PAGE

15. *Diagram Methods in Superconductivity* 214
- 15.1 Introduction 214
- 15.2 Hamiltonian for coupled electron–phonon system . . 215
- 15.3 Short review of BCS theory 217
- 15.4 Breakdown of perturbation theory in a superconductor . 223
- 15.5 A brief look at Nambu formalism 226
- 15.6 Treatment of retardation effects by Nambu formalism . . 229

16. *Phonons From a Many-Body Viewpoint (Reprint)* 231

Appendices

- A. Dirac formalism 243
- B. The time development operator, $U(t)$ 249
- C. Finding the ground state energy from the vacuum amplitude . 251
- D. The $\tilde{U}(t)$ operator and its expansion 252
- E. Expansion of the single-particle propagator and vacuum amplitude 255
- F. Evaluating matrix elements by Wick's theorem . . . 258
- G. Derivation of the graphical expansion for propagator and vacuum amplitude 263
- H. The spectral density function 267
- I. How the $i\delta$ factor is used 268
- J. Electron propagator in normal electron–phonon system . . 270

Answers to Exercises 277

References 285

Index 289

CHAPTER 1

Feynman Diagrams and the Many-Body Problem

1.1 What the many-body problem and Feynman diagrams are about

A reasonable starting point for a discussion of the many-body problem might be the question of how many bodies are required before we have a problem. Prof. G. E. Brown has pointed out that, for those interested in exact solutions, this can be answered by a look at history. In eighteenth-century Newtonian mechanics, the three-body problem was insoluble. With the birth of general relativity around 1910 and quantum electrodynamics in 1930, the two- and one-body problems became insoluble. And within modern quantum field theory, the problem of zero bodies (vacuum) is insoluble. So, if we are out after exact solutions, no bodies at all is already too many.

Of course we are not really interested in exact solutions, so let us look around for a better statement of the problem. Suppose we have a system containing a large number of particles, such as water molecules in a glass of water, or protons and neutrons in a lead nucleus, or oxygen molecules in a flask of oxygen gas. A system of this sort is indicated schematically in Fig. 1.1.

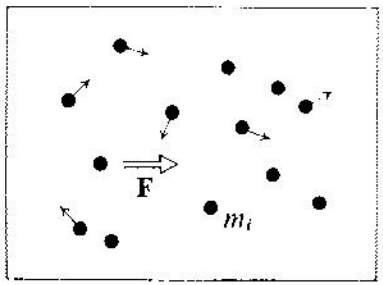


Fig. 1.1 *Many-Body System*

The problem we shall be concerned with is to describe the observed properties of the system in terms of the behaviour of the particles composing it. Thus, we might be interested in calculating the specific heat of the water, or the magnetic moment of the nucleus, or the compressibility of the oxygen.

The first thing to realize is that it takes more than just the presence of many bodies in our system for the problem to be a many-body problem. For

example, imagine that the particles do not interact with one another. This would be approximately true in the oxygen flask if the density were low enough, since then the molecules would be so far apart that collisions between them would be rare. It is seen that, in this case, each particle acts independently of the others, so that one can simply investigate the behaviour of each particle separately. (Note that in a system of identical non-interacting bosons or fermions, the particle motions are interdependent because of the fact that the total system wave function is symmetric or antisymmetric. However, during a calculation the particles may be treated separately anyway, since the symmetrization can always be done at the end.) In other words, we don't really have one many-body problem, but rather, many one-body problems. Of course, for identical particles, all these one-body problems are the same.

The real many-body problem begins with a system of particles which interact with one another. Here we can no longer consider the particles to act independently but must take into account the enormously complicated influence that each particle has on the behaviour of all the others. Almost all physical systems besides gases are of this type—molecules in a liquid, electrons in a solid, protons and neutrons in a nucleus, and so on.

This leads us to the following definition: *The many-body problem is the study of the effects of interactions between particles on the behaviour of a many-particle system.* For example, we are interested in the influence interactions have on the ground and excited state energies, on thermodynamic properties, electrical and magnetic properties, etc. In general, the many-body problem is extremely difficult, because of the incredibly intricate motions of the particles in an interacting system.

One of the most successful of the early methods of approaching the problem, and one which is still used extensively today, is the *canonical transformation* technique, to be described in the next section. This involves transforming the Schrödinger equation to a new set of co-ordinates in which the interaction term becomes small. The principal drawback with this technique is that it is not as systematic as one would like, and this sometimes makes it difficult to apply. It was this lack of a systematic method which kept the many-body field in its cradle well up into the 1950's.

The situation changed radically in 1956–7. In a series of pioneering papers, it was shown that the methods of *quantum field theory*, already famous for its success in elementary particle physics, provided a powerful, unified way of attacking the many-body problem. The new key opened many doors, and in rapid succession the idea was applied to nuclei, superfluids, superconductors, electrons in metals, phonons, ferromagnets, plasmas, atoms, molecules, etc. In the last decade, many-body theory has come of age, making possible ever-increasing amounts of exciting and fundamental research into

the nature of matter. It has penetrated so deeply into so many branches of modern physics that it has become a necessity for all physicists to acquire at least a rudimentary knowledge of the subject. To convey this minimal knowledge is our purpose here.

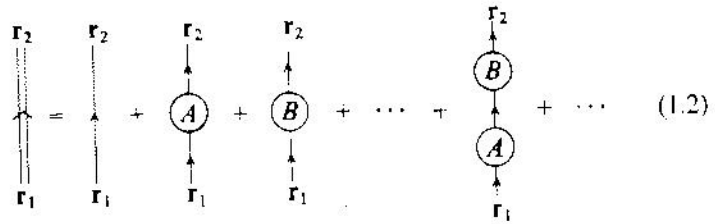
In this book, we shall be mainly concerned with that field theoretic technique known as the *propagator* method. This is based on the idea that in order to find the important physical properties of a system it is not necessary to know the detailed behaviour of each particle in the system but, rather, just the average behaviour of one or two typical particles. The quantities which describe this average behaviour are called the *one-particle propagator* and *two-particle propagator*, respectively.

Consider the one-particle propagator first. It is obviously hopeless to try to describe in detail the tremendously complicated motion of a particle moving from one point to another in an interacting system. But we can describe the motion in an 'average' way by giving the probability (or in quantum systems, the probability *amplitude*) for the motion. Thus, the one-particle propagator, $G(\mathbf{r}_2,t_2;\mathbf{r}_1,t_1)$ is defined as the probability (amplitude) that a single particle in the system will move or 'propagate' to the point $\mathbf{r}_2$ at time t_2 if it starts out from the point $\mathbf{r}_1$ at time t_1. The two-particle propagator is defined in a similar way. From these propagators, it is possible to obtain the physical properties of the many-body system.

The method of calculating the propagators which we will use in this book is the method of *Feynman diagrams*. Just to get an idea of what these diagrams are, consider the following simple example: A man who has had too much to drink, leaves a party at point $\mathbf{r}_1$, and on the way to his home at point $\mathbf{r}_2$, he can stop off at one or more bars—bar A, B, C..., etc. We ask for the probability, $P(\mathbf{r}_2,\mathbf{r}_1)$, that he gets home. This probability, which is just the propagator here (with time omitted for simplicity), is the sum of the probabilities for all the different ways he can propagate from $\mathbf{r}_1$ to $\mathbf{r}_2$ interacting with the various bars. Assuming, for simplicity, that the various processes involved are independent, this is just $P_0(\mathbf{r}_2,\mathbf{r}_1)$ (=probability that he will go 'freely' from $\mathbf{r}_1$ to $\mathbf{r}_2$, i.e., without stopping at a bar), plus $P_0(\mathbf{r}_A,\mathbf{r}_1)\times P(A)\times P_0(\mathbf{r}_2,\mathbf{r}_A)$ (=probability he will go freely from $\mathbf{r}_1$ to bar A, times the probability that he will come out of A in condition to continue, times the probability that he then proceeds freely to $\mathbf{r}_2$), plus $P_0(\mathbf{r}_B,\mathbf{r}_1)\times P(B)\times P_0(\mathbf{r}_2,\mathbf{r}_B)$ (=probability for route $\mathbf{r}_1$—bar B—$\mathbf{r}_2$) plus etc. ... plus $P_0(\mathbf{r}_A,\mathbf{r}_1)\times P(A)\times P_0(\mathbf{r}_B,\mathbf{r}_A)\times P(B)\times P_0(\mathbf{r}_2,\mathbf{r}_B)$ (=probability for route $\mathbf{r}_1$—A—B—$\mathbf{r}_2$) plus etc. ... This gives us an infinite 'perturbation' series for the propagator:

$$P(\mathbf{r}_2,\mathbf{r}_1) = P_0(\mathbf{r}_2,\mathbf{r}_1)+P_0(\mathbf{r}_A,\mathbf{r}_1)\,P(A)\,P_0(\mathbf{r}_2,\mathbf{r}_A)+P_0(\mathbf{r}_B,\mathbf{r}_1)\,P(B)\,P_0(\mathbf{r}_2,\mathbf{r}_B)+\ldots$$
$$+P_0(\mathbf{r}_A,\mathbf{r}_1)\,P(A)\,P_0(\mathbf{r}_B,\mathbf{r}_A)\,P(B)\,P_0(\mathbf{r}_2,\mathbf{r}_B)+\ldots. \qquad (1.1)$$

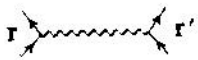
Each term in this series may be represented by a diagram in the following way: Let us represent $P_0(\mathbf{r}_j,\mathbf{r}_i)$ (the probability of free motion from point $\mathbf{r}_i$ to point $\mathbf{r}_j$) by a directed line: $\mathbf{r}_i \longrightarrow \mathbf{r}_j$, and $P(X)$ (the probability of emerging from bar X) by a circle: (X). Then the series may be drawn as



(1.2)

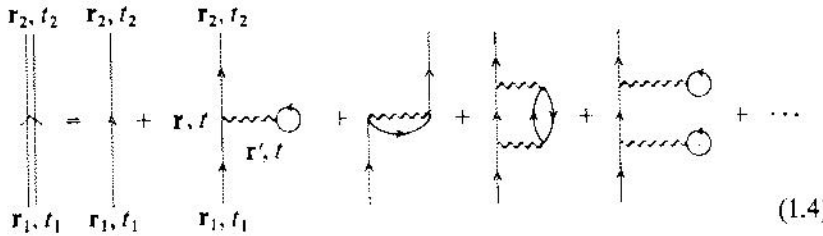
Since each diagram element stands for a factor, this is completely equivalent to (1.1). However, it has the great advantage that it also reveals the physical meaning of the series, giving us a 'map' which helps us to keep track of all the sequences of interactions the drunken man can have in going from $\mathbf{r}_1$ to $\mathbf{r}_2$.

In a many-body system, instead of a propagating drunken man interacting with various bars, we have a propagating particle interacting with the other particles of the system. Let us represent the interaction between a particle at $\mathbf{r}$ and one at $\mathbf{r}'$ by a wiggly line, thus:



(1.3)

Then, analogous to the drunken man case, the propagator, $G(\mathbf{r}_2,t_2;\mathbf{r}_1,t_1)$, can be represented as the sum of all diagrams showing the particle beginning at the point $\mathbf{r}_1$ at time t_1, interacting zero, one, or more times with the other particles in the system, and winding up at the point $\mathbf{r}_2$ at time t_2:



(1.4)

(a) (b) (c) (d) (e)

Diagram (*a*) shows 'free' propagation from $\mathbf{r}_1,t_1$ to $\mathbf{r}_2,t_2$. Diagrams (*b*) and (*c*) show the particle undergoing a single collision with another particle. In (*d*) and (*e*) there are two collisions, etc. (The detailed interpretation of these

diagrams is more difficult than in the drunken man case, so we postpone it to chapter 4.) As with the drunken man propagator, each diagram in (1.4) corresponds to a term in the perturbation expansion of the many-body propagator, as will be discussed in chapter 4. Similar diagrams are used in the case of the two-particle propagator.

The pictures in (1.4) are called *Feynman diagrams* after their inventor, Richard P. Feynman, who employed them in his Nobel prize-winning work on quantum electrodynamics. They are used very extensively in elementary particle physics.

The way in which these diagrams are employed in the actual calculation of the propagator will be discussed at the end of this chapter. But first we review the canonical transformation method for solving the many-body problem, since this provides the necessary background for understanding the significance of the new quantum field theoretic technique.

1.2 Canonical transformation method of solving the many-body problem

Let us first express quantitatively our remarks about a system of N non-interacting particles. Suppose that these particles have masses $m_1, m_2, \ldots, m_N$, and that they are placed in a time-independent external force field $\mathbf{F}(\mathbf{r})$, with associated potential $V(\mathbf{r})$. Our problem is to find out how they behave. In the classical case, the system is described by the N independent equations of motion

$$\mathbf{F}(\mathbf{r}_i) = m_i \frac{d^2\mathbf{r}_i}{dt^2}, \quad i = 1, 2, \ldots, N, \tag{1.5}$$

with solutions of the form $\mathbf{r}_i = \mathbf{r}_i(t)$. In the quantum mechanical case, this is replaced by the Schrödinger equation

$$H\Psi = E\Psi, \quad \text{with} \quad H = \sum_{i=1}^{N} H_i, \quad H_i = \frac{p_i^2}{2m_i} + V(\mathbf{r}_i), \tag{1.6a}$$

where H, Ψ, E are the total system Hamiltonian, wave function, and energy, respectively, and H_i, $\mathbf{p}_i$, $V(\mathbf{r}_i)$ are the single particle Hamiltonian, momentum, and potential energy. If Ψ is written in the product form (neglect symmetry requirements for simplicity):

$$\Psi(\mathbf{r}_1 \ldots \mathbf{r}_N) = \prod_{i=1}^{N} \phi_{k_i}(\mathbf{r}_i) \tag{1.6b}$$

and substituted into (1.6a), it is found that (1.6a) separates into the N single particle Schrödinger equations

$$H_i \phi_{k_i}(\mathbf{r}_i) = E_{k_i} \phi_{k_i}(\mathbf{r}_i), \quad i = 1, \ldots, N \tag{1.6c}$$

and the total energy is just the sum of the single particle energies:

$$E = \sum_i E_{k_i} \tag{1.6d}$$

Thus, in both the classical and quantum mechanical non-interacting systems we find N independent equations, which means that we have just N one-body problems.

In the real many-body problem, we have seen that the particles interact with one another. This means that in the classical case it is necessary to solve the N coupled equations

$$\mathbf{F}(\mathbf{r}_i) + \sum_{j=1}^{N} \mathbf{F}(\mathbf{r}_i, \mathbf{r}_j) = m_i \frac{d^2 \mathbf{r}_i}{dt^2}, \quad i = 1, 2, \ldots, N, \tag{1.7}$$

where $\mathbf{F}(\mathbf{r}_i, \mathbf{r}_j)$ is the interaction force between two particles. In the quantum case, we find a non-separable Schrödinger equation:

$$\left(\sum_{i=1}^{N} \left[\frac{p_i^2}{2m_i} + V(\mathbf{r}_i) \right] + \tfrac{1}{2} \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} V(\mathbf{r}_i, \mathbf{r}_j, \mathbf{p}_i, \mathbf{p}_j) \right) \Psi(\mathbf{r}_1 \ldots \mathbf{r}_N) = E \Psi(\mathbf{r}_1 \ldots \mathbf{r}_N) \tag{1.8}$$

where $V(\mathbf{r}_i, \mathbf{r}_j, \mathbf{p}_i, \mathbf{p}_j)$ is the two-particle interaction potential, considered to be momentum-dependent, for the sake of generality.

It will be convenient in what follows to make a distinction between 'weak' and 'strong' interactions. We will call the interaction term in (1.8) 'weak' or 'small' if it causes just a small perturbation to the solutions in the non-interacting case, i.e., if it can be handled by ordinary finite-order perturbation theory. If it cannot be handled this way, the interaction will be referred to as 'strong' or 'large'. Most of the interactions we have to deal with are of the strong type. For example, consider the Coulomb interaction between two electrons in a metal. This has the form

$$V(\mathbf{r}_i, \mathbf{r}_j) = \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

If the ground state energy of the system is calculated using this as the perturbation, we obtain the result

$$E_0 = E_0^{(0)} + E_0^{(1)} + \infty + \infty + \infty + \ldots,$$

i.e., infinity to all orders of perturbation theory above the first! (It should be noted that there are some interactions which are small in magnitude but which cannot be treated as small perturbations, such as the small attraction between electrons which gives rise to superconductivity. According to the above scheme, these will also be classified as 'strong'.)

Since visualizing the motion of a strongly interacting N particle system is roughly like trying to watch a basketball game played with N balls, the early attacks on the many-body problem tried to reduce it to a one-body problem by getting rid of the interaction. This could be done either by pretending it didn't exist, or more legally, by transforming it away. In the classical case, such a transformation implies that we change to a new set of co-ordinates in which the equations of motion (1.7) become approximately decoupled. For instance, in simple situations it might be possible to define new co-ordinates $\mathbf{R}_k$ given by

$$\mathbf{r}_i = \mathbf{r}_i(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_k, \ldots, \mathbf{R}_N) \tag{1.9}$$

which, when introduced into (1.7) change it into:

$$f(\mathbf{R}_k) = M_k \frac{d^2 \mathbf{R}_k}{dt^2} + \underbrace{\sum_l h(\mathbf{R}_k, \mathbf{R}_l)}_{small}. \tag{1.10}$$

The M_k are referred to as 'effective masses'. Equation (1.10) constitutes a set of N nearly independent 'one-body' problems which can be more or less accurately solved, the remaining small interaction $h(\mathbf{R}_k, \mathbf{R}_l)$ being treated by perturbation methods. The 'bodies' here are of course not real but rather *fictitious* bodies.

The idea of transforming a system of interacting real particles into a system of approximately non-interacting fictitious bodies can be easily illustrated by means of two interacting particles in a gravitational field. Let the masses of the two particles be m_1, m_2, positions $\mathbf{r}_1$, $\mathbf{r}_2$, gravitational force $\mathbf{F}_1 = m_1\mathbf{g}$, $\mathbf{F}_2 = m_2\mathbf{g}$, and interaction force $\mathbf{F}(\mathbf{r}_1 - \mathbf{r}_2)$. These obey the coupled equations of motion

$$\begin{aligned} \mathbf{F}_1 + \mathbf{F}(\mathbf{r}_1 - \mathbf{r}_2) &= m_1 \ddot{\mathbf{r}}_1 \\ \mathbf{F}_2 - \mathbf{F}(\mathbf{r}_1 - \mathbf{r}_2) &= m_2 \ddot{\mathbf{r}}_2. \end{aligned} \tag{1.11}$$

The problem may be reduced to two independent one-body problems by making the transformation to new co-ordinates

$$\begin{aligned} (m_1 + m_2)\mathbf{R} &= m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2 \quad \text{(centre of mass co-ordinate)} \\ \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2 \qquad\quad \text{(relative co-ordinate).} \end{aligned} \tag{1.12}$$

Adding the two equations yields

$$\mathbf{F}_{\text{total}} = (m_1 + m_2)\ddot{\mathbf{R}}, \tag{1.13}$$

while multiplying by m_2 and m_1 and subtracting gives

$$\mathbf{F}(\mathbf{r}) = \frac{m_1 m_2}{m_1 + m_2} \ddot{\mathbf{r}}. \tag{1.14}$$

Thus, we have two new independent equations: one for a fictitious particle-like body of effective mass m_1+m_2 with position at mass centre $\mathbf{R}$ and the other for a fictitious particle-like body of effective mass $m_1m_2/(m_1+m_2)$ and position at the relative co-ordinate $\mathbf{r}$.

The new non-interacting fictitious bodies are not always 'particle-like' in their appearance, however. Consider for instance the well-known case of a one-dimensional chain of N atoms of mass m coupled by nearest-neighbour

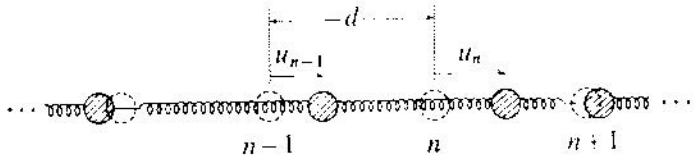


Fig. 1.2 *Chain of Atoms with Harmonic Coupling*

harmonic forces shown in Fig. 1.2. The classical equation of motion for such a system is

$$-2k_c u_n + k_c(u_{n+1}+u_{n-1}) = m\frac{d^2u_n}{dt^2} \tag{1.15}$$

where u_n is the displacement of the nth atom from equilibrium and k_c is the spring constant. The transformation (1.9) here is just the simple Fourier transform:

$$u_n = \sum_k U_k e^{-iknd}. \tag{1.16}$$

Substituting this in (1.15) produces decoupled equations of form (1.10):

$$2k_c(\cos kd - 1)\,U_k = m\frac{d^2U_k}{dt^2} + 0, \tag{1.17}$$

which have the solution

$$U_k = A_k e^{i\omega_k t}; \quad \omega_k = \sqrt{\left\{\frac{2k_c}{m}(1-\cos kd)\right\}}. \tag{1.18}$$

If all the A_k's are zero except one, then this becomes

$$u_n = A_k e^{-i(knd-\omega_k t)} \tag{1.19}$$

which is just the equation of a sinusoidal longitudinal vibration or 'sound wave' on the chain, of frequency ω_k and wavelength $\lambda = 2\pi/k$. Thus, the fictitious 'single bodies' here are wave-like instead of particle-like.

The quantum case may often be handled in a parallel fashion by trans-

forming the Hamiltonian, H, canonically, so that its interaction term becomes small. Introducing the new co-ordinates $\mathbf{R}_k$ and momenta $\mathbf{P}_k$ by

$$\begin{aligned}\mathbf{r}_i &= \mathbf{r}_i(\mathbf{R}_1,\ldots,\mathbf{R}_k,\ldots,\mathbf{R}_N;\mathbf{P}_1,\ldots,\mathbf{P}_k,\ldots,\mathbf{P}_N)\\ \mathbf{p}_i &= \mathbf{p}_i(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{P}_1,\ldots,\mathbf{P}_N),\end{aligned} \tag{1.20}$$

(Note: The definition of a canonical transformation is that the new co-ordinates, $\mathbf{R}_i$, $\mathbf{P}_i$, must obey the same canonical commutation relations which are obeyed by $\mathbf{r}_i$, $\mathbf{p}_i$, i.e.

$$[\mathbf{r}_i,\mathbf{p}_j] = i\hbar\delta_{ij}, \quad [\mathbf{r}_i,\mathbf{r}_j] = 0, \quad [\mathbf{p}_i,\mathbf{p}_j] = 0.) \tag{1.20'}$$

yields the transformation

$$H = \sum_i H(\mathbf{p}_i,\mathbf{r}_i) + \tfrac{1}{2}\sum_{i,j} V(\mathbf{r}_i,\mathbf{r}_j;\mathbf{p}_i,\mathbf{p}_j)$$

$$\to H' = \sum_q H'(\mathbf{P}_q,\mathbf{R}_q) + \tfrac{1}{2}\sum_{q,m} \underbrace{V'(\mathbf{R}_q,\mathbf{R}_m;\mathbf{P}_q,\mathbf{P}_m)}_{small}. \tag{1.21}$$

If this can be done, then the problem reduces to the set of N approximately independent one-body problems:

$$H'(\mathbf{P}_q,\mathbf{R}_q)\,\phi'_q = E'_q\phi'_q \tag{1.22}$$

with V' as small perturbation. These are just the equations for the independent fictitious bodies in the quantum case. The energy levels of the quantum system are the sum of the fictitious body energies:

$$E = \sum_q E'_q. \tag{1.23}$$

A simple example of transformation (1.21) is provided by the system of two interacting particles treated quantum mechanically. The system obeys the equation (assume no gravitational field)

$$H\Psi(\mathbf{r}_1,\mathbf{r}_2) = E\Psi(\mathbf{r}_1,\mathbf{r}_2) \tag{1.24}$$

where

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\mathbf{r}_1-\mathbf{r}_2); \quad \mathbf{p} = \frac{\hbar}{i}\boldsymbol{\nabla}. \tag{1.25}$$

Making the same transformation (1.12), to centre of mass and relative co-ordinates, we find

$$H = H(\mathbf{R}) + H(\mathbf{r})$$

where

$$H(\mathbf{R}) = \frac{p_R^2}{2(m_1+m_2)}, \quad H(\mathbf{r}) = \frac{p_r^2}{2\left(\frac{m_1m_2}{m_1+m_2}\right)} + V(\mathbf{r}) \tag{1.26}$$

which yields the two Schrödinger equations

$$H(\mathbf{R})\phi_k(\mathbf{R}) = E_k\phi_k(\mathbf{R})$$
$$H(\mathbf{r})\gamma_l(\mathbf{r}) = E_l\gamma_l(\mathbf{r}) \tag{1.27}$$

showing two fictitious particle-like objects just like those in the corresponding classical case.

We can also demonstrate the transformation (1.21) for the chain of atoms in Fig. 1.2 (for details, see Ziman (1962), p. 6 ff., or H. Højgaard Jensen (1964), p. 1). The Hamiltonian for the chain is (neglecting end effects)

$$H = \sum_{n=1}^{N}\left(\frac{p_n^2}{2m}+k_c u_n^2\right)-\tfrac{1}{2}k_c\sum_{n-1}^{N}(u_n u_{n+1}+u_n u_{n-1})$$
$$= \sum_{n-1}^{N}\left(\frac{p_n^2}{2m}+k_c u_n^2\right)-k_c\sum_{n-1}^{N}u_n u_{n+1}. \tag{1.28}$$

The first term describes a set of independent harmonic oscillators, one on each atom site, while the second is the interaction between each atom and its nearest neighbour. The transformation (1.20) in this case turns out to be

$$u_n = \frac{1}{\sqrt{N}}\sum_q\left(\mathscr{U}_q\cos qnd-\frac{1}{m\omega_q}\mathscr{P}_q\sin qnd\right) \tag{1.29}$$

$$p_n = \frac{1}{\sqrt{N}}\sum_q(m\omega_q\mathscr{U}_q\sin qnd+\mathscr{P}_q\cos qnd) \tag{1.30}$$

where

$$\omega_q = \sqrt{\left\{\frac{2k_c}{m}(1-\cos qd)\right\}}. \tag{1.31}$$

The $\mathscr{U}_q$, $\mathscr{P}_q$ obey the canonical commutation rules

$$[\mathscr{U}_q,\mathscr{P}_{q'}] = i\hbar\delta_{qq'},\quad [\mathscr{U}_q,\mathscr{U}_{q'}] = 0,\quad [\mathscr{P}_q,\mathscr{P}_{q'}] = 0, \tag{1.32}$$

which may be proved by substituting (1.29, 30) into (1.20'), with $\mathbf{r}_i\equiv u_i$. Placing (1.29, 30) into (1.28) and using (1.32) we get, after some tedious calculation, the result:

$$H' = \sum_q\left[\frac{\mathscr{P}_q^2}{2m}+\frac{m\omega_q^2}{2}\mathscr{U}_q^2\right], \tag{1.33}$$

which is just the sum of a set of ordinary harmonic oscillator Hamiltonians of various frequencies. (Note: the usual transformation which is made is not (1.29, 30) but rather

$$u_n = \frac{1}{\sqrt{N}}\sum_q U_q e^{-iqnd},\quad p_n = \frac{1}{\sqrt{N}}\sum_q P_q e^{+iqnd}.$$

However, this leads to a Hamiltonian which is not completely decoupled since it mixes modes of wavenumber q and $-q$. Transformation (1.29, 30) produces complete decoupling.) The Schrödinger equation and energies of the qth oscillator are the well-known

$$H_q'\phi_q' = \left(\frac{\mathscr{P}_q^2}{2m}+\frac{m\omega_q^2}{2}\mathscr{U}_q^2\right)\phi_q' = E_q'\phi_q'$$
$$E_q' = \hbar\omega_q[n_q+\tfrac{1}{2}],\quad n_q = 0,1,2,3,\ldots, \tag{1.34}$$

so that the total system energy and wave functions are

$$E = \sum_q\hbar\omega_q(n_q+\tfrac{1}{2})$$
$$\Psi = \phi_{q_1}'\phi_{q_2}'\ldots\phi_q'\ldots. \tag{1.35}$$

Thus the independent 'fictitious bodies' here are just quantized longitudinal sound waves.

It will be useful for us to recall the operator algebra method of deriving results (1.35) (see, for example, Park (1964) p. 110 ff.). This is done by performing an additional transformation on H_q' in (1.34) which involves the 'ladder' operators, b_q, $b_q^\dagger$ defined by:

$$b_q = \sqrt{\frac{1}{2m\hbar\omega_q}}\mathscr{P}_q-i\sqrt{\frac{m\omega_q}{2\hbar}}\mathscr{U}_q$$
$$b_q^\dagger = \sqrt{\frac{1}{2m\hbar\omega_q}}\mathscr{P}_q+i\sqrt{\frac{m\omega_q}{2\hbar}}\mathscr{U}_q \tag{1.36}$$

From the commutation rules (1.32), it is easily verified that the b_q's obey the rules:

$$(a)\ [b_q,b_{q'}^\dagger] = \delta_{qq'},\quad (b)\ [b_q,b_{q'}] = 0,\quad (c)\ [b_q^\dagger,b_{q'}^\dagger] = 0. \tag{1.37}$$

Substituting the inverse of transformation (1.36) into (1.34) and using (1.37a), yields the new Hamiltonian and Schrödinger equation

$$H_q'' = \hbar\omega_q(b_q^\dagger b_q+\tfrac{1}{2}),\quad H_q''\phi_q'' = E_q'\phi_q''. \tag{1.38}$$

Using (1.37, 38), it may be shown (see above reference) that if we let ψ_{0q} be the lowest-energy eigenfunction of H_q'', then all the other eigenfunctions are given by

$$\phi_q^* \equiv \psi_{n_q} = \frac{1}{\sqrt{n_q!}}(b_q^\dagger)^{n_q}\psi_{0q},\quad n_q = 0,1,2,\ldots \tag{1.39a}$$

(ψ_{n_q} is short for $\psi_{(n_q)_q}$). The corresponding energies are

$$E_q' = \hbar\omega_q(n_q+\tfrac{1}{2}), \tag{1.39b}$$

thus establishing (1.34). It also follows that the b-operators have the following important properties when operating on the energy eigenfunctions:

$$\begin{aligned} &(a)\ b_q^\dagger \psi_{n_q} = \sqrt{n_q+1}\,\psi_{n_q+1}, \\ &(b)\ b_q \psi_{n_q} = \sqrt{n_q}\,\psi_{n_q-1}, \\ &(c)\ b_q^\dagger b_q \psi_{n_q} = n_q \psi_{n_q}. \end{aligned} \tag{1.40}$$

Observe that the additional transformation, (1.36), changes H' in (1.33) to

$$H'' = \sum_q \hbar\omega_q (b_q^\dagger b_q + \tfrac{1}{2}) = \underbrace{\tfrac{1}{2}\sum_q \hbar\omega_q}_{E_0} + \sum_q \hbar\omega_q b_q^\dagger b_q, \tag{1.41}$$

with associated Schrödinger equation

$$H''\Psi_{n_{q_1}, n_{q_2}, \ldots, n_q, \ldots} = E\Psi_{n_{q_1}, n_{q_2}, \ldots, n_q, \ldots}$$

where

$$\Psi_{n_{q_1}, n_{q_2}, \ldots, n_q, \ldots} = \psi_{n_{q_1}} \psi_{n_{q_2}} \ldots \psi_{n_q} \ldots \tag{1.42}$$

1.3 Elementary excitations

The results in the last section show how the problem of a strongly coupled classical or quantum many-body system may often be solved by transforming to a set of approximately (or exactly, in the simple cases considered) independent fictitious bodies. There is a more modern (but equivalent) way of viewing these fictitious bodies which has the advantage of giving a unified picture of many-body systems. It is based on the concept of *elementary excitations*, and is the viewpoint which will be taken throughout this book.

In order to understand what an elementary excitation is, and to see how it is related to the fictitious bodies, let us look at a specific case, the *phonon*. Recall first that light waves may be regarded either as quantized radiation oscillators or as consisting of particles ('quanta') called photons each of which has energy $\hbar\omega$. This suggests that it may be possible to look at sound waves in the same way. If we examine result (1.34), we see that instead of regarding the sound wave of wavenumber q as one fictitious body (the harmonic oscillator) having quantized energy $E_q' = \hbar\omega_q(n_q + \frac{1}{2})$, we could alternatively regard it as a set of n_q quanta each having energy $\hbar\omega_q$, together with a ground state of energy $\frac{1}{2}\hbar\omega_q$. These quanta of the sound wave are called *phonons* and, like photons, they behave very much as particles (i.e., particles in the quantum-mechanical sense—they are not necessarily localized, although they can be—see Højgaard Jensen (1964)). It should be pointed out here that it is common to call a phonon a 'quantized sound wave', but that according to the above, this is not correct. For a given n_q there is only one quantized sound wave of wavenumber q (this is just the fictitious body of energy E_q'), but there are

many, i.e., n_q, phonons of wavenumber q. Hence it is more proper to call the phonon a quantum or particle of sound.

The energy $\hbar\omega_q$ is evidently just the least unit of excitation energy above the zero-point energy $\frac{1}{2}\hbar\omega_q$. Since the phonon carries this least unit, it is referred to as an '*elementary excitation*'. The 'compound excitations' are then just excitations involving many phonons.

The phonon way of viewing the sound wave provides a new interpretation of the wave function and ladder operators, $b_q^\dagger$, b_q. Evidently, $\Psi_{n_{q_1}, n_{q_2}, \ldots, n_q, \ldots}$ in (1.42) describes a system with n_{q_1} phonons of wavenumber q_1, n_{q_2} of wavenumber q_2, etc. Therefore, by (1.40), $b_q^\dagger$ is an operator which creates a phonon of wavenumber q, while b_q destroys such a phonon, and $b_q^\dagger b_q$ is the 'number operator' for phonons of wavenumber q.

An important feature of phonons, in contrast to the quantized sound waves, is that the total system energy is equal to the sum of the energies of all the quantized sound waves, by (1.35), but it is not equal to the sum of the energies for all the phonons. That is, (1.23) does not hold true for phonons. This is obvious from (1.41) where we see that to get the total energy, we must add the ground state energy to that of the phonons. Thus (1.41) gives us a picture of any excited state of the system as being composed of a ground state plus a collection of independent phonons above the ground state.

This result for the phonon case turns out to be extremely general. It appears now that, in most many-body systems, it is possible to perform a transformation from the system of strongly interacting particles to a set of approximately independent elementary excitations above the ground state. Thus, we may write, using (1.21) and by analogy with (1.41), the transformation in the form:

$$\begin{aligned} H &= \sum_i H(\mathbf{p}_i, \mathbf{r}_i) + \tfrac{1}{2}\sum_{ij} V(\mathbf{r}_i, \mathbf{r}_j; \mathbf{p}_i, \mathbf{p}_j) \\ \rightarrow H' &= E_0 + \sum_q \epsilon_q' A_q^\dagger A_q + \underbrace{f(\ldots A_k \ldots A_k^\dagger \ldots)}_{\text{small}} \end{aligned} \tag{1.43}$$

where E_0 is the ground state energy of the interacting system, ϵ_q' is the energy of the elementary excitation, $A_q^\dagger$, A_q, $A_q^\dagger A_q$ are the creation, destruction and number operators for the elementary excitations. (The ϵ_q' is often called the 'dispersion law' or 'excitation spectrum'.)

The small term in (1.43) describes the interactions between elementary excitations. These give rise to a broadening, $\Delta\epsilon_q'$, of the energy levels, ϵ_q'. By the uncertainty principle, we have $\Delta E \Delta t \sim \hbar$, which means that the elementary excitations have a *lifetime*, $\tau_q \sim \hbar(\Delta\epsilon_q')^{-1}$. This lifetime must of course be reasonably long (i.e., level width $\hbar\tau_q^{-1}$ must be $\ll \epsilon_q'$) for the elementary excitations to really be considered well-defined and independent of one another.

Elementary excitations are often (Pines (1961), p. 1) divided into two general

categories: '*collective excitations*', and '*quasi particles*', although this practice is far from being universal. (For example, some writers, like Ter Haar (1960), call all elementary excitations quasi particles.) The collective excitations are the quanta associated with collective motions of macroscopic groups of particles in the system, i.e., with motions of the system as a whole. Examples of collective excitations are:

1. *Phonons:* in a regular array of atoms such as found in a crystal, the collective motions are sound waves. The corresponding excitations as discussed above are the sound quanta or phonons.

2. *Plasmons:* in the electron gas in a metal, one can have wave-like fluctuations in the electron density similar to sound waves. These are the approximately independent fictitious bodies known as 'plasma oscillations'. The quanta of these oscillations are the collective excitations called plasmons.

3. *Magnons:* in ferromagnets there are regular fluctuations in the density of spin angular momentum, referred to as 'spin waves'. The collective excitation here is the spin wave quantum, known as the magnon.

4. *Nuclear quanta:* in nuclei, one finds various vibrational and rotational motions; the associated quanta are the collective excitations in this case.

The collective excitations show no more resemblance to the real particles of the system than water waves show to water molecules. In contrast to this, *quasi particles* resemble the real particles quite closely. The idea is roughly this: if we consider a single particle moving through the system, it pushes or pulls on the particles in its neighbourhood and becomes surrounded by a 'cloud' of agitated particles similar to the dust cloud kicked up by a galloping horse in a western. The real particle plus its cloud constitutes the quasi particle. Just as the dust cloud hides the horse, so the particle cloud 'screens' the real particle, greatly reducing the effect of its force field. Hence a quasi particle interacts only weakly with other quasi particles and can be treated as approximately independent of them. The presence of the cloud also makes the properties of the quasi particle different from that of the real particle—for example, it may have an effective mass. (It should be noted that, in the quantum case, the particles in the cloud are in virtual energy states. This is because the collisions between the particle we are considering and the other particles (i.e., the collisions which kick up the cloud) do not in general conserve energy (see paragraph after (4.47)). Despite the fact that the states are virtual, the cloud itself is a physically real object.) Some examples of quasi particles are:

1. *Quasi electron:* an electron in an electron gas with a uniform positive charge background repels other electrons, thus becoming surrounded by a positive screening cloud. The electron plus screening cloud constitutes the quasi electron. The effective interaction between two quasi electrons is a screened interaction which is much weaker (shorter range) than the original Coulomb interaction.

2. *Polaron:* an electron moving through an insulating polar crystal interacts with the crystal lattice ions, displacing them from their equilibrium positions and causing local excitation of sound waves, i.e., phonons. The polaron is the electron plus a cloud of phonons.

3. *Quasi nucleon:* despite powerful short-range forces between nucleons in a nucleus, they behave in many respects as if they were independent of each other (as indicated by the success of the nuclear shell model). The nearly independent particles here are not the nucleons themselves but the nucleon surrounded by a cloud of other nucleons, i.e., the quasi nucleon.

4. *Conduction electron:* an electron interacting with the periodic potential caused by the fixed lattice ions in a crystal has no cloud around it in the sense above. Nevertheless, the influence of the potential may be described in terms of an effective mass, so the conduction electron may be regarded as a primitive sort of quasi particle.

There are in addition a few elementary excitations which do not fit very easily into either of the above categories, although they are often placed in one or the other. One example is the *exciton*, which is a bound electron–'hole' pair moving as a hydrogen-like 'atom' through the crystal. It is often called a collective excitation. Another is the *bogolon*, or 'Bogoliubov quasi particle' which consists of a linear combination of an electron in state $(+k,\uparrow)$ and a 'hole' in $(-k,\downarrow)$. The bogolon is the elementary excitation in a superconductor. Excitations similar to bogolons also exist in certain even–even nuclei which in many respects resemble superconductors.

It is important to notice that there may be more than one kind of elementary excitation in a given system. For example, in the electron gas in a metal, there are both quasi electrons and plasmons, while in a nucleus we have quasi nucleons and vibrational and rotational collective excitations existing simultaneously. Thus, in general, the right-hand side of (1.43) may be written

$$H' = E_0 + \underbrace{\sum_q \epsilon'_q A^\dagger_q A_q}_{\text{quasi particles}} + \underbrace{\sum_k \epsilon''_k B^\dagger_k B_k}_{\text{collective excitations}} + \textit{small terms}. \tag{1.44}$$

1.4 Quantum field theory method of solving the many-body problem

The picture of a strongly interacting many-body system in terms of a set of approximately independent elementary excitations above a ground state is an appealingly simple one. However, the problems involved in actually finding the energies of the ground state and elementary excitations are enormous. The canonical transformation method is easy enough for two particles or for phonons, and has even been used with great success in some very complicated systems—take for example the Bohm–Pines theory of quasi electrons and plasmons in the electron gas (Pines (1963), p. 104 ff.), or the Bohr–Mottelson theory of collective excitations in nuclei (Thouless (1961), p. 78).

But in the general case there is no recipe for how to carry out the transformation, so the method can be difficult to apply.

What we would like, essentially, is a systematic way of getting the energy of the ground state, and the energies and lifetimes of the elementary excitations. It was shown in a series of revolutionary papers appearing during 1955–7 (and also in some lesser known papers prior to that time) that quantum field theory, previously restricted to elementary particle physics, provides just the systematic method we are looking for. Not only does it give us a unified way of getting the ground energy and excitation energies and lifetimes, but it also provides direct ways of obtaining many other system properties as well. Let us take a bird's-eye look at the new method.

The hero roles in the field theoretic treatment of the many-body problem are played by the *Green's functions* or *propagators* of the system. These are essentially a generalization of the ordinary familiar undergraduate Green's function. They come in all sizes and shapes—one-particle, two-particle, ..., n-particle, advanced, retarded, causal, zero temperature, finite temperature, real time, imaginary time—an assortment to suit every situation and taste. There are essentially three reasons for the popularity propagators are enjoying these days:

1. They yield in a direct way the most important physical properties of the system.
2. They have a simple physical interpretation.
3. They can be calculated in a systematic way which appeals to one's physical intuition.

Take the *single-particle propagator*, $G(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1)$, for instance. This is the probability amplitude that if we put a particle into the interacting system at point $\mathbf{r}_1$ at time t_1 and let it collide with the other particles for a while (i.e., 'propagate' through the system), then it will be observed at the point $\mathbf{r}_2$ at time t_2. The propagator, G, yields directly the energies and lifetimes of quasi particles. It gives also the momentum distribution, spin and particle density, and can be used as well to calculate the ground state energy. All these properties may be obtained at temperatures greater than zero by using the finite temperature version of G.

The *two-particle propagator*, G_2, is the probability amplitude for observing one particle at $\mathbf{r}_3, t_3$ and another at $\mathbf{r}_4, t_4$ if one was put into the system at $\mathbf{r}_1, t_1$ and another at $\mathbf{r}_2, t_2$. This G_2 also has a wide range of talents. It gives directly the energies and lifetimes of collective excitations, as well as the magnetic susceptibility, electrical conductivity, and a host of other non-equilibrium properties at both zero and finite temperatures.

There is in addition a field theoretic quantity called the '*vacuum amplitude*' which plays a less central role in many-body theory, but is nevertheless

of considerable importance. The zero temperature vacuum amplitude can be used to calculate the ground state energy; its finite temperature edition yields the grand partition function from which all the equilibrium properties of the system may be determined.

How are the Green's functions calculated? There are two equivalent ways. The first is to solve the chain of differential equations they satisfy. That is, the single particle G obeys a differential equation involving the unknown two-particle G_2, G_2 obeys an equation involving G_3, ..., etc. This means that one has to grapple with an 'infinite hierarchy' of coupled non-linear differential equations. In practice, we usually cut the Gordian knot by making some sort of approximation for G_2 in the first equation, and simply dropping all the other equations in the chain. The differential equation method will not be discussed in this book—those interested will find some references in the *Further Reading* section at the end of chapter 14.

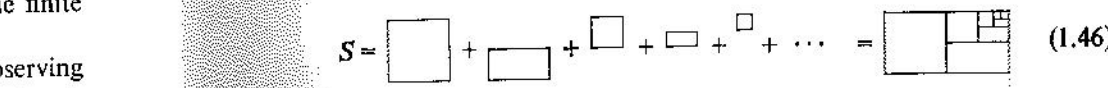
The other method is to expand the propagator (or vacuum amplitude) in an infinite perturbation series and evaluate the series approximately. The usual method of doing this, i.e., summing all terms up to second or third order, doesn't work for the propagator because the series converges too slowly. In fact, it often happens that all the terms in the series are infinite! Therefore, what is done instead is to sum over certain types of terms to infinite order, a procedure called '*partial*' or '*selective*' *summation*. This new '*infinite-order perturbation theory*' is radically different from the daily kind, and to carry it out requires a new technique. The technique is the method of *Feynman diagrams* which will be briefly described now.

1.5 Feynman diagrams and infinite-order perturbation theory

It is easy to find examples from everyday life showing how diagrams can be useful in summing infinite series. Take for instance the simple geometric series

$$S = 1+\tfrac{1}{2}+\tfrac{1}{4}+\tfrac{1}{8}+\tfrac{1}{16}+\ldots = 2. \tag{1.45}$$

If each term is represented by a rectangle of area equal to the value of the term, this can be translated into

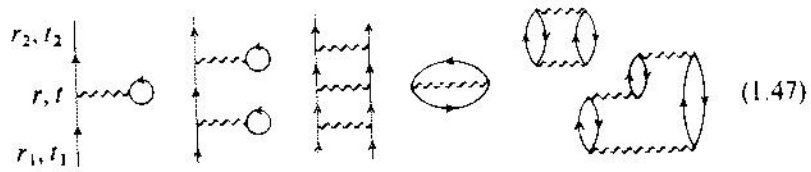


(1.46)

This 'diagrammatic' form has the advantage of revealing the structure of the series (1.45) in a 'physical' way which makes the manner of summing it obvious even to an average ten-year old.

Much the same philosophy underlies the Feynman diagram method. It was indicated in §1.1 how the single particle propagator could be expanded in a perturbation series in which each term consisted of complicated chains

of factors. Analogous to the above, where each number is represented by a rectangle, in the propagator case each factor was represented as a directed line or a wiggle. The same thing holds true for the other field theoretic quantities, and in (1.47) we have drawn, besides some single particle propagator 'bubbles', a few typical diagrams occurring in the perturbation expansions of the two-particle propagator (such as the 'ladder') and vacuum amplitude (such as the 'oyster' and 'rings'):



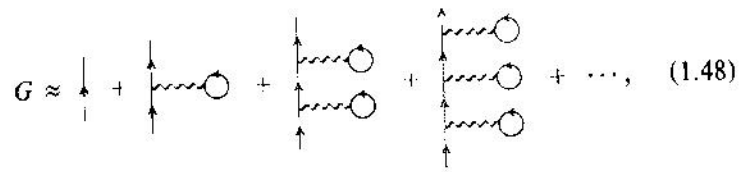
(1.47)

1st order 2nd order 3rd order 'Oyster' 'Rings'

'Bubble' diagrams 'Ladder'

Analogous to the way in which each rectangle revealed the 'structure' of the corresponding term in (1.45), each Feynman diagram reveals the structure of the perturbation term it represents. However, unlike (1.46), the size or shape of a Feynman diagram has no significance. Instead, like an electric circuit diagram, the important property of a Feynman diagram is how the various lines in it are connected to each other, i.e., the *topology* of the diagram.

It is this topology which is the key to infinite-order perturbation theory. When the perturbation series is written out in diagrammatic form, it is observed that the diagrams may be arranged in classes having similar topological structure—like, for example, all orders of 'bubble' diagrams or all 'rings'. We have done a bit of this grouping in (1.47). Then a remarkable fact emerges, i.e., that certain classes of diagrams (hence perturbation terms) may be easily summed to infinite order. For example, it is possible to sum over all orders of bubble diagrams, thus:



(1.48)

since the perturbation series terms corresponding to these diagrams turn out to constitute just a simple geometric series. This is just the partial summation mentioned at the end of the last section, and it gives us the new sort of approxi-

mation for G we talked about there. That is, the perturbation series for the various propagators and the vacuum amplitude may be evaluated approximately by summing to infinite order over certain types of diagrams. The partial summation method will be the basic technique employed throughout this book.

Feynman diagrams have other appealing features besides their utility as a calculational tool. One thing which was already pointed out in §1.1 is the fact that they show directly the physical meaning of the perturbation term they represent. Another thing is that they reveal at a glance the structure of very complicated approximations by showing which sets of diagrams have been summed over. In this way, they have introduced a new language into physics, and one often sees phrases like 'ladder approximation' or 'ring approximation' even in articles in which no diagrams appear. And finally, one cannot be immune to the Klee-like charm of the diagrams. Including in their ranks, in addition to the above, such characters as the 'necklace', the 'potato' and the 'tadpole', plus infinite numbers yet unnamed, they constitute what might indeed be called 'perturbation theory in comic-book form'.

In the next couple of chapters we are going to show how to evaluate the propagator diagrammatically for a classical system containing only one particle, and for its quantum analogue. Then we shall go on to describe how the same technique may be used to find the energies of the ground state and elementary excitations, in many-body systems.

Further reading

Ter Haar (1960).
Patterson (1964).
Pines (1963), chap. I.

Exercises

1.1 Prove the commutation rule (1.37a).
1.2 Verify (1.38).
1.3 Calculate: $b^\dagger_{q_3} \Psi_{3q_3}$.
1.4 Prove (1.40c) from (1.40*a*, *b*).
1.5 Calculate the following:

(*a*) $b^\dagger_{q_3} \Psi_{0_{q_1}, 3_{q_2}, 0_{q_3}, 0, 0, \ldots}$.

(*b*) $b_{q_3} \Psi_{0_{q_1}, 0_{q_2}, 0, 0 \ldots}$.

(*c*) $b^\dagger_{q_3} b_{q_2} b^\dagger_{q_1} \Psi_{1_{q_1}, 5_{q_2}, 0_{q_3}, 0, 0 \ldots}$.

1.6 How many phonons are in the atomic chain described by the wave function: $\Psi_{0_{q_1}, 0_{q_2}, 2_{q_3}, 0_{q_4}, 3_{q_5}, 0, 0 \ldots}$.
1.7 What is the total energy of the system in Ex. 1.6?