dagger(x) a^\dagger(x') V(x,x') a(x') a(x)$$

i.e. annihilation operators check for presence of particles at x and x' — if they exist, asign the potential energy and then recreate particles in correct order (viz. statistics). Factor of two for double-counting.

check:

$$a^\dagger(x)a^\dagger(x')a(x')a(x)|x_1, x_2, \cdots x_N\rangle = a^\dagger(x)a^\dagger(x')a(x')a(x) \quad a^\dagger(x_1)\cdots a^\dagger(x_N)|\Omega\rangle$$

$$= \sum_{n=1}^{N} \zeta^{n-1}\delta(x-x_n) a^\dagger(x_n)\ \overbrace{a^\dagger(x')a(x')}^{n(x')} \quad a^\dagger(x_1)\cdots a^\dagger(x_{n-1})a^\dagger(x_{n+1})\cdots a^\dagger(x_N)|\Omega\rangle$$

$$= \sum_{n=1}^{N} \zeta^{n-1}\delta(x-x_n) \sum_{m(\neq n)}^{N} \delta(x'-x_m) a^\dagger(x_n) \quad a^\dagger(x_1)\cdots a^\dagger(x_{n-1})a^\dagger(x_{n+1})\cdots a^\dagger(x_N)|\Omega\rangle$$

$$= \sum_{n,m\neq n}^{N} \delta(x-x_n)\delta(x'-x_m)|x_1, x_2, \cdots x_N\rangle$$

then multiplying by $V(x,x')/2$, and integrate over x and x' $\mapsto \hat{V}$

N.B. $\displaystyle\frac{1}{2}\int dx \int dx'\, V(x,x')\hat{n}(x)\hat{n}(x')$ does *not* reproduce the two-body operator

▷ Turning to a non-diagonal basis

$$\boxed{\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\mu,\mu',\lambda,\lambda'} a^\dagger_\mu a^\dagger_{\mu'} a_\lambda a_{\lambda'}, \qquad \mathcal{O}_{\mu,\mu',\lambda,\lambda'} \equiv \langle \mu,\mu'|\hat{\mathcal{O}}_2|\lambda,\lambda'\rangle}$$

▷ <u>Applications of Second Quantisation</u>

1. Phonons

   Oscillator states $|k\rangle$ form a Fock space:
   for each mode k, an arbitrary state of excitation can be created from the vacuum

   $$|k\rangle = a^\dagger_k|\Omega\rangle, \qquad a_k|\Omega\rangle = 0, \qquad [a_k, a^\dagger_{k'}] = \delta_{kk'}, \qquad \hat{H} = \sum_k \hbar\omega_k \left(a^\dagger_k a_k + 1/2\right)$$

   In this case, the Hamiltonian is <u>diagonal</u>: any state $|k_1,k_2,\cdots\rangle = a^\dagger_{k_1} a^\dagger_{k_2}\cdots|\Omega\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $\hbar\omega_{k_1} + \hbar\omega_{k_2} + \cdots$

2. Interacting Electron Gas

   (i) Free-electron Hamiltonian

   $$\hat{H}^{(0)} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\sigma} c_{k\sigma}, \qquad [c_{k\sigma}, c^\dagger_{k'\sigma'}] = \delta_{kk'}\delta_{\sigma\sigma'}$$

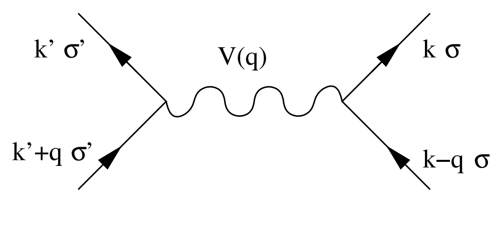
   also diagonal in plain wave basis

   (ii) Two-body interactions:

   $$\hat{H} = \hat{H}^{(0)} + \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c^\dagger_\sigma(x) c^\dagger_{\sigma'}(x') V(x-x') c_{\sigma'}(x') c_\sigma(x)$$

   N.B. off-diagonal in Fourier basis! $\displaystyle\sum_{kk'q}\sum_{\sigma\sigma'} V(q)\, c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c_{k'+q,\sigma} c_{k-q,\sigma}$

   Feynman diagram:



▷ COMMENTS:

- Phonon Hamiltonian is example of 'free field theory':
  involves field operators at quadratic order but no higher...
- (whereas) electron Hamiltonian is typical of an interacting field theory:
  here there are two-body terms!
- As compared to free theories, analysis of interacting theories is infinitely harder...

▷ To familiarise ourselves with the second quantisation,
in the following lectures we will look at SEVERAL CASE STUDIES:

- 'Atomic limit' of strongly interacting electron gas:
  electron crystallisation and Mott transition
- Quantum magnetism
- Weakly interacting Bose gas