1 Lecture 3: The many body problem

In this lecture the *many body problem* is introduced in the context of *first* and *second quantisation*.

2 The Schrödinger equation

We consider N particles; in many cases of interest in this course the hamiltonian for the particles takes the form

$$H = \sum_{k=1}^{N} T(\mathbf{x}_k) + \frac{1}{2}\sum_{k\neq l=1}^{N} V(\mathbf{x}_k, \mathbf{x}_l), \tag{1}$$

where $\mathbf{x}_k$ is the position of the kth particle, T is the kinetic energy, and V is the potential energy of interaction, *counted once*, between the particles. (It is often convenient to assume that the position variable $\mathbf{x}_k$ includes not only the particle's coordinates in $\mathbb{R}^3$, but also its internal configurations such as spin, etc.) The time-independent Schrödinger equation then reads

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t) = H\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t), \tag{2}$$

together with some appropriate choice of boundary conditions for the wavefunction.

Suppose that $\psi_j(\mathbf{x})$, $j = 1, 2, \ldots$, is a complete set of orthonormalised single-particle wavefunctions. For example, $\psi_{j_k}(\mathbf{x}_k)$ could be the eigenfunctions of the harmonic oscillator. Then any product $\psi_{j_1}(\mathbf{x}_1)\psi_{j_2}(\mathbf{x}_2)\cdots\psi_{j_N}(\mathbf{x}_N)$ is a valid many-body wavefunction. Further, these products are *complete*, in that any many-body wavefunction can be expressed as a linear combination of them:

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t) = \sum_{j_1, j_2, \ldots, j_N} C(j_1, j_2, \ldots, j_N, t)\psi_{j_1}(\mathbf{x}_1)\psi_{j_2}(\mathbf{x}_2)\cdots\psi_{j_N}(\mathbf{x}_N). \tag{3}$$

(This is a consequence of the *tensor product rule*. That this should be true follows from general information-theoretic considerations emerging from the assumption that it is possible to perform *tomography* of the entire wavefunction by separately measuring the particles.)

Substituting (3) into the Schrödinger equation (2) yields

$$i\hbar\frac{\partial}{\partial t}C(j_1, j_2, \ldots, j_N, t) = \sum_{k=1}^{N}\sum_{l}\int d\mathbf{x}_k \overline{\psi}_{j_k}(\mathbf{x}_k)T(\mathbf{x}_k)\psi_l(\mathbf{x}_k)C(j_1, \ldots, l, \ldots j_N, t) \tag{4}$$

$$+\frac{1}{2}\sum_{k\neq k'}^{N}\sum_{l}\sum_{m}\int d\mathbf{x}_k d\mathbf{x}_{k'}\overline{\psi}_{j_k}(\mathbf{x}_k)\overline{\psi}_{j_{k'}}(\mathbf{x}_{k'})V(\mathbf{x}_k, \mathbf{x}_{k'})\psi_l(\mathbf{x}_k)\psi_m(\mathbf{x}_{k'})\times \tag{5}$$

$$C(j_1, \ldots, l, \ldots, m, \ldots j_N, t). \tag{6}$$

We now accommodate the indistinguishability of the particles into the wavefunction by demanding that an exchange of particles cannot lead to an observable consequence. This means that

$$\Psi(\ldots,\mathbf{x}_j,\ldots,\mathbf{x}_k,\ldots) = e^{i\phi_{jk}}\Psi(\ldots,\mathbf{x}_k,\ldots,\mathbf{x}_j,\ldots), \tag{7}$$

i.e., the wavefunction must be the same *up to a phase*. Since a further exchange of particles j and k yields the original wavefunction the phase $e^{i\phi_{jk}} = \pm 1$ in order to ensure that Ψ is not multiple valued. (In geometries with nontrivial topologies, or in two dimensions the wavefunction may possibly be multiple valued, yielding the possibility of *anyons*, and other exotic particles.) A necessary and sufficient condition to ensure the (anti-)symmetry of the wavefunction is that the coefficients in (3) satisfy

$$C(\ldots,j_k,\ldots,j_l,\ldots) = \pm C(\ldots,j_l,\ldots,j_k,\ldots) \tag{8}$$

Exercise: prove this.

2.1 Bosons

The particles described by a wavefunction Ψ that is completely symmetric under interchange are known as *bosons*. The symmetry of the coefficients allows us to reorder the indices of the coefficient C in the summation (3). Suppose the state 1 occurs n_1 times, and the state 2 occurs n_2 times, etc. Then all such terms with the same numbers n_k have the same coefficient. It is thus convenient to rename the coefficient function

$$\overline{C}(n_1,n_2,\ldots,n_k,\ldots,t) \equiv C(\underbrace{11\cdots1}_{n_1}\underbrace{22\cdots2}_{n_2}\cdots,t) \tag{9}$$

We now define another coefficient function

$$f(n_1,n_2,\ldots,n_k,\ldots,t) \equiv \sqrt{\frac{N!}{n_1!n_2!\cdots}}\,\overline{C}(n_1,n_2,\ldots,n_k,\ldots,t). \tag{10}$$

The condition that the wavefunction Ψ is normalised becomes

$$\sum_{n_1,n_2,\ldots} |f(n_1,n_2,\ldots,n_k,\ldots,t)|^2 = 1, \tag{11}$$

where the coefficients n_j must satisfy

$$\sum_{j=1}^{\infty} n_j = N. \tag{12}$$

Exercise: prove this.

We can now use the f coefficients to rewrite the original wavefunction in terms of a new convenient complete orthonormal basis

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,t) = \sum_{\substack{n_1,n_2,\ldots,n_k,\ldots \\ \sum_k n_k = N}} f(n_1,n_2,\ldots,t)\Phi_{n_1n_2\cdots n_k\cdots}(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N), \tag{13}$$

where

$$\Phi_{n_1 n_2 \cdots n_k \cdots}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \sqrt{\frac{n_1! n_2! \cdots}{N!}} \sum_{\substack{j_1, j_2, \ldots, j_N \\ (n_1, n_2, \ldots,)}} \psi_{j_1}(\mathbf{x}_1)\psi_{j_2}(\mathbf{x}_2) \cdots \psi_{j_N}(\mathbf{x}_N), \quad (14)$$

and the summation is over all indices j_k with the given pattern $(n_1, n_2, \ldots,)$ of 1s, 2s, etc. Note that the functions $\Phi_{n_1 n_2 \cdots n_k \cdots}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$ are completely symmetrised.

Exercise: prove that the functions $\Phi_{n_1 n_2 \cdots n_k \cdots}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$ form a symmetrised complete orthonormal set.

Here is an example of a $\Phi_{n_1 n_2 \cdots n_k \cdots}$ function:

$$\Phi_{210 \cdots 0 \cdots}(\mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3) = \frac{1}{\sqrt{3}}(\psi_1(\mathbf{x}_1)\psi_1(\mathbf{x}_2)\psi_2(\mathbf{x}_3) + \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)\psi_1(\mathbf{x}_3) + \psi_2(\mathbf{x}_1)\psi_1(\mathbf{x}_2)\psi_1(\mathbf{x}_3)). \quad (15)$$

Substituting the expansion (11) into the Schrödinger equation (2) leads to

$$i\hbar \frac{\partial}{\partial t} f(n_1, n_2, \ldots, n_k, \ldots, t) = \sum_j \langle j|T|j\rangle n_j f(n_1, \ldots, n_k, \ldots n_k, \ldots, t) + \quad (16)$$

$$\sum_{j \neq j'} \langle j|T|j'\rangle \sqrt{n_j(n_{j'}+1)} f(n_1, \ldots, n_j - 1, \ldots, n_{j'} + 1, \ldots n_k, \ldots, t) + \quad (17)$$

$$\frac{1}{2} \sum_{j \neq j' \neq k \neq k'} \langle jj'|V|kk'\rangle \sqrt{n_j n_{j'}(n_k + 1)(n_{k'} + 1)} \times \quad (18)$$

$$f(n_1, \ldots, n_j - 1, \ldots, n_{j'} - 1, \ldots, n_k + 1, \ldots, n_{k'} + 1, \ldots, t) + etc., \quad (19)$$

where there is an additional term for all possible sets of occupation numbers so that two particles are removed, multiplied by an overall factor $\langle jj'|V|kk'\rangle \times \sqrt{productofns}$, and then subsequently added back in at different places. This expression appears very complicated, however, there is a way to write it in an equivalent form which is much more compact.

2.2 Fermions

If a minus sign is chosen in (5) then the Cs are antisymmetric under the exchange of any two particles:

$$C(\ldots, j_k, \ldots, j_l, \ldots) = -C(\ldots, j_l, \ldots, j_k, \ldots), \quad (20)$$

which shows that j_l must be different from j_k or else the coefficient vanishes. This, in turn, shows that the occupation numbers n_l can only be 0 or 1. Any coefficients with the same states occupied are equal up to a minus sign, allowing us to define a new coefficient $\overline{C}$

$$\overline{C}(n_1, n_2, \ldots, t) = C(\cdots j_k < j_l < j_m \cdots, t), \quad (21)$$

where all of the numbers $j_1, j_2, \ldots$ are first arranged in increasing order.

Exactly as in the bosonic case the many particle wavefunction Ψ can be expanded as

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t) = \sum_{\substack{n_1, n_2, \ldots, n_k, \ldots \\ \sum_k n_k = N}} f(n_1, n_2, \ldots, t) \Phi_{n_1 n_2 \cdots n_k \cdots}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N), \qquad (22)$$

where now

$$\Phi_{n_1 n_2 \cdots n_k \cdots}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \sqrt{\frac{n_1! n_2! \cdots}{N!}} \begin{vmatrix} \psi_{j_1}(\mathbf{x}_1) & \psi_{j_1}(\mathbf{x}_2) & \cdots & \psi_{j_1}(\mathbf{x}_N) \\ \vdots & & \ddots & \vdots \\ \psi_{j_N}(\mathbf{x}_1) & \psi_{j_N}(\mathbf{x}_2) & \cdots & \psi_{j_N}(\mathbf{x}_N) \end{vmatrix}, \qquad (23)$$

and $j_1 < j_2 < \cdots < j_N$. These *Slater determinants* form a complete set of orthonormal antisymmetric wavefunctions.

We postpone the task of writing out the Schrödinger equation until next section where we'll develop a much more compact representation.

3 Many particle hilbert space; creation and annihilation operators

In this section we introduce a new orthonormal basis for hilbert space describing the *number* of particles in each state. This must be initially understood as an *abstract* construction until such time we can show it is equivalent to the first-quantised treatments of the previous section. The basis we introduce is denoted

$$|n_1 n_2 \cdots n_k \cdots\rangle, \quad n_j \in \mathbb{Z}^+, \qquad (24)$$

which is meant to mean that n_j particles are in the single-particle eigenstate ψ_j. This basis is demanded to be complete and orthonormal, meaning that

$$\langle n'_1 n'_2 \cdots n'_k \cdots | n_1 n_2 \cdots n_k \cdots \rangle = \delta_{n'_1 n_1} \delta_{n'_2 n_2} \cdots \qquad (25)$$

and

$$\sum_{n_1 n_2 \cdots} |n_1 n_2 \cdots n_k \cdots\rangle\langle n_1 n_2 \cdots n_k \cdots| = \mathbb{I}. \qquad (26)$$

3.1 Bosons

In the bosonic case, associated with this occupation number basis, we introduce the *annihilation* and *creation* operators $b_k, b_k^\dagger$, satisfying the *canonical commutation relations* (CCR)

$$[b_j, b_k^\dagger] = \delta_{jk}, \quad [b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0. \qquad (27)$$

These operators are taken to act in the standard way on the number basis, e.g.,

$$b_k^\dagger |n_1 n_2 \cdots n_k \cdots\rangle = \sqrt{n_j + 1} |n_1 n_2 \cdots n_k + 1 \cdots\rangle, \qquad (28)$$

etc. The *mode number operators* n_k are defined to be

$$n_k = b_k^\dagger b_k. \tag{29}$$

We now use the occupation number basis to rewrite the Schrödinger equation. Form the following state

$$|\Psi(t)\rangle = \sum_{n_1 n_2 \cdots} f(n_1, n_2, \ldots, n_k, \ldots, t)|n_1 n_2 \cdots n_k \cdots\rangle, \tag{30}$$

where the fs are taken to be the expansion coefficients of (11) which satisfy the coupled differential equations (14). This state vector in our abstract hilbert space obeys the differential equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \sum_{n_1 n_2 \cdots} i\hbar\frac{\partial}{\partial t} f(n_1, n_2, \ldots, n_k, \ldots, t)|n_1 n_2 \cdots n_k \cdots\rangle \tag{31}$$

Relabelling dummy indices, using the properties of CCR, and rewriting the appropriate operations in terms of the annihiliation and creation operators leads us to the consequence that the abstract state vector $|\Psi(t)\rangle$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \widehat{H}|\Psi(t)\rangle, \tag{32}$$

where the operator $\widehat{H}$ is given by

$$\widehat{H} = \sum_{j,k} b_j^\dagger \langle j|T|k\rangle b_k + \frac{1}{2}\sum_{j,k,l,m} b_j^\dagger b_k^\dagger \langle jk|V|lm\rangle b_l b_m. \tag{33}$$

These equations restate the Schrödinger equation in *second quantisation*. All the statistics and operators properties are expressed via the CCR. The physical problem is unchanged by the new formulation, and the coefficients express the connection between first and second quantisations. Thus any solution to the Schrödinger equation in first quantisation yields a solution in second quantisation and vice versa.

3.2 Fermions

In the fermionic case we introduce the *annihilation* and *creation* operators $a_k, a_k^\dagger$, satisfying the *canonical anticommutation relations* (CAR)

$$\{a_j, a_k^\dagger\} = \delta_{jk}, \quad \{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0. \tag{34}$$

The action of these operators on the vacuum state $|0\rangle$ is expressed by

$$|n_1 n_2 \cdots n_k \cdots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots(a_k^\dagger)^{n_k}\cdots|0\rangle. \tag{35}$$

If we now introduce, as before, the abstract state vector $|\Psi(t)\rangle$

$$|\Psi(t)\rangle = \sum_{n_1 n_2 \cdots} f(n_1, n_2, \ldots, n_k, \ldots, t)|n_1 n_2 \cdots n_k \cdots\rangle, \tag{36}$$

where the fs are taken to be the expansion coefficients of (17) obeying the coupled differential equations coming from substitution into the Schrödinger equation, then we find that

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \widehat{H}|\Psi(t)\rangle, \tag{37}$$

where the operator $\widehat{H}$ is given by

$$\widehat{H} = \sum_{j,k} a_j^\dagger \langle j|T|k\rangle a_k + \frac{1}{2}\sum_{j,k,l,m} a_j^\dagger a_k^\dagger \langle jk|V|lm\rangle a_l a_m. \tag{38}$$