Introduction to Quantum Physics

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Abstract

The video channel with the title "Professor M does Science" in YouTube offers a simple step-by-step but all the same very valuable and rigorous introduction into the world of quantum physics. This script covers quantum fields and helps to digest the topic covered by a group of those videos but is not meant as a replacement for them.

8 Quantum Fields

8.1 Quantum Field Operators

A field in physics is a mathematical object that is defined at every point in space, and a quantum field is a field in quantum mechanics. The quantum field operators to be defined are the basic quantities of quantum field theory. They are the creation and annihilation operators in the position representation and allow to create and annihilate particles at any point in space. Two ingredients are needed in order to determine them.

A change of the basis from $\{|u_i\rangle\}$ to $\{|v_j\rangle\}$ for both the bosonic and fermionic creation and annihilation operators as the first ingredient means

$$\hat{a}^\dagger_{v_j} = \sum_i \langle u_i|v_j\rangle\, \hat{a}^\dagger_{u_i} \qquad\qquad \hat{a}_{v_j} = \sum_i \langle v_j|u_i\rangle\, \hat{a}_{u_i}$$

in the occupation number representation, and the second ingredient for defining the quantum field operators is the position representation with the eigenvalue equation $\hat{\underline{r}}\,|\underline{r}\rangle = \underline{r}\,|\underline{r}\rangle$. As a Hermitian operator the eigenstates of the position operator $|\underline{r}\rangle$ span an orthonormal basis for the state space where the orthonormality is written as $\langle\underline{r}|\underline{r}'\rangle = \delta(\underline{r}-\underline{r}')$ using the Dirac delta-function. A state $|\varphi\rangle$ is

$$|\varphi\rangle = \int d\,\underline{r}\,\varphi(\underline{r})\,|\underline{r}\rangle \qquad\qquad \varphi(\underline{r}) = \langle\underline{r}\,|\,\varphi\rangle$$

where the expansion coefficient $\varphi(\underline{r})$ is called a wave function.

The creation quantum field operator is defined as

$$\hat{a}^\dagger_{\underline{r}} = \sum_i \langle u_i\,|\,\underline{r}\rangle\, \hat{a}^\dagger_{u_i} = \sum_i u_i^*(\underline{r})\, \hat{a}^\dagger_{u_i} \qquad\qquad \langle u_i\,|\,\underline{r}\rangle = u_i^*(\underline{r})$$

by going from the basis $\{|u_i\rangle\}$ and to the position representation basis $\{|\underline{r}\rangle\}$. Changing the notation from $\hat{a}^\dagger_{\underline{r}}$ to $\hat{\psi}^\dagger(\underline{r})$ as common in quantum field theory gives

$$\hat{\psi}^\dagger(\underline{r}) = \sum_i u_i^*(\underline{r})\, \hat{a}^\dagger_{u_i}$$

and

$$\hat{\psi}^\dagger(\underline{r})\,|0\rangle = \sum_i u_i^*(\underline{r})\,\hat{a}_{u_i}^\dagger\,|0\rangle = \sum_i \langle u_i\,|\,\underline{r}\rangle\,|u_i\rangle = \left(\sum_i |u_i\rangle\,\langle u_i|\right)|\underline{r}\rangle = \mathbb{I}\,|\underline{r}\rangle = |\underline{r}\rangle$$

shows that the creation operator indeed creates a particle at position $\underline{r}$ when acting on the vacuum state. The annihilation operator is the adjoint of the creation operator and is therefore

$$\hat{\psi}(\underline{r}) = \left(\sum_i u_i^*(\underline{r})\,\hat{a}_{u_i}^\dagger\right)^\dagger = \sum_i \left(u_i^*(\underline{r})\,\hat{a}_{u_i}^\dagger\right)^\dagger = \sum_i u_i(\underline{r})\,\hat{a}_{u_i}$$

and it can be shown that it indeed removes a particle at position $\underline{r}$.

To summarize, starting from a discrete basis $\{|u_i\rangle\}$ the corresponding creation and annihilation operators $\hat{a}_{u_i}^\dagger$ and $\hat{a}_{u_i}$, respectively, have been transformed to the basis $\{|\underline{r}\rangle\}$ of the position eigenstates

$$\hat{\psi}^\dagger(\underline{r}) = \sum_i u_i^*(\underline{r})\,\hat{a}_{u_i}^\dagger \qquad\qquad \hat{\psi}(\underline{r}) = \sum_i u_i(\underline{r})\,\hat{a}_{u_i} \tag{8.1}$$

and are called the *quantum field operators* or simply the field operators. The expansion coefficients are the wave functions

$$u_i^*(\underline{r}) = \langle u_i\,|\,\underline{r}\rangle \qquad\qquad u_i(\underline{r}) = \langle \underline{r}\,|\,u_i\rangle$$

associated with the basis states.

It is often useful to invert the relations (8.1) to go from the quantum field operators to the operators in the basis $\{|u_i\rangle\}$. The derivation of the corresponding expressions just involves the projection of the field operators onto the basis $\{|u_i\rangle\}$. They are given here as

$$\hat{a}_{u_i}^\dagger = \int d\underline{r}\,u_i(\underline{r})\,\hat{\psi}^\dagger(\underline{r}) \qquad\qquad \hat{a}_{u_i} = \int d\underline{r}\,u_i^*(\underline{r})\,\hat{\psi}(\underline{r}) \tag{8.2}$$

without derivation.

For particles with spin s, the eigenvalues of the operator $\hat{s}_z$ can take any of the $(2s+1)$ possible values $-s, -s+1, -s+2, ..., s-2, s-1, s$. The spin of the electron, for example, can therefore take one of the two values $-\frac{1}{2}$ and $+\frac{1}{2}$. The position representation for a spin this particles is spanned by the states in the basis $\{|\underline{r}\rangle\}$. When working with particles of spin s the augmented basis states labeled by $\{|\underline{r}\rangle\,,\sigma\}$ are used to describe the position representation, but now each position eigentate is associated with a particular spin eigenvalue σ where σ can take any of the allowed values $-s, -s+1, ..., s-1, s$. In this augmented basis of particles with spin, a general quantum state can be written as

$$|\varphi\rangle = \sum_{\sigma=-s}^{s} \int d\underline{r}\,\varphi(\underline{r},\sigma)\,|\underline{r},\sigma\rangle$$

where the wave function $\varphi(\underline{r},\sigma) = \langle \underline{r},\sigma\,|\,\varphi\rangle$ depends on position and the spin labels. Note that $\underline{r}$ is a continuous label leading to an integral and σ is a discrete label leading to a summation. Thus, the quantum field operators become

$$\hat{\psi}_\sigma^\dagger(\underline{r}) = \sum_i u_i^*(\underline{r},\sigma)\,\hat{a}_{u_i}^\dagger \qquad\qquad \hat{\psi}_\sigma(\underline{r}) = \sum_i u_i(\underline{r},\sigma)\,\hat{a}_{u_i} \tag{8.3}$$

given $\{|u_i\rangle\}$ and $\{|\underline{r}\rangle\,,\sigma\}$.

8.2 Commutators and Anticommutators of the Quantum Field Operators

The quantum field operators (8.1) describe creation and annihilation of particles in space. Bosonic field operators obey a set of commutation relations and fermionic field operators obey a set of anticommutation relations. Since the field operators are creation and annihilation operators, they obey the same commutation and anticommutation relations of all the other creation and annihilation operators. As a reminder, the commutator is defined as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$, and the anticommutator is defined as $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$.

The field operators for bosons obey commutation relations. These relations for creation and annihilation operators are

$$[\hat{a}^\dagger_{u_i}, \hat{a}^\dagger_{u_j}] = 0 \qquad [\hat{a}_{u_i}, \hat{a}_{u_j}] = 0 \qquad [\hat{a}_{u_i}, \hat{a}^\dagger_{u_j}] = \delta_{ij}$$

in the basis $\{|u_i\rangle\}$. Thus, the commutation relations are

$$\begin{aligned}
[\hat{\psi}^\dagger(\underline{r}), \hat{\psi}^\dagger(\underline{r}')] &= \left[\sum_i u_i^*(\underline{r})\,\hat{a}^\dagger_{u_i}, \sum_j u_j^*(\underline{r}')\,\hat{a}^\dagger_{u_j}\right] = \sum_{ij} u_i^*(\underline{r})\,u_j^*(\underline{r}')\,[\hat{a}^\dagger_{u_i}, \hat{a}^\dagger_{u_j}] = 0 \\
[\hat{\psi}(\underline{r}), \hat{\psi}(\underline{r}')] &= \left[\sum_i u_i(\underline{r})\,\hat{a}_{u_i}, \sum_j u_j(\underline{r}')\,\hat{a}_{u_j}\right] = \sum_{ij} u_i(\underline{r})\,u_j(\underline{r}')\,[\hat{a}_{u_i}, \hat{a}_{u_j}] = 0 \\
[\hat{\psi}(\underline{r}), \hat{\psi}^\dagger(\underline{r}')] &= \left[\sum_i u_i(\underline{r})\,\hat{a}_{u_i}, \sum_j u_j^*(\underline{r}')\,\hat{a}^\dagger_{u_j}\right] = \sum_{ij} u_i(\underline{r})\,u_j^*(\underline{r}')\,[\hat{a}_{u_i}, \hat{a}^\dagger_{u_j}] = \sum_{ij} u_i(\underline{r})\,u_j^*(\underline{r}')\,\delta_{ij} \\
&= \sum_i u_i(\underline{r})\,u_i^*(\underline{r}') = \sum_i \langle \underline{r}\,|\,u_i\rangle\,\langle u_i\,|\,\underline{r}'\rangle = \langle \underline{r}|\left(\sum_i |u_i\rangle\,\langle u_i|\right)|\underline{r}'\rangle = \langle \underline{r}|\,\mathbb{I}\,|\underline{r}'\rangle \\
&= \langle \underline{r}\,|\,\underline{r}'\rangle = \delta(\underline{r} - \underline{r}')
\end{aligned}$$

in the basis $\{|\underline{r}\rangle\}$. The anticommutator relations for fermions can be derived similarly. To summarize, the commutation relations are

$$[\hat{\psi}^\dagger(\underline{r}), \hat{\psi}^\dagger(\underline{r}')] = 0 \qquad [\hat{\psi}(\underline{r}), \hat{\psi}(\underline{r}')] = 0 \qquad [\hat{\psi}(\underline{r}), \hat{\psi}^\dagger(\underline{r}')] = \delta(\underline{r} - \underline{r}') \tag{8.4}$$

for the bosonic field operators, and the anticommutator relations are

$$\{\hat{\psi}^\dagger(\underline{r}), \hat{\psi}^\dagger(\underline{r}')\} = 0 \qquad \{\hat{\psi}(\underline{r}), \hat{\psi}(\underline{r}')\} = 0 \qquad \{\hat{\psi}(\underline{r}), \hat{\psi}^\dagger(\underline{r}')\} = \delta(\underline{r} - \underline{r}') \tag{8.5}$$

for the fermionic field operators. These results are expected for a continuous basis.

The two relations for the bosons and the fermions show certain similarities, and they can with

$$[\hat{A}, \hat{B}]_{-\eta} = \hat{A}\hat{B} - \eta\,\hat{B}\hat{A} \qquad \eta = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases}$$

be combined into a compact expression such that

$$[\hat{\psi}^\dagger(\underline{r}), \hat{\psi}^\dagger(\underline{r}')]_{-\eta} = 0 \qquad [\hat{\psi}(\underline{r}), \hat{\psi}(\underline{r}')]_{-\eta} = 0 \qquad [\hat{\psi}(\underline{r}), \hat{\psi}^\dagger(\underline{r}')]_{-\eta} = \delta(\underline{r} - \underline{r}')$$

cover the relations for bosons and fermions. In this compact form, the commutation and anticommutation relations for the field operators with spin $\sigma = -s, -s+1, ..., s-1, s$ are

$$[\hat{\psi}^\dagger_\sigma(\underline{r}), \hat{\psi}^\dagger_{\sigma'}(\underline{r}')]_{-\eta} = 0 \qquad [\hat{\psi}_\sigma(\underline{r}), \hat{\psi}_{\sigma'}(\underline{r}')]_{-\eta} = 0 \qquad [\hat{\psi}_\sigma(\underline{r}), \hat{\psi}^\dagger_{\sigma'}(\underline{r}')]_{-\eta} = \delta(\underline{r} - \underline{r}')\,\delta_{\sigma\sigma'}$$

using (8.3) in the orthonormal basis $\{|\underline{r}\rangle, \sigma\}$ such that $\langle \underline{r}, \sigma\,|\,\underline{r}', \sigma'\rangle = \delta(\underline{r} - \underline{r}')\,\delta_{\sigma\sigma'}$

8.3 Operators in Terms of Quantum Field Operators

The quantum field operators (8.1) are the building blocks for quantum field theory. As such all relevant quantities should be expressed in terms of these two field operators $\hat{\psi}^\dagger(\underline{r})$ that creates a particle at position $\underline{r}$ and $\hat{\psi}(\underline{r})$ that annihilates a particle at position $\underline{r}$. The commutation and anticommutation relations in (8.4) and (8.5) belong to bosons and fermions, respectively.

The operators in quantum field theory generally act on systems with many identical particles, and one-body operators among them act on one particle at a time. Given the single-particle state space V_q and an operator $\hat{f}_q$ acting on it, the operator $\mathbb{I}_1 \otimes \mathbb{I}_2 \otimes ... \otimes \hat{f}_q \otimes ... \otimes \mathbb{I}_N$ acts on the full state space $V = V_1 \otimes V_2 \otimes ... \otimes V_q \otimes ... \otimes V_N$ of the N-particle system but its action only affects one particle in the subspace V_q. For simplicity one writes just $\hat{f}_q$ instead of $\mathbb{I}_1 \otimes \mathbb{I}_2 \otimes ... \otimes \hat{f}_q \otimes ... \otimes \mathbb{I}_N$. In the context is should be clear whether $\hat{f}_q$ acts on the state space V_q only or on the full N-particle state space V but only affects particles in V_q while the identity operators $\mathbb{I}_{q'}$ leave the particle in $V_{q'}$ with $q' \neq q$ untouched.

One can build a symmetric one-body operator $\hat{F}$ acting on the full state space V

$$\hat{F} = \sum_{q=1}^{N} \hat{f}_q$$

defined as the sum over all particles of the individual operators acting on each of the individual particles. This one-body operator acts on all particles but does so by acting on each particle separately. Operators of this form are very common for the description of quantum systems. The kinetic energy operator is an example.

In the basis $\{|u_i\rangle\}$ the operator $\hat{F}$ can be written as

$$\hat{F} = \sum_{q=1}^{N} \hat{f}_q = \sum_{ij} \langle u_i \,|\, \hat{f} \,|\, u_j \rangle \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j} = \sum_{ij} f_{ij} \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j}$$

where f_{ij} are the matrix elements in a more compact form. In terms of the field operators the one-body operator becomes

$$\hat{F} = \int d\underline{r}_1 \int d\underline{r}_2 \, \langle \underline{r}_1 | \, \hat{f} \, | \underline{r}_2 \rangle \, \hat{\psi}^\dagger(\underline{r}_1) \, \hat{\psi}(\underline{r}_2) \tag{8.6}$$

because the field operators are nothing more than a continuous version of the creation and annihilation operators in the basis $\{|\underline{r}\rangle\}$.

It is a good exercise to convert the one-body operator from the discrete basis $\{|u_i\rangle\}$ to the continuous basis $\{|\underline{r}\rangle\}$. Thus, inserting (8.2)

$$\begin{aligned}
\hat{F} &= \sum_{ij} \langle u_i \,|\, \hat{f} \,|\, u_j \rangle \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j} = \sum_{ij} \langle u_i \,|\, \hat{f} \,|\, u_j \rangle \left(\int d\underline{r}_1 \, \langle \underline{r}_1 | \, u_i \rangle \; \hat{\psi}^\dagger(\underline{r}_1) \right) \left(\int d\underline{r}_2 \, \langle u_j | \, \underline{r}_2 \rangle \; \hat{\psi}(\underline{r}_2) \right) \\
&= \int d\underline{r}_1 \int d\underline{r}_2 \, \langle \underline{r}_1 | \left(\sum_i |u_i\rangle \, \langle u_i| \right) \hat{f} \left(\sum_j |u_j\rangle \, \langle u_j| \right) |\underline{r}_2\rangle \, \hat{\psi}^\dagger(\underline{r}_1) \, \hat{\psi}(\underline{r}_2) \\
&= \int d\underline{r}_1 \int d\underline{r}_2 \, \langle \underline{r}_1 | \mathbb{I} \hat{f} \mathbb{I} | \, \underline{r}_2 \rangle \, \hat{\psi}^\dagger(\underline{r}_1) \, \hat{\psi}(\underline{r}_2) = \int d\underline{r}_1 \int d\underline{r}_2 \, \langle \underline{r}_1 | \, \hat{f} \, | \, \underline{r}_2 \rangle \, \hat{\psi}^\dagger(\underline{r}_1) \, \hat{\psi}(\underline{r}_2)
\end{aligned}$$

gives the result in (8.6).

The other important type of operators in quantum field theory are the two-body operators used, for example, for the Coulomb interaction between two charged particles. A two-body operator has the form

$$\hat{G} = \frac{1}{2} \sum_{\substack{q,q'=1 \\ q \neq q'}}^{N} \hat{g}_{qq'}$$

where $\hat{g}_{qq'}$ acts on $V_q \otimes V_{q'}$. This operator is

$$\hat{G} = \frac{1}{2} \sum_{ijk\ell} {}_1\langle u_i|_2 \langle u_j| \, \hat{g}_{12} \, |u_k\rangle_1 \, |u_\ell\rangle_2 \, \hat{a}^\dagger_{u_i} \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} \hat{a}_{u_k}$$

in the discrete basis $\{|u_i\rangle\}$, and the two-body operator becomes

$$\hat{G} = \frac{1}{2} \int d\underline{r}_1 \int d\underline{r}_2 \int d\underline{r}_3 \int d\underline{r}_4 \, {}_1\langle \underline{r}_1|_2 \langle \underline{r}_2| \, \hat{g}_{12} \, |\underline{r}_3\rangle_1 \, |\underline{r}_4\rangle_2 \, \hat{\psi}^\dagger(\underline{r}_1) \, \hat{\psi}^\dagger(\underline{r}_2) \, \hat{\psi}(\underline{r}_4) \, \hat{\psi}(\underline{r}_3) \tag{8.7}$$

in the continuous basis $\{|\underline{r}\rangle\}$. Note that the matrix elements are in the order u_k, u_ℓ and $\underline{r}_3, \underline{r}_4$, respectively, but the order in the creation and annihilation operators is u_ℓ, u_k and $\underline{r}_4, \underline{r}_3$, respectively.

To understand the one-body and the two-body operator conceptually, one can look at the field operators at the end of the two expressions. To understand the one-body and two-body operators, one can first look at the field operators. The integrand of the one-body operator involves an annihilation of a particle at position $\underline{r}_2$ and immediate creation of a particle at position $\underline{r}_1$. This process is associated with the matrix elements $\langle \underline{r}_1 | \hat{f} \, | \underline{r}_2 \rangle$ giving the relative amplitude associated with this transition. Thus, a very natural way to interpret this expression is in terms of scatterings of particles from a position $\underline{r}_2$ to a position $\underline{r}_1$ with each transition associated with a certain amplitude given by the corresponding matrix elements. The full one-body operator includes all scatterings for single particles from all possible starting positions to all possible final positions, and each is associated with its own amplitude. All one-body operators have this form and they only differ in the matrix elements which determine the relative importance of each scattering event.

The two-body operator can be understood in a similar way. It describes the scattering of two particles at position $\underline{r}_3$ and $\underline{r}_4$ to the new positions at $\underline{r}_1$ and $\underline{r}_2$. Again the amplitude of this process is associated with the corresponding matrix element ${}_1\langle \underline{r}_1 |_2 \langle \underline{r}_2 | \, \hat{g}_{12} \, | \underline{r}_3 \rangle_1 \, | \underline{r}_4 \rangle_2$. From this point of view, the one-body operator involves the scattering of individual particles while two-body operators involve the scattering of pairs of particles.

The one-body and the two-body operator become

$$\begin{aligned}
\hat{F} &= \sum_{\sigma_1=-s}^{s} \sum_{\sigma_2=-s}^{s} \int d\underline{r}_1 \int d\underline{r}_2 \, \langle \underline{r}_1, \sigma_1 | \, \hat{f} \, | \underline{r}_2, \sigma_2 \rangle \, \hat{\psi}^\dagger_{\sigma_1}(\underline{r}_1) \, \hat{\psi}_{\sigma_2}(\underline{r}_2) \\
\hat{G} &= \frac{1}{2} \sum_{\sigma_1=-s}^{s} \sum_{\sigma_2=-s}^{s} \sum_{\sigma_3=-s}^{s} \sum_{\sigma_4=-s}^{s} \int d\underline{r}_1 \int d\underline{r}_2 \int d\underline{r}_3 \int d\underline{r}_4 \\
&\quad {}_1\langle \underline{r}_1, \sigma_1 |_2 \langle \underline{r}_2, \sigma_2 | \, \hat{g}_{12} \, | \underline{r}_3, \sigma_3 \rangle_1 \, | \underline{r}_4, \sigma_4 \rangle_2 \, \hat{\psi}^\dagger_{\sigma_1}(\underline{r}_1) \, \hat{\psi}^\dagger_{\sigma_2}(\underline{r}_2) \, \hat{\psi}_{\sigma_4}(\underline{r}_4) \, \hat{\psi}_{\sigma_3}(\underline{r}_3)
\end{aligned} \tag{8.8}$$

when including the spin σ for particles with spin. The basic states $|\underline{r}, \sigma\rangle$ include now both position and spin.

As an example the operator $\hat{f} = |\underline{r}\rangle\langle\underline{r}|$ is used. To see what this operator does, consider the expectation value

$$\langle \varphi \, | \, \hat{f} \, | \varphi \rangle = \langle \varphi \, | \, \underline{r} \rangle\langle \underline{r} \, | \, \varphi \rangle = \varphi^*(\underline{r}) \, \varphi(\underline{r}) = |\varphi(\underline{r})|^2$$

where $\langle \underline{r} \, | \, \varphi \rangle$ is the state in the position representation which is the wave function $\varphi(\underline{r})$. This is the probability distribution of finding the quantum particle at a given location in space. Thus, the operator $\hat{f}$ is associated with the local single-particle density at position $\underline{r}$, and it can be written as $\hat{f} = \hat{n}(\underline{r})$ in the usual form.

The associated local particle density one-body operator for a system of N identical particles

$$\hat{F} = \sum_{q=1}^{N} |\underline{r}\rangle_{qq}\langle\underline{r}|$$

is

$$\hat{F} = \sum_{ij} \langle u_i \, | \, \underline{r} \rangle\langle \underline{r} \, | \, u_j \rangle \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j} = \sum_{ij} u_i^*(\underline{r}) \, u_j(\underline{r}) \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j}$$

in the basis $\{|u_i\rangle\}$ and

$$\hat{F} = \int d\underline{r}_1 \int d\underline{r}_2 \, \langle \underline{r}_1 \, | \, \underline{r} \rangle\langle \underline{r} \, | \, \underline{r}_2 \rangle \, \hat{\psi}^\dagger(\underline{r}_1) \hat{\psi}(\underline{r}_2) = \int d\underline{r}_1 \int d\underline{r}_2 \, \delta(\underline{r}_1 - \underline{r}) \, \delta(\underline{r} - \underline{r}_2) \, \hat{\psi}^\dagger(\underline{r}_1) \hat{\psi}(\underline{r}_2) = \hat{\psi}^\dagger(\underline{r}) \, \hat{\psi}(\underline{r})$$

in the position basis $\{\underline{r}\}$. Thus, the local particle density operator in terms of field operators take a particularly simple form. It annihilates a particle at position $\underline{r}$ and then it creates it at the same point. In another basis, the expression looks less simple.

8.4 The Hamiltonian Operator

The Hamiltonian operator is associated with the total energy of a given quantum system. One of its key features is that it drives the time evolution of quantum systems. When studying systems of many identical quantum particles the formalism derived above will be used.

The Hamiltonian of a system of N identical particles $\hat{H}$ consists of the three terms $\hat{T}$ for the kinetic energy, $\hat{V}$ for the external potential and $\hat{W}$ for the pairwise interaction term between the particles of the system. The three terms of the Hamiltonian $\hat{H} = \hat{T} + \hat{V} + \hat{W}$ are

$$\hat{T} = \sum_{q=1}^{N} \hat{t}_q \quad \hat{t} = \frac{\hat{p}^2}{2m} \qquad \hat{V} = \sum_{q=1}^{N} \hat{v}_q \quad \hat{v} = v(\hat{\underline{r}}) \qquad \hat{W} = \frac{1}{2} \sum_{\substack{q,q'=1 \\ q \neq q'}}^{N} \hat{w}_{qq'} \quad \hat{w}_{12} = w(\hat{\underline{r}}_1, \hat{\underline{r}}_2) \tag{8.9}$$

where $\hat{v}$ can be anything from an applied field to the Coulomb potential from surrounding atomic nuclei, and where two widely used examples for the pairwise interaction between two particles are

$$\frac{1}{4\pi\epsilon_0} \frac{e^2}{|\underline{r}_1 - \underline{r}_2|} \qquad\qquad -g^2 \frac{e^{\alpha m |\underline{r}_1 - \underline{r}_2|}}{|\underline{r}_1 - \underline{r}_2|}$$

the Coulomb potential on the left side and the Yukawa potential on the right side. (Note that they are both only dependent on $|\underline{r}_1 - \underline{r}_2|$.)

The Hamiltonian can be written in terms of the occupation number representation. Given a basis $\{|u_i\rangle\}$ and the creation and annihilation operators (for bosons or fermions) $\hat{a}^\dagger_{u_i}$ and $\hat{a}_{u_i}$, respectively, a one-body operator can be written in the form

$$\hat{F} = \sum_{q=1}^{N} \hat{f}_q = \sum_{ij} \langle u_i | \hat{f} | u_j \rangle \hat{a}^\dagger_{u_i} \hat{a}_{u_j}$$

as shown above. Thus,

$$\hat{T} = \sum_{q=1}^{N} \hat{t}_q = \sum_{ij} \langle u_i | \hat{t} | u_j \rangle \hat{a}^\dagger_{u_i} \hat{a}_{u_j} \qquad\qquad \hat{V} = \sum_{q=1}^{N} \hat{v}_q = \sum_{ij} \langle u_i | \hat{v} | u_j \rangle \hat{a}^\dagger_{u_i} \hat{a}_{u_j}$$

are the two one-body terms in the Hamiltonian $\hat{H}$. A two-body operator has the form

$$\hat{G} = \frac{1}{2} \sum_{\substack{q,q'=1 \\ q \neq q'}}^{N} \hat{g}_{qq'} = \sum_{ijk\ell} {}_1\langle u_i |_2 \langle u_j | \hat{g} | u_k \rangle_1 | u_\ell \rangle_2 \, \hat{a}^\dagger_{u_i} \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} \hat{a}_{u_k}$$

according as introduced above. The interaction term of the Hamiltonian becomes

$$\hat{W} = \frac{1}{2} \sum_{\substack{q,q'=1 \\ q \neq q'}}^{N} \hat{w}_{qq'} = \frac{1}{2} \sum_{ijk\ell} {}_1\langle u_i |_2 \langle u_j | \hat{w} | u_k \rangle_1 | u_\ell \rangle_2 \, \hat{a}^\dagger_{u_i} \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} \hat{a}_{u_k}$$

without the subindices of the operator $\hat{w}$ to simplify notation. The Hamiltonian of N identical particles is therefore

$$\begin{aligned} \hat{H} = \hat{T} + \hat{V} + \hat{W} &= \sum_{q=1}^{N} \hat{t}_q + \sum_{q=1}^{N} \hat{v}_q + \frac{1}{2} \sum_{\substack{q,q'=1 \\ q \neq q'}}^{N} \hat{w}_{qq'} \\ &= \sum_{ij} \langle u_i | \hat{t} | u_j \rangle \hat{a}^\dagger_{u_i} \hat{a}_{u_j} + \sum_{ij} \langle u_i | \hat{v} | u_j \rangle \hat{a}^\dagger_{u_i} \hat{a}_{u_j} + \frac{1}{2} \sum_{ijk\ell} {}_1\langle u_i |_2 \langle u_j | \hat{w} | u_k \rangle_1 | u_\ell \rangle_2 \, \hat{a}^\dagger_{u_i} \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} \hat{a}_{u_k} \end{aligned} \tag{8.10}$$

in terms of the occupation number representation.

The two one-body terms $\hat{T}$ and $\hat{V}$ lead usually to rather simple calculations, but the two-body term $\hat{W}$ is often extremely challenging to evaluate. A useful starting point to study a Hamiltonian like this is to first write it down in the basis defined by the eigenstates of the non-interacting part of the Hamiltonian. It facilitates the development of approximate methods for the interacting part. In order to separate the one-body operators from the two-body operators the Hamiltonian is split into the two parts $\hat{H}_0 = \hat{T} + \hat{V}$ and $\hat{W}$.

The non-interacting Hamiltonian $\hat{H}_0$ can be written as

$$\hat{H}_0 = \sum_{ij} \langle u_i| (\hat{t} + \hat{v}) |u_j\rangle \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j} = \sum_{ij} \langle u_i| \, \hat{h}_0 \, |u_j\rangle \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j}$$

with $\hat{h}_0 = \hat{t} + \hat{v}$. Because $\hat{h}_0$ is a Hermitian operator, the eigenstates $|v_k\rangle$ from the eigenvalue equation $\hat{h}_0 |v_k\rangle = E_k |v_k\rangle$ span a basis of the full state space. The non-interacting Hamiltonian becomes

$$\hat{H}_0 = \sum_{k\ell} \langle v_k| \, \hat{h}_0 \, |v_\ell\rangle \, \hat{a}^\dagger_{v_k} \hat{a}_{v_\ell} = \sum_{k\ell} E_\ell \, \langle v_k|v_\ell\rangle \, \hat{a}^\dagger_{v_k} \hat{a}_{v_\ell} = \sum_{k\ell} E_\ell \delta_{k\ell} \, \hat{a}^\dagger_{v_k} \hat{a}_{v_\ell} = \sum_{k} E_k \, \hat{a}^\dagger_{v_k} \hat{a}_{v_k} = \sum_{k} E_k \, \hat{n}_{v_k}$$

with the number operator $\hat{n}_{v_k}$ in the orthonormal basis of the eigenstates $\{|v_i\rangle\}$. In the basis of its own eigenstates the non-interacting Hamiltonian $\hat{H}_0$ takes a very simple form. All it does is count the number of particles in each state and scale that by the associated energies.

The full Hamiltonian is

$$\hat{H} = \sum_{ij} \langle u_i| \, \hat{h}_0 \, |u_j\rangle \, \hat{a}^\dagger_{u_i} \hat{a}_{u_j} + \frac{1}{2} \sum_{ijk\ell} {}_1\langle u_i|_2\langle u_j| \, \hat{w} \, |u_k\rangle_1 \, |u_\ell\rangle_2 \, \hat{a}^\dagger_{u_i} \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} \hat{a}_{u_k}$$

in the basis $\{|u_i\rangle\}$ and becomes

$$\hat{H} = \sum_{k} E_k \, \hat{n}_{v_k} + \frac{1}{2} \sum_{ijk\ell} {}_1\langle v_i|_2\langle v_j| \, \hat{w} \, |v_k\rangle_1 \, |v_\ell\rangle_2 \, \hat{a}^\dagger_{v_i} \hat{a}^\dagger_{v_j} \hat{a}_{v_\ell} \hat{a}_{v_k}$$

in the basis $\{|v_i\rangle\}$. The one-body term has been simplified but the two-body term still has the same complicated form. This is one of the outstanding challenges in physics. A good progress can be made with this form using suitable approximations.