Many-Particle Quantum Systems

1 Identical particles in quantum mechanics

Many-particle quantum systems are always made up of many *identical particles*, possibly of several different kinds. Symmetry under exchange of identical particles has very important consequences in quantum mechanics, and the formalism of many-particle quantum mechanics is designed to build these consequences properly into the theory. We start by reviewing these ideas.

Consider a system of N identical particles with coordinates $\mathbf{r}_1, \ldots \mathbf{r}_N$ described by a wavefunction $\psi(\mathbf{r}_1 \ldots \mathbf{r}_N)$. For illustration, suppose that the Hamiltonian has the form

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N}V(\mathbf{r}_i) + \sum_{i<j}U(\mathbf{r}_i - \mathbf{r}_j)\ .$$

Here there are three contributions to the energy: the kinetic energy of each particle (∇_i^2 operates on the coordinates $\mathbf{r}_i$); the one-body potential energy $V(\mathbf{r})$; and the two-particle interaction potential $U(\mathbf{r}_i - \mathbf{r}_j)$. To discuss symmetry under exchange of particles, we define the exchange operator $\mathcal{P}_{ij}$ via its action on wavefunctions:

$$\mathcal{P}_{ij}\psi(\ldots\mathbf{r}_i\ldots\mathbf{r}_j\ldots) = \psi(\ldots\mathbf{r}_j\ldots\mathbf{r}_i\ldots)\ .$$

Since $[\mathcal{H}, \mathcal{P}_{ij}] = 0$, we can find states that are simultaneous eigenstates of $\mathcal{H}$ and $\mathcal{P}_{ij}$. Moreover, a system that is initially in an eigenstate of $\mathcal{P}_{ij}$ will remain in one under time evolution with $\mathcal{H}$. For these reasons we examine the eigenvalues of $\mathcal{P}_{ij}$. Since $(\mathcal{P}_{ij})^2 = 1$, these are $+1$ and -1. Now, it is an observational fact (explained in relativistic quantum field theory by the spin-statistics theorem) that particles come in two kinds and that particles of a given kind are always associated with the same eigenvalue of the exchange operator: $+1$ for bosons and -1 for fermions.

1.1 Many particle basis states

In a discussion of many-particle quantum systems we should restrict ourselves to wavefunctions with the appropriate symmetry under particle exchange. We can do this by using a set of basis states that has the required symmetry. As a starting point, suppose that we have a complete, orthonormal set of single-particle states $\phi_1(\mathbf{r}), \phi_2(\mathbf{r})\ldots$. Next we would like to write down a wavefunction representing an N-particle system with one particle in state l_1, one in state l_2 and so on. The choice

$$\phi_{l_1}(\mathbf{r})\phi_{l_2}(\mathbf{r})\ldots\phi_{l_N}(\mathbf{r})$$

is unsatisfactory because for general $l_1, l_2\ldots$ it has no particular exchange symmetry. Instead we take

$$\psi(\mathbf{r}_1\ldots\mathbf{r}_N) = \mathcal{N}\sum_{\text{distinct perms.}}(\pm1)^P\phi_{k_1}(\mathbf{r}_1)\ldots\phi_{k_N}(\mathbf{r}_N)\ . \tag{1}$$

Several aspects of the notation in Eq. (1) require comment. The sign inside the brackets in $(\pm1)^P$ is $+1$ for bosons and -1 for fermions. The set of labels $\{k_1\ldots k_N\}$ is a permutation of the set $\{l_1\ldots l_N\}$. The permutation is called *even* if it can be produced by an even number of exchanges of adjacent pairs of labels, and is *odd* otherwise; the integer P is even or odd accordingly. The sum is over all *distinct* permutations of the labels. This means that if two or more of the labels l_n are the same, then permutations amongst equal labels do not appear as multiple contributions to the sum. Finally, $\mathcal{N}$ is a normalisation, which we determine next.

To normalise the wavefunction, we must evaluate

$$\int \mathrm{d}^d\mathbf{r}_1\ldots\int \mathrm{d}^d\mathbf{r}_N\,\psi^*(\mathbf{r}_1\ldots\mathbf{r}_N)\psi\ \ (\mathbf{r}_1\ldots\mathbf{r}_N)\ .$$

Substituting from Eq. (1), we obtain a double sum (over permutations $k_1\ldots k_N$ and $h_1\ldots h_N$) of terms of the form

$$\int \mathrm{d}^d\mathbf{r}_1\,\phi^*_{k_1}(\mathbf{r})\phi_{h_1}(\mathbf{r}_1)\ldots\int \mathrm{d}^d\mathbf{r}_N\,\phi^*_{k_N}(\mathbf{r})\phi_{h_N}(\mathbf{r}_1)\ .$$

These terms are zero unless $k_1 = h_1$, $k_2 = h_2$, and $\ldots k_N = h_N$, in which case they are unity. Therefore only the diagonal terms in the double sum contribute, and we have

$$\int \ldots \int |\psi|^2 = |\mathcal{N}|^2 \sum_{\text{dist. perms.}} (\pm 1)^{2P} = |\mathcal{N}|^2 \, \frac{N!}{n_1! \, n_2! \, \ldots}$$

where the n_1, $n_2 \ldots$ are the numbers of times that each distinct orbital appears in the set $\{l_1 \ldots l_N\}$, and the ratio of factorials is simply the number of distinct permutations. Hence we normalise the wavefunction to unity by taking

$$\mathcal{N} = \left(\frac{n_1! \; n_2! \; \ldots}{N!} \right)^{1/2} .$$

1.2 Slater determinants

For fermion wavefunctions we can get the correct signs by thinking of Eq. (1) as a determinant

$$\psi(\mathbf{r}_1 \ldots \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{l_1}(\mathbf{r_1}) & \ldots & \phi_{l_1}(\mathbf{r_N}) \\ & \ldots & \\ \phi_{l_N}(\mathbf{r_1}) & \ldots & \phi_{l_N}(\mathbf{r_N}) \end{vmatrix} . \tag{2}$$

Note that this determinant is zero either if two orbitals are the same ($l_i = l_j$) or if two coordinates coincide ($\mathbf{r}_i = \mathbf{r}_j$), so the Pauli exclusion principle is correctly built in. Note also that, since the sign of the determinant is changed if we exchange two adjacent rows, it is necessary to keep in mind a definite ordering convention for the single particle orbitals $\phi_l(\mathbf{r})$ to fix the phase of the wavefunction.

For bosons, we should use an object similar to a determinant, but having all terms combined with a positive sign: this is known as a *permanent*.

1.3 Occupation numbers

We can specify the basis states we have constructed by giving the number of particles n_l in each orbital l. Clearly, for fermions $n_l = 0$ or 1, while for bosons $n_l = 0, 1, \ldots$. These occupation numbers are used within Dirac notation as labels for a state: $|n_1, n_2, \ldots\rangle$.

1.4 Fock space

Combining states $|n_1, n_2, \ldots\rangle$ with all possible values of the occupation numbers, we have basis vectors for states with any number of particles. This vector space is known as *Fock space*. Using it, we can discuss processes in which particles are created or annihilated, as well as ones with fixed particle number, described by wavefunctions of the form $\psi(\mathbf{r}_1 \ldots \mathbf{r}_N)$.

1.5 The vacuum state

It is worth noting that one of the states in Fock space is the vacuum: the wavefunction for the quantum system when it contains no particles, written as $|0\rangle$. Clearly, in recognising this as a quantum state we have come some way from the notation of single-body and few-body quantum mechanics, with wavefunctions written as functions of particle coordinates. Of course, $|0\rangle$ is different from 0, and in particular $\langle 0|0\rangle = 1$.

1.6 Creation and annihilation operators

Many of the calculations we will want to do are carried out most efficiently by introducing creation operators, which add particles when they act to the right on states from Fock space. Their Hermitian conjugates are annihilation operators, which remove particles. Their definition rests on the set of single particle orbitals from which we built Fock space: $c_l^\dagger$ adds particles to the orbital $\phi_l(\mathbf{r})$. More formally, we define

$$c_{l_1}^\dagger c_{l_2}^\dagger \ldots c_{l_N}^\dagger |0\rangle \tag{3}$$

to be the state with coordinate wavefunction

$$\psi(\mathbf{r}_1, \ldots \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \sum_{\text{all perms}} (\pm 1)^P \phi_{k_1}(\mathbf{r}_1) \ldots \phi_{k_N}(\mathbf{r}_N) = (n_1! \, n_2! \, \ldots)^{1/2} |n_1, n_2 \ldots\rangle \, . \tag{4}$$

A detail to note is that the sum in Eq. (4) is over all permutations, while that in Eq. (1) included only distinct permutations. The difference (which is significant only for bosons, since it is only for bosons that we can have $n_l > 1$), is the reason for the factor $(n_1!\, n_2!\, \ldots)^{1/2}$ appearing on the right of Eq. (4). This choice anticipates what is necessary in order for boson creation and annihilation operators to have convenient commutation relations.

Annihilation operators appear when we take the Hermitian conjugate of Eq. (3), obtaining $\langle 0|\, c_{l_N} \ldots c_{l_2} c_{l_1}$. Let's examine the effect of creation and annihilation operators when they act on various states. Since $c_l^\dagger|0\rangle$ is the state with coordinate wavefunction $\phi_l(\mathbf{r})$, we know that $\langle 0|c_l\, c_l^\dagger|0\rangle = 1$, but for any choice of the state $|\phi\rangle$ other than the vacuum, $c_l^\dagger|\phi\rangle$ contains more than one particle and hence $\langle 0|c_l\, c_l^\dagger|\phi\rangle = 0$. From this we can conclude that

$$c_l\, c_l^\dagger|0\rangle = |0\rangle\ ,$$

demonstrating that the effect of c_l is to remove a particle from the state $|n_l{=}1\rangle \equiv c_l^\dagger|0\rangle$. We also have for any $|\phi\rangle$ the inner products $\langle 0|c_l^\dagger|\phi\rangle = \langle\phi|c_l\,|0\rangle = 0$, and so we can conclude that

$$c_l\,|0\rangle = \langle 0|c_l^\dagger = 0\ .$$

1.7 Commutation and anticommutation relations

Recalling the factor of $(\pm 1)^P$ in Eq. (4), we have for any $|\phi\rangle$

$$c_l^\dagger c_m^\dagger|\phi\rangle = \pm c_m^\dagger c_l^\dagger|\phi\rangle\ ,$$

where the upper sign is for bosons and the lower one for fermions. From this we conclude that boson creation operators commute, and fermion creation operators anticommute: that is, for bosons

$$[c_l^\dagger, c_m^\dagger] = 0$$

and for fermions

$$\{c_l^\dagger, c_m^\dagger\} = 0\ ,$$

where we use the standard notation for an anticommutator of two operators A and B: $\{A, B\} = AB + BA$. Taking Hermitian conjugates of these two equations, we have for bosons

$$[c_l, c_m] = 0$$

and for fermions

$$\{c_l, c_m\} = 0\ .$$

Note for fermions we can conclude that $(c_l)^2{=}(c_l^\dagger)^2{=}0$, which illustrates again how the Pauli exclusion principle is built into our approach.

Finally, one can check that to reproduce the values of inner products of states appearing in Eq. (4), we require for bosons

$$[c_l\,, c_m^\dagger] = \delta_{lm}$$

and for fermions

$$\{c_l\,, c_m^\dagger\} = \delta_{lm}\ .$$

To illustrate the correctness of these relations, consider for a single boson orbital the value of $|[(c^\dagger)^n|0\rangle]|^2$. From Eq. (4) we have $|[(c^\dagger)^n|0\rangle]|^2 = n!$. Let's recover the same result by manipulating commutators: we have

$$\begin{aligned}
\langle 0|(c)^n(c^\dagger)^n|0\rangle &= \langle 0|(c)^{n-1}([c, c^\dagger] + c^\dagger c)(c^\dagger)^{n-1}|0\rangle \\
&= m\langle 0|(c)^{n-1}(c^\dagger)^{n-1}|0\rangle + \langle 0|c^\dagger(c)^{n-m}c^\dagger c(c)^m(c^\dagger)^{n-1}|0\rangle \\
&= n\langle 0|(c)^{n-1}(c^\dagger)^{n-1}|0\rangle + \langle 0|c^\dagger(c)^{n-1}(c^\dagger)^{n-1}|0\rangle \\
&= n(n-1)\ldots(n-l)\langle 0|(c^\dagger)^{n-l}(c)^{n-l}|0\rangle \\
&= n!\,\langle 0|0\rangle\ .
\end{aligned}$$

Of course, manipulations like these are familiar from the theory of raising and lowering operators for the harmonic oscillator.

1.8 Number operators

From Eq. (4) as the defining equation for the action of creation operators in Fock space we have

$$c_l^\dagger |n_1 \dots n_l \dots\rangle = (\pm 1)^{n_1+\dots+n_{l-1}} \sqrt{n_l+1}\, |n_1 \dots n_l + 1 \dots\rangle \ ,$$

or zero for fermions if n_l=1. Similarly, by considering the Hermitian conjugate of a similar equation, we have

$$c_l |n_1 \dots n_l \dots\rangle = (\pm 1)^{n_1+\dots+n_{l-1}} \sqrt{n_l}\, |n_1 \dots n_l - 1 \dots\rangle \ ,$$

or zero for both bosons and fermions if n_l=0. In this way we have

$$c_l^\dagger c_l \, |\dots n_l \dots\rangle = n_l |\dots n_l \dots\rangle$$

where the possible values of n_l are n_l=0, 1, 2 . . . for bosons and n_l=0, 1 for fermions. Thus the combination $c_l^\dagger c_l$, which we will also write as $\hat{n}_l$, is the number operator and counts particles in the orbital ϕ_l.

1.9 Transformations between bases

In the context of single-particle quantum mechanics it is often convenient to make transformations between different bases. Since we used a particular set of basis functions in our definition of creation and annihilation operators, we should understand what such transformations imply in operator language.

Suppose we have two complete, orthonormal sets of single-particle basis functions, $\{\phi_l(\mathbf{r})\}$ and $\{\rho_\alpha(\mathbf{r})\}$, which we also write as $\{|\phi_i\rangle\}$ and $\{|\rho_\alpha\rangle\}$. Then we can expand one in terms of the other, writing

$$\rho_\alpha(\mathbf{r}) = \sum_l \phi_l(\mathbf{r}) U_{l\alpha} \tag{5}$$

with $U_{l\alpha} = \langle\phi_l|\rho_\alpha\rangle$. Note that U is a unitary matrix, since

$$\begin{aligned} (\mathrm{U}\mathrm{U}^\dagger)_{ml} &= \sum_\alpha \langle\phi_m|\rho_\alpha\rangle\langle\rho_\alpha|\phi_l\rangle \\ &= \langle\phi_m|\phi_l\rangle \qquad \text{since} \qquad \sum_\alpha |\rho_\alpha\rangle\langle\rho_\alpha| = \mathbf{1} \\ &= \delta_{ml} \ . \end{aligned}$$

Now let $c_l^\dagger$ create a particle in orbital $\phi_l(\mathbf{r})$, and let $d_\alpha^\dagger$ create a particle in orbital $\rho_\alpha(\mathbf{r})$. We can read off from Eq. (5) an expression for $d_\alpha^\dagger$ in terms of $c_l^\dagger$:

$$d_\alpha^\dagger = \sum_l c_l^\dagger U_{l\alpha} \ .$$

From the Hermitian conjugate of this equation we also have

$$d_\alpha = \sum_l U_{l\alpha}^* c_l = \sum_l (\mathrm{U}^\dagger)_{\alpha l} c_l \ .$$

1.9.1 Effect of transformations on commutation relations

We should verify that such transformations preserve commutation relations. For example, suppose that c_l and $c_l^\dagger$ are fermion operators, obeying $\{c_l\,, c_m^\dagger\} = \delta_{lm}$. Then

$$\{d_\alpha, d_\beta^\dagger\} = \sum_{lm} U_{l\alpha}^* U_{m\beta} \{c_l\,, c_m^\dagger\} = (\mathrm{U}^\dagger \mathrm{U})_{\alpha\beta} = \delta_{\alpha\beta} \ .$$

Similarly, for boson operators commutation relations are preserved under unitary transformations.

1.10 General single-particle operators in second-quantised form

To continue our programme of formulating many-particle quantum mechanics in terms of creation and annihilation operators, we need to understand how to transcribe operators from coordinate representation or first-quantised form to so-called second-quantised form. In the first instance, we examine how to do this for one-body operators – those which involve the coordinates of one particle at a time. An example is the kinetic energy operator. Suppose in general that $A(\mathbf{r})$ represents such a quantity for a single-particle system. Then for a system of N particles in first-quantised notation we have

$$\hat{A} = \sum_{i=1}^{N} A(\mathbf{r}_i) \ .$$

We want to represent $\hat{A}$ using creation and annihilation operators. As a first step, we can characterise $A(\mathbf{r})$ by its matrix elements, writing

$$A_{lm} = \int \phi_l^*(\mathbf{r}) A(\mathbf{r}) \phi_m(\mathbf{r}) \mathrm{d}^d\mathbf{r} \ .$$

Then

$$A(\mathbf{r})\phi_m(\mathbf{r}) = \sum_l \phi_l(\mathbf{r}) A_{lm} \ . \tag{6}$$

The second-quantised representation is

$$\hat{A} = \sum_{pq} A_{pq} c_p^\dagger c_q \ . \tag{7}$$

To justify this, we should verify that reproduces the correct matrix elements between all states from the Fock space. We will simply check the action of $\hat{A}$ on single particles states. We have

$$\hat{A}|\phi_m\rangle = \sum_{pq} A_{pq} c_p^\dagger c_q c_m^\dagger |0\rangle \ .$$

Now, taking as an example bosons,

$$c_p^\dagger c_q c_m^\dagger |0\rangle = c_p^\dagger ([c_q, c_m^\dagger] + c_m^\dagger c_q)|0\rangle = c_p^\dagger \delta_{qm}|0\rangle$$

so

$$\hat{A}|\phi_m\rangle = \sum_p |\phi_p\rangle A_{pm} \ ,$$

reproducing Eq. (6), as required.

1.11 Two-particle operators in second-quantised form

Two-body operators depend on the coordinates of a pair of particles, an example being the two-body potential in an interacting system. Writing the operator in first-quantised form as $A(\mathbf{r}_1, \mathbf{r}_2)$, it has matrix elements which carry four labels:

$$A_{lmpq} = \int \phi_l^*(\mathbf{r}_1)\phi_m^*(\mathbf{r}_2) A(\mathbf{r}_1, \mathbf{r}_2) \phi_p(\mathbf{r}_2)\phi_q(\mathbf{r}_1) \mathrm{d}^d\mathbf{r}_1 \mathrm{d}^d\mathbf{r}_2 \ .$$

Its second-quantised form is

$$\hat{A} \equiv \sum_{ij} A(\mathbf{r}_i, \mathbf{r}_j) = \sum_{lmpq} A_{lmpq} c_l^\dagger c_m^\dagger c_p c_q \ . \tag{8}$$

Again, to justify this one should check matrix elements of the second-quantised form between all states in Fock space. We will content ourselves with matrix elements for two-particle states, evaluating

$$\langle A \rangle = \langle 0 | c_y c_x \hat{A} c_a^\dagger c_b^\dagger |0\rangle$$

by two routes. In a first-quantised calculation with $\pm$ signs for bosons and fermions, we have

$$\begin{aligned}
\langle A \rangle &= \frac{1}{2} \int\int [\phi_x^*(\mathbf{r}_1)\phi_y^*(\mathbf{r}_2) \pm \phi_x^*(\mathbf{r}_2)\phi_y^*(\mathbf{r}_1)] \cdot [A(\mathbf{r}_1, \mathbf{r}_2) + A(\mathbf{r}_2, \mathbf{r}_1)] \cdot [\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) \pm \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)] \mathrm{d}^d\mathbf{r}_1 \mathrm{d}^d\mathbf{r}_2 \\
&= \frac{1}{2}[A_{xyba} \pm A_{xyab} + A_{yxab} \pm A_{yxba} + A_{xyba} \pm A_{xyab} + A_{yxab} \pm A_{yxba}] \\
&= (A_{xyba} + A_{yxab}) \pm (A_{xyab} + A_{yxba}) \ .
\end{aligned} \tag{9}$$

Using the proposed second-quantised form for $\hat{A}$, we have

$$\langle A\rangle = \sum_{lmpq} A_{lmpq}\langle 0|c_y c_x c_l^\dagger c_m^\dagger c_p c_q c_a^\dagger c_b^\dagger|0\rangle \ .$$

We can simplify the vacuum expectation value of products of creation and annihilation operators such as the one appearing here by using the appropriate commutation or anticommutation relation to move annihilation operators to the right, or creation operators to the left, whereupon acting on the vacuum they give zero. In particular

$$c_p c_q c_a^\dagger c_b^\dagger|0\rangle \ = (\delta_{aq}\delta_{bp} \pm \delta_{ap}\delta_{bq})|0\rangle$$

and

$$\langle 0|c_y c_x c_l^\dagger c_m^\dagger = \langle 0|(\delta_{ym}\delta_{xl} \pm \delta_{yl}\delta_{xm}) \ .$$

Combining these, we recover Eq. (9).

2 Diagonalisation of quadratic Hamiltonians

If a Hamiltonian is quadratic (or, more precisely, bilinear) in creation and annihilation operators we can diagonalise it, meaning we can reduce it to a form involving only number operators. This is an approach that applies directly to Hamiltonians for non-interacting systems, and also to Hamiltonians for interacting systems when interactions are treated within a mean field approximation.

2.1 Number-conserving quadratic Hamiltonians

Such Hamiltonians have the form

$$\mathcal{H} = \sum_{ij} H_{ij} a_i^\dagger a_j \ .$$

Note that in order for the operator $\mathcal{H}$ to be Hermitian, we require the matrix H to be Hermitian. Since the matrix H is Hermitian, it can be diagonalised by unitary transformation. Denote this unitary matrix by U and let the eigenvalues of H be ε_n. The same transformation applied to the creation and annihilation operators will diagonalise $\mathcal{H}$. The details of this procedure are as follows. Let

$$\alpha_l^\dagger = \sum_i a_i^\dagger U_{il} \ .$$

Inverting this, we have

$$\sum \alpha_l^\dagger (\mathrm{U}^\dagger)_{lj} = a_j^\dagger$$

and taking a Hermitian conjugate

$$\sum_l U_{jl}\alpha_l = a_j \ .$$

Substituting for $a^\dagger$'s and a's in terms of $\alpha^\dagger$'s and α's, we find

$$\mathcal{H} = \sum_{lm} \alpha_l^\dagger (\mathrm{U}^\dagger \mathrm{H}\mathrm{U})_{lm}\alpha_m = \sum_n \varepsilon_n \alpha_n^\dagger \alpha_n \equiv \sum_n \varepsilon_n \hat{n}_n \ .$$

Thus the eigenstates of $\mathcal{H}$ are the occupation number eigenstates in the basis generated by the creation operators $\alpha_n^\dagger$.

2.2 Mixing creation and annihilation operators: Bogoliubov transformations

There are a number of physically important systems which, when treated approximately, have bilinear Hamiltonians that include terms with two creation operators, and others with two annihilation operators. Examples include superconductors, superfluids and antiferromagnets. These Hamiltonians can be diagonalised by what are known as *Bogoliubov transformations*, which mix creation and annihilation operators, but, as always, preserve commutation relations. We now illustrate these transformations, discussing fermions and bosons separately.

2.2.1 Fermions

Consider for fermion operators the Hamiltonian

$$\mathcal{H} = \epsilon(c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda(c_1^\dagger c_2^\dagger + c_2 c_1) \ ,$$

which arises in the BCS theory of superconductivity. Note that λ must be real for $\mathcal{H}$ to be Hermitian (more generally, with complex λ the second term of $\mathcal{H}$ would read $\lambda c_1^\dagger c_2^\dagger + \lambda^* c_2 c_1$). Note as well the opposite ordering of labels in the terms $c_1^\dagger c_2^\dagger$ and $c_2 c_1$, which is also a requirement of Hermiticity.

The fermionic Bogoliubov transformation is

$$\begin{aligned} c_1^\dagger &= u d_1^\dagger + v d_2 \\ c_2^\dagger &= u d_2^\dagger - v d_1 \ , \end{aligned} \tag{10}$$

where u and v are c-numbers, which we can in fact take to be real, because we have restricted ourselves to real λ. The transformation is useful only if fermionic anticommutation relations apply to both sets of operators. Let us suppose they apply to the operators d and $d^\dagger$, and check the properties of the operators c and $c^\dagger$. The coefficients of the transformation have been chosen to ensure that $\{c_1^\dagger, c_2^\dagger\} = 0$, while

$$\{c_1^\dagger, c_1\} = u^2\{d_1^\dagger, d_1\} + v^2\{d_2^\dagger, d_2\}$$

and so we must require $u^2 + v^2 = 1$, suggesting the parameterisation $u = \cos\theta$, $v = \sin\theta$.

The remaining step is to substitute in $\mathcal{H}$ for $c^\dagger$ and c in terms of $d^\dagger$ and d, and pick θ so that terms in $d_1^\dagger d_2^\dagger + d_2 d_1$ have vanishing coefficient. The calculation is clearest when it is set out using matrix notation. First, we can write $\mathcal{H}$ as

$$\mathcal{H} = \frac{1}{2}\begin{pmatrix} c_1^\dagger & c_2 & c_2^\dagger & c_1 \end{pmatrix} \begin{pmatrix} \epsilon & \lambda & 0 & 0 \\ \lambda & -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon & -\lambda \\ 0 & 0 & -\lambda & -\epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix} + \epsilon$$

where we have used the anticommutator to make substitutions of the type $c^\dagger c = 1 - c\, c^\dagger$.

For conciseness, consider just the upper block

$$\begin{pmatrix} c_1^\dagger & c_2 \end{pmatrix} \begin{pmatrix} \epsilon & \lambda \\ \lambda & -\epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix}$$

and write the Bogoliubov transformation also in matrix form as

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix} \ .$$

We pick θ so that

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \epsilon & \lambda \\ \lambda & -\epsilon \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} \tilde{\epsilon} & 0 \\ 0 & -\tilde{\epsilon} \end{pmatrix} \ ,$$

where $\tilde{\epsilon} = \sqrt{\epsilon^2 + \lambda^2}$. Including the other 2×2 block of $\mathcal{H}$, we conclude that

$$\mathcal{H} = \tilde{\epsilon}(d_1^\dagger d_1 + d_2^\dagger d_2) + \epsilon - \tilde{\epsilon} \ .$$

2.2.2 Bosons

The Bogoliubov transformation for a bosonic system is similar in principle to what we have just set out, but different in detail. We are concerned with a Hamiltonian of the same form, but now written using boson creation and annihilation operators:

$$\mathcal{H} = \epsilon(c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda(c_1^\dagger c_2^\dagger + c_2 c_1) \ .$$

We use a transformation of the form

$$\begin{aligned} c_1^\dagger &= u d_1^\dagger + v d_2 \\ c_2^\dagger &= u d_2^\dagger + v d_1 \ . \end{aligned}$$

Note that one sign has been chosen differently from its counterpart in Eq. (10) in order to ensure that bosonic commutation relations for the operators d and $d^\dagger$ imply the result $[c_1^\dagger, c_2^\dagger] = 0$. We also require

$$[c_1, c_1^\dagger] = u^2[d_1, d_1^\dagger] - v^2[d_2, d_2^\dagger] = 1$$

and hence $u^2 - v^2 = 1$. The bosonic Bogoliubov transformation may therefore be parameterised as $u = \cosh\theta$, $v = \sinh\theta$.

We can introduce matrix notation much as before (but note some crucial sign differences), with

$$\mathcal{H} = \frac{1}{2}\begin{pmatrix} c_1^\dagger & c_2 & c_2^\dagger & c_1 \end{pmatrix}\begin{pmatrix} \epsilon & \lambda & 0 & 0 \\ \lambda & \epsilon & 0 & 0 \\ 0 & 0 & \epsilon & \lambda \\ 0 & 0 & \lambda & \epsilon \end{pmatrix}\begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix} - \epsilon\,,$$

where for bosons we have used the commutator to write $c^\dagger c = c\,c^\dagger - 1$. Again, we focus on one 2×2 block

$$\begin{pmatrix} c_1^\dagger & c_2 \end{pmatrix}\begin{pmatrix} \epsilon & \lambda \\ \lambda & \epsilon \end{pmatrix}\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix}$$

and write the Bogoliubov transformation also in matrix form as

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix}\begin{pmatrix} u & v \\ v & u \end{pmatrix}\begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}\,.$$

Substituting for c and $c^\dagger$ in terms of d and $d^\dagger$, this block of the Hamiltonian becomes

$$\begin{pmatrix} d_1^\dagger & d_2 \end{pmatrix}\begin{pmatrix} u & v \\ v & u \end{pmatrix}\begin{pmatrix} \epsilon & \lambda \\ \lambda & \epsilon \end{pmatrix}\begin{pmatrix} u & v \\ v & u \end{pmatrix}\begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}\,.$$

In the fermionic case the matrix transformation was simply an orthogonal rotation. Here it is not, and so we should examine it in more detail. We have

$$\begin{pmatrix} u & v \\ v & u \end{pmatrix}\begin{pmatrix} \epsilon & \lambda \\ \lambda & \epsilon \end{pmatrix}\begin{pmatrix} u & v \\ v & u \end{pmatrix} = \begin{pmatrix} \epsilon[u^2+v^2] + 2\lambda uv & 2\epsilon uv + \lambda[u^2+v^2] \\ 2\epsilon uv + \lambda[u^2+v^2] & \epsilon[u^2+v^2] + 2\lambda uv \end{pmatrix}\,.$$

It is useful to recall the double angle formulae $u^2 + v^2 = \cosh 2\theta$ and $2uv = \sinh 2\theta$. Then, setting $\tanh 2\theta = -\lambda/\epsilon$ we arrive at

$$\mathcal{H} = \tilde{\epsilon}(d_1^\dagger d_1 + d_2^\dagger d_2) - \epsilon + \tilde{\epsilon}\,.$$

with

$$\tilde{\epsilon} = \sqrt{\epsilon^2 - \lambda^2}. \tag{11}$$

Note that in the bosonic case the transformation requires $\epsilon > \lambda$: if this is not the case, $\mathcal{H}$ is not a Hamiltonian for normal mode oscillations about a stable equilibrium, but instead represents a system at an unstable equilibrium point.

2.3 Fourier transform conventions

We will use Fourier transforms extensively, because much of the time we will be considering systems that are translation-invariant, and the plane waves used in these transforms are eigenfunctions of translation operators. For convenience, we collect here some definitions. Although we are generally interested in the thermodynamic limit (the limit of infinite system size), it is usually clearest and cleanest to write transforms in the first instance for a finite system. In order to preserve translation invariance, we take this finite system to have periodic boundary conditions. Since some details differ, we consider lattice and continuum problems separately.

2.3.1 Lattice systems

Consider a three-dimensional Bravais lattice with basis vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. Lattice sites have coordinates

$$\mathbf{r} = l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \tag{12}$$

with l,m and n integer. Periodic boundary conditions mean that $l + N_1 \equiv l$, $m + N_2 \equiv m$, and $n + N_3 \equiv n$, and the number of lattice sites is then $N = N_1N_2N_3$. In the usual way, reciprocal lattice vectors $\mathbf{G}_1$, $\mathbf{G}_2$ and $\mathbf{G}_3$ satisfy $\mathbf{G}_1 \cdot \mathbf{a} = 2\pi$, $\mathbf{G}_1 \cdot \mathbf{b} = \mathbf{G}_1 \cdot \mathbf{c} = 0$ and so on. Then the wave $\mathrm{e}^{\mathrm{i}\mathbf{kr}}$ satisfies periodic boundary conditions if

$$\mathbf{k} = 2\pi \left(\frac{n_1}{N_1}\mathbf{G}_1, \frac{n_2}{N_2}\mathbf{G}_2, \frac{n_3}{N_3}\mathbf{G}_3 \right) \tag{13}$$

with n_1, n_2 and n_3 integer. Note that we have N values of $\mathbf{k}$ in the Brillouin zone.

Let $c^\dagger_{\mathbf{r}}$ be a (boson or fermion) creation operator at the site $\mathbf{r}$. We define the Fourier transform and inverse transform by

$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} \mathrm{e}^{-\mathrm{i}\mathbf{kr}} c^\dagger_{\mathbf{r}} \quad \text{and} \quad c^\dagger_{\mathbf{r}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{kr}} c^\dagger_{\mathbf{k}} \,. \tag{14}$$

There are several points to make here. First, one should check for consistency by substituting one expression into the other. Second, these definitions use the unitary $N \times N$ matrix U, which has elements

$$U_{\mathbf{kr}} = \frac{1}{\sqrt{N}} \mathrm{e}^{\mathrm{i}\mathbf{kr}} \,.$$

Third, if we consider time-dependence in the Heisenberg picture with a Hamiltonian $\mathcal{H} = \hbar\omega(\mathbf{k}) c^\dagger_{\mathbf{k}} c_{\mathbf{k}}$ we have

$$c^\dagger_{\mathbf{k}}(t) \equiv \mathrm{e}^{\mathrm{i}\mathcal{H}t} c^\dagger_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathcal{H}t} = c^\dagger_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\omega_{\mathbf{k}}t} \qquad \text{and} \qquad c^\dagger_{\mathbf{r}}(t) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}[\mathbf{kr} - \omega(\mathbf{k})t]} c^\dagger_{\mathbf{k}} \,,$$

which has the usual traveling wave form.

2.3.2 Continuum systems

Consider a cube of side L and volume V with periodic boundary conditions. Take

$$\mathbf{k} = \frac{2\pi}{L} (n_1, n_2, n_3)$$

with n_1, n_2 and n_3 integer. Then the wavefunctions

$$\psi_{\mathbf{k}}(\mathbf{r}) = V^{-1/2} \mathrm{e}^{\mathrm{i}\mathbf{kr}}$$

form a normalised single-particle basis.

Let $c^\dagger(\mathbf{r})$ be a (boson or fermion) creation operator for a particle at the point $\mathbf{r}$. Then the creation operator for a particle in the state with wavefunction $\psi_{\mathbf{k}}(\mathbf{r})$ is

$$c^\dagger_{\mathbf{k}} = V^{-1/2} \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-\mathrm{i}\mathbf{kr}}\, c^\dagger(\mathbf{r}) \tag{15}$$

and the inverse transform is

$$c^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{kr}} c^\dagger_{\mathbf{k}} \,. \tag{16}$$

2.3.3 Thermodynamic limit

In the thermodynamic limit sums on wavevectors can be replaced by integrals. On a lattice we have

$$N^{-1} \sum_{\mathbf{k}} \;\to\; \frac{1}{\Omega} \int_{\mathrm{BZ}} \mathrm{d}^d\mathbf{k} \,, \tag{17}$$

where the integral is over the Brillouin zone of volume Ω. In the continuum we have

$$V^{-1} \sum_{\mathbf{k}} \;\to\; (2\pi)^{-d} \int \mathrm{d}^d\mathbf{k} \,. \tag{18}$$