Notes on Second Quantisation

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1 Introduction

- When we deal with a system of identical particles, it becomes inconvenient to write the many-body wavefunction in the form

$$\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,...,\mathbf{r}_N).$$

- Instead, we make use of the fact that identical quantum mechanical particles are indistinguishable, and express the state in terms of the occupation numbers n_i of a complete set of single particle states.

2 Free Particles

- We consider particles in a cubic volume of side length L. This will be our quantisation volume $V = L^3$ for normalisation, and we impose periodic boundary conditions.
- In this volume, the momentum is quantised as

$$\mathbf{p} = \frac{2\pi}{L}(m_1, m_2, m_3)\hbar$$

where m_i are integers.

- The state of the system is then characterised by the number of particles $n_{\mathbf{p}}$ having momentum $\mathbf{p}$:

$$|\psi\rangle = |n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, ..., n_{\mathbf{p}_i}, ...\rangle = \prod_i |n_{\mathbf{p}_i}\rangle$$

- We choose the normalisation of the states as

$$\langle n'_{\mathbf{p}_1}, n'_{\mathbf{p}_2}, ..., n'_{\mathbf{p}_i}, ... \,|\, n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, ..., n_{\mathbf{p}_i}, ...\rangle = \delta_{n'_{\mathbf{p}_1},n_{\mathbf{p}_1}}\, \delta_{n'_{\mathbf{p}_1},n_{\mathbf{p}_2}} ... \delta_{n'_{\mathbf{p}_i},n_{\mathbf{p}_i}} ...$$

- These states for all combinations of $\{n_{\mathbf{p}_i}\}$ form a complete basis for our many-particle system.

2.1 Identical Bosons

- We now define the *annihilation* operator for mode $\mathbf{p}$ as

$$\hat{b}_{\mathbf{p}}\, |...n_{\mathbf{p}}...\rangle = \sqrt{n_{\mathbf{p}}}\, |...(n_{\mathbf{p}} - 1)...\rangle$$

- The adjoint of this operator is then the creation operator $b^\dagger_{\mathbf{p}}$, and it can be shown that

$$\hat{b}^\dagger_{\mathbf{p}}\, |...n_{\mathbf{p}}...\rangle = \sqrt{n_{\mathbf{p}} + 1}\, |...(n_{\mathbf{p}} + 1)...\rangle$$

- The relevant commutator relations are given by

$$[\hat{b}_{\mathbf{p}}, \hat{b}^{\dagger}_{\mathbf{p}'}] = \delta_{\mathbf{p},\mathbf{p}'}$$
$$[\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = [\hat{b}^{\dagger}_{\mathbf{p}}, \hat{b}^{\dagger}_{\mathbf{p}'}] = 0$$

- Because

$$\hat{b}^{\dagger}_{\mathbf{p}}\hat{b}^{\dagger}_{\mathbf{p}'} |\phi\rangle = \hat{b}^{\dagger}_{\mathbf{p}'}\hat{b}^{\dagger}_{\mathbf{p}} |\phi\rangle$$

  these states are symmetric under interchange of particles, and we are dealing with a system of Bosons.

- These states are called Fock states, or number states, because they are eigenstates of the particle number operator

$$\hat{N}_{\mathbf{p}} = \hat{b}^{\dagger}_{\mathbf{p}}\hat{b}_{\mathbf{p}}$$
$$\hat{N}_{\mathbf{p}} |...n_{\mathbf{p}}...\rangle = n_{\mathbf{p}} |...n_{\mathbf{p}}...\rangle$$

- $\{N_{\mathbf{p}}\}$ forms a complete set of commuting observables, and thus all other possible many-body states can be constructed from superpositions of Fock states.

- Using the number operator, we can construct the momentum operator as

$$\hat{\mathbf{P}} = \sum_{\mathbf{p}} \mathbf{p}\hat{N}_{\mathbf{p}} = \sum_{\mathbf{p}} \mathbf{p}\, \hat{b}^{\dagger}_{\mathbf{p}}\hat{b}_{\mathbf{p}}$$

- The kinetic energy operator is then similarly written as

$$\hat{H}_{KE} = \sum_{\mathbf{p}} E_{\mathbf{p}}\hat{N}_{\mathbf{p}} = \sum_{\mathbf{p}} \frac{p^2}{2m}\, \hat{b}^{\dagger}_{\mathbf{p}}\hat{b}_{\mathbf{p}}$$

  so that the Schrödinger equation for non-interacting particles reads

$$\hat{H}_{KE} |\psi\rangle = i\hbar\frac{\partial}{\partial t} |\psi\rangle$$

- Note the similarities between this formalism, and the formalism for the harmonic oscillator with creation and annihilation operators for the excitations. Here, each state behaves as an independent harmonic oscillator, and the number of particles in the state are the excitation level of that oscillator.

2.2 Identical Fermions

- The state for Fermions must be antisymmetric under interchange of particles, and therefore the fermion creation and annihilation operators must obey the relations

$$\hat{c}^{\dagger}_{\mathbf{p}}\hat{c}^{\dagger}_{\mathbf{p}'} = -\hat{c}^{\dagger}_{\mathbf{p}'}\hat{c}^{\dagger}_{\mathbf{p}}, \quad \hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}'} = -\hat{c}_{\mathbf{p}'}\hat{c}_{\mathbf{p}}$$

  and

$$\hat{c}_{\mathbf{p}}\hat{c}^{\dagger}_{\mathbf{p}'} + \hat{c}^{\dagger}_{\mathbf{p}'}\hat{c}_{\mathbf{p}} = \delta_{\mathbf{p},\mathbf{p}'}$$

- These are so-called anticommutation relations, defined as

$$\{A, B\} = [A, B]_{+} = AB + BA$$

- We can thus write the relations for Fermionic operators as

$$[\hat{c}_{\mathbf{p}}, \hat{c}^{\dagger}_{\mathbf{p}'}]_{+} = \delta_{\mathbf{p},\mathbf{p}'}$$
$$[\hat{c}_{\mathbf{p}}, \hat{c}_{\mathbf{p}'}]_{+} = [\hat{c}^{\dagger}_{\mathbf{p}}, \hat{c}^{\dagger}_{\mathbf{p}'}]_{+} = 0$$

- Note that these operators obey the Pauli exclusion principle, as

$$\hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}} = -\hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}}, \;\Rightarrow \hat{c}^2_{\mathbf{p}} = 0,$$

  and thus

$$\hat{N}^2_{\mathbf{p}} = \hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}}\hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}} = \hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}} - \hat{c}^{\dagger}_{\mathbf{p}}\hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}} = \hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}} = \hat{N}_{\mathbf{p}}$$

  so that the only allowed eigenvalues for $\hat{N}_{\mathbf{p}}$ for Fermions are 0 and 1.

- As for Bosons, the momentum and kinetic energy operators are given by

$$\hat{\mathbf{P}} = \sum_{\mathbf{p}} \mathbf{p}\, \hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}}, \quad \hat{H}_{KE} = \sum_{\mathbf{p}} \frac{p^2}{2m}\, \hat{c}^{\dagger}_{\mathbf{p}}\hat{c}_{\mathbf{p}}$$

3 Field Operators

- We define the field operators

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} \mathrm{e}^{i(\mathbf{k}.\mathbf{r}-\omega_p t)}\hat{a}_{\mathbf{p}}$$
$$\hat{\psi}^{\dagger}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} \mathrm{e}^{-i(\mathbf{k}.\mathbf{r}-\omega_p t)}\hat{a}^{\dagger}_{\mathbf{p}}$$

  where $\mathbf{k} = \mathbf{p}/\hbar$, $\omega_p = E_p/\hbar = p^2/(2m\hbar)$.

- This operator obeys the commuator (or equivalent anticommutator for fermions)

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^{\dagger}(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}')$$

- These operators can be interpreted as the creation and annihilation operators for a state in which a particle is located at the point $\mathbf{r}$, and are the Fourier transforms of the momentum space operators.

$$|\mathbf{r}\rangle = \hat{\psi}^{\dagger}(\mathbf{r})\,|0\rangle$$

- We can compute the commutators

$$[\hat{H}_{KE}, \hat{\psi}^{\dagger}(\mathbf{r})] = -\frac{\hbar^2}{2m}\nabla^2\hat{\psi}^{\dagger}(\mathbf{r})$$
$$[\hat{H}_{KE}, \hat{\psi}(\mathbf{r})] = \frac{\hbar^2}{2m}\nabla^2\hat{\psi}(\mathbf{r})$$

- In the Heisenberg picture, the equation of motion for the field operator of a free particle is

$$i\hbar\frac{\partial\hat{\psi}}{\partial t} = [\hat{\psi}, \hat{H}] = [\hat{\psi}, \hat{H}_{KE}] = -\frac{\hbar^2}{2m}\nabla^2\hat{\psi}$$

- This has the same form as the usual Schrödinger equation for a single particle, except that ψ is now an operator. This is why this formulation of many-body quantum mechanics is known as second quantisation: This is the same theory that would result from taking the single particle wavefunction to be a classical field, and then imposing commutation relations on that field.

- Many useful forms involving the field operators can be proven using the wavefunction for a particle of momentum $\mathbf{p}$ in a box of volume V,

$$\langle \mathbf{r} | \, \mathbf{p} \rangle = \frac{1}{\sqrt{V}} \mathrm{e}^{i(\mathbf{k}.\mathbf{r} - \omega_p t)}$$

together with the identity

$$\int_V d^3 r \; \mathrm{e}^{i\mathbf{k}.\mathbf{r}} = \begin{cases} V, & k = 0 \\ 0, & k \neq 0 \end{cases} = V \, \delta_{\mathbf{k},\mathbf{0}}$$

- For example,

$$\begin{aligned} \hat{H}_{KE} &= \int d^3 r \, \hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(\mathbf{r}) \\ \hat{P} &= \int d^3 r \, \hat{\psi}^\dagger(\mathbf{r}) \; (-i\hbar\nabla) \; \hat{\psi}(\mathbf{r}) \\ \hat{N} &= \int d^3 r \, \hat{\psi}^\dagger(\mathbf{r}) \, \hat{\psi}(\mathbf{r}) \end{aligned}$$

- With an external field $V_1(\mathbf{r})$, the Hamiltonian is written

$$\hat{H}_0 = \int d^3 r \, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_1(\mathbf{r}) \right] \hat{\psi}(\mathbf{r})$$

- Interactions between two atoms described by a potential $V_2(\mathbf{r}_1 - \mathbf{r}_2)$ produce a Hamiltonian of the form $\hat{H} = \hat{H}_0 + \hat{H}_{int}$, with

$$\hat{H}_{int} = \frac{1}{2} \int d^3 r \int d^3 r' \, \hat{\psi}^\dagger(\mathbf{r}, t) \, \hat{\psi}^\dagger(\mathbf{r}', t) \, V_2(\mathbf{r}' - \mathbf{r}) \, \hat{\psi}(\mathbf{r}', t) \, \hat{\psi}(\mathbf{r}, t)$$