

Lesson 9 - Second Quantization of Matter

Unit 9.1 Schrödinger field for bosons and fermions

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Structure of Matter - MSc in Physics

Time-dependent Schrödinger equation (I)

In 1927 Paul Dirac suggested that the light field is composed of an infinite number of quanta, the photons.

In the same year Eugene Wigner and Pascual Jordan proposed something similar for the matter.

In non-relativistic quantum mechanics the matter field is nothing but the single-particle Schrödinger field $\psi(\mathbf{r}, t)$ of quantum mechanics, which satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \psi(\mathbf{r}, t), \quad (1)$$

where $U(\mathbf{r})$ is the external potential acting on the quantum particle.

Time-dependent Schrödinger equation (II)

The Schrödinger field $\psi(\mathbf{r}, t)$ can be expanded as

$$\psi(\mathbf{r}, t) = \sum_{\alpha} c_{\alpha}(t) \phi_{\alpha}(\mathbf{r}) \quad (2)$$

where $\phi_{\alpha}(\mathbf{r})$ are the eigenfunctions of the stationary equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \phi_{\alpha}(\mathbf{r}) = \epsilon_{\alpha} \phi_{\alpha}(\mathbf{r}) \quad (3)$$

with ϵ_{α} the eigenvalues and α the label which represents the set of quantum numbers. The eigenfunctions are orthonormal, namely

$$\int d^3\mathbf{r} \phi_{\alpha}^*(\mathbf{r}) \phi_{\beta}(\mathbf{r}) = \delta_{\alpha\beta} . \quad (4)$$

Inserting Eq. (2) into the time-dependent Schrödinger equation (1) one easily finds

$$c_{\alpha}(t) = c_{\alpha}(0) e^{-i\epsilon_{\alpha} t/\hbar} . \quad (5)$$

Schrödinger energy (I)

The constant of motion associated to the Schrödinger field $\psi(\mathbf{r}, t)$ is the average total energy of the system, given by

$$H = \int d^3\mathbf{r} \psi^*(\mathbf{r}, t) \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \psi(\mathbf{r}, t). \quad (6)$$

Inserting the expansion (2) into the total energy we find

$$H = \sum_{\alpha} \frac{\epsilon_{\alpha}}{2} (c_{\alpha}^* c_{\alpha} + c_{\alpha} c_{\alpha}^*). \quad (7)$$

This energy is obviously independent on time: the time dependence of the complex amplitudes $c_{\alpha}^*(t)$ and $c_{\alpha}(t)$ cancels due to Eq. (5).

Schrödinger energy (II)

Instead of using the complex amplitudes $c_\alpha^*(t)$ and $c_\alpha(t)$ one can introduce the real variables

$$q_\alpha(t) = \sqrt{\frac{2\hbar}{\omega_\alpha}} \frac{1}{2} (c_\alpha(t) + c_\alpha^*(t)) \quad (8)$$

$$p_\alpha(t) = \sqrt{2\hbar\omega_\alpha} \frac{1}{2i} (c_\alpha(t) - c_\alpha^*(t)) \quad (9)$$

such that the Schrödinger energy of the matter field reads

$$H = \sum_{\alpha} \left(\frac{p_\alpha^2}{2} + \frac{1}{2} \omega_\alpha^2 q_\alpha^2 \right), \quad (10)$$

where

$$\omega_\alpha = \frac{\epsilon_\alpha}{\hbar} \quad (11)$$

is the eigenfrequency associated to the eigenenergy ϵ_α .

This energy is written in terms of an infinite set of real harmonic oscillators: one oscillator for each mode characterized by quantum numbers α and frequency ω_α .

Second quantization (I)

The canonical quantization of the classical Hamiltonian (10) is obtained by promoting the real coordinates q_α and the real momenta p_α to operators:

$$q_\alpha \rightarrow \hat{q}_\alpha , \quad (12)$$

$$p_\alpha \rightarrow \hat{p}_\alpha , \quad (13)$$

satisfying the commutation relations

$$[\hat{q}_\alpha, \hat{p}_\beta] = i\hbar \delta_{\alpha\beta} , \quad (14)$$

The quantum Hamiltonian is thus given by

$$\hat{H} = \sum_{\alpha} \left(\frac{\hat{p}_\alpha^2}{2} + \frac{1}{2} \omega_\alpha^2 \hat{q}_\alpha^2 \right) . \quad (15)$$

The formal difference between Eq. (10) and Eq. (15) is simply the presence of the “hat symbol” in the canonical variables.

Second quantization (II)

We now introduce annihilation and creation operators

$$\hat{c}_\alpha = \sqrt{\frac{\omega_\alpha}{2\hbar}} \left(\hat{q}_\alpha + \frac{i}{\omega_\alpha} \hat{p}_\alpha \right), \quad (16)$$

$$\hat{c}_\alpha^+ = \sqrt{\frac{\omega_\alpha}{2\hbar}} \left(\hat{q}_\alpha - \frac{i}{\omega_\alpha} \hat{p}_\alpha \right), \quad (17)$$

which satisfy the commutation relations

$$[\hat{c}_\alpha, \hat{c}_\beta^+] = \delta_{\alpha,\beta}, \quad [\hat{c}_\alpha, \hat{c}_\beta] = [\hat{c}_\alpha^+, \hat{c}_\beta^+] = 0, \quad (18)$$

and the quantum Hamiltonian (15) becomes

$$\hat{H} = \sum_\alpha \epsilon_\alpha \left(\hat{c}_\alpha^+ \hat{c}_\alpha + \frac{1}{2} \right). \quad (19)$$

Second quantization (III)

The operators \hat{c}_α and \hat{c}_α^+ act in the Fock space of the “particles” of the Schrödinger field. A generic state of this Fock space is given by

$$| \dots n_\alpha \dots n_\beta \dots n_\gamma \dots \rangle , \quad (20)$$

meaning that there are n_α particles in the single-particle state $|\alpha\rangle$, n_β particles in the single-particle state $|\beta\rangle$, n_γ particles in the single-particle state $|\gamma\rangle$, et cetera.

The operators \hat{c}_α and \hat{c}_α^+ are called annihilation and creation operators because they respectively destroy and create one particle in the single-particle state $|\alpha\rangle$, namely

$$\hat{c}_\alpha | \dots n_\alpha \dots \rangle = \sqrt{n_\alpha} | \dots n_\alpha - 1 \dots \rangle , \quad (21)$$

$$\hat{c}_\alpha^+ | \dots n_\alpha \dots \rangle = \sqrt{n_\alpha + 1} | \dots n_\alpha + 1 \dots \rangle . \quad (22)$$

These properties follow directly from the commutation relations (18).

Second quantization (IV)

The vacuum state, where there are no particles, can be written as

$$|0\rangle = |\dots 0 \dots 0 \dots 0 \dots\rangle, \quad (23)$$

and

$$\hat{c}_\alpha |0\rangle = 0, \quad (24)$$

$$\hat{c}_\alpha^+ |0\rangle = |1_\alpha\rangle = |\alpha\rangle, \quad (25)$$

where $|\alpha\rangle$ is such that

$$\langle \mathbf{r} | \alpha \rangle = \phi_\alpha(\mathbf{r}). \quad (26)$$

From Eqs. (21) and (22) it follows immediately that

$$\hat{N}_\alpha = \hat{c}_\alpha^+ \hat{c}_\alpha \quad (27)$$

is the number operator which counts the number of particles in the single-particle state $|\alpha\rangle$, i.e.

$$\hat{N}_\alpha |\dots n_\alpha \dots\rangle = n_\alpha |\dots n_\alpha \dots\rangle. \quad (28)$$

Bosonic vs fermionic matter field (I)

The annihilation and creation operators \hat{c}_α and \hat{c}_α^+ which satisfy the commutation rules (18) are called bosonic operators and the corresponding quantum field operator

$$\hat{\psi}(\mathbf{r}, t) = \sum_{\alpha} \hat{c}_\alpha(t) \phi_\alpha(\mathbf{r}) \quad (29)$$

is the bosonic field operator. Indeed the commutation rules (18) imply Eqs. (21) and (22) and, as expected for bosons, there is no restriction on the number of particles n_α which can occupy in the single-particle state $|\alpha\rangle$.

To obtain fermionic properties it is sufficient to impose anti-commutation rules for the operators \hat{c}_α and \hat{c}_α^+ , i.e.

$$\{\hat{c}_\alpha, \hat{c}_\beta^+\} = \delta_{\alpha\beta}, \quad \{\hat{c}_\alpha, \hat{c}_\beta\} = \{\hat{c}_\alpha^+, \hat{c}_\beta^+\} = 0, \quad (30)$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ are the anti-commutation brackets.

An important consequence of anti-commutation is that

$$(\hat{c}_\alpha^+)^2 = 0. \quad (31)$$

Moreover, the eigenvalues of \hat{N}_α can be only 0 and 1. This is exactly the Pauli exclusion principle.