and the z component of this part of the field is

$$\sum_l \{z_l^2[(3F(\sqrt{\eta}r_l)/r_l^5) + (6/r_l^4)(\eta/\pi)^{1/2}\exp(-\eta r_l^2)$$

$$+ (4/r_l^2)(\eta^3/\pi)^{1/2}\exp(-\eta r_l^2)] - [(F(\sqrt{\eta}r_l)/r_l^3) \tag{9}$$

$$+ (2/r_l^2)(\eta/\pi)^{1/2}\exp(-\eta r_l^2)]\} \ .$$

The total E_z is given by the sum of (8) and (9). The effects of any number of lattices may be added.

APPENDIX C: QUANTIZATION OF ELASTIC WAVES: PHONONS

Phonons were introduced in Chapter 4 as quantized elastic waves. How do we quantize an elastic wave? As a simple model of phonons in a crystal, consider the vibrations of a linear lattice of particles connected by springs. We can quantize the particle motion exactly as for a harmonic oscillator or set of coupled harmonic oscillators. To do this we make a transformation from particle coordinates to phonon coordinates, also called wave coordinates because they represent a traveling wave.

Let N particles of mass M be connected by springs of force constant C and length a. To fix the boundary conditions, let the particles form a circular ring. We consider the transverse displacements of the particles out of the plane of the ring. The displacement of particle s is q_s and its momentum is p_s. The Hamiltonian of the system is

$$H = \sum_{s=1}^{n} \left\{ \frac{1}{2M} p_s^2 + \frac{1}{2} C(q_{s+1} - q_s)^2 \right\} \ . \tag{1}$$

The Hamiltonian of a harmonic oscillator is

$$H = \frac{1}{2M} p^2 + \frac{1}{2} Cx^2 \ , \tag{2}$$

and the energy eigenvalues are, where $n = 0, 1, 2, 3, \ldots,$

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega \ . \tag{3}$$

The eigenvalue problem is also exactly solvable for a chain with the different Hamiltonian (1).

To solve (1) we make a Fourier transformation from the coordinates p_s, q_s to the coordinates P_k, Q_k, which are known as phonon coordinates.

Phonon Coordinates

The transformation from the particle coordinates q_s to the phonon coordinates Q_k is used in all periodic lattice problems. We let

$$q_s = N^{-1/2} \sum_k Q_k \exp(iksa) \quad , \tag{4}$$

consistent with the inverse transformation

$$Q_k = N^{-1/2} \sum_s q_s \exp(-iksa) \quad . \tag{5}$$

Here the N values of the wavevector k allowed by the periodic boundary condition $q_s = q_{s+N}$ are given by:

$$k = 2\pi n/Na \; ; \; n = 0, \pm 1, \pm 2, \ldots, \pm\left(\frac{1}{2}N - 1\right), \frac{1}{2}N \quad . \tag{6}$$

We need the transformation from the particle momentum p_s to the momentum P_k that is canonically conjugate to the coordinate Q_k. The transformation is

$$p_s = N^{-1/2} \sum_k P_k \exp(-iksa); \quad P_k = N^{-1/2} \sum_s p_s \exp(iksa) \quad . \tag{7}$$

This is not quite what one would obtain by the naive substitution of p for q and P for Q in (4) and (5), because k and $-k$ have been interchanged between (4) and (7).

We verify that our choice of P_k and Q_k satisfies the quantum commutation relation for canonical variables. We form the commutator

$$\begin{aligned} [Q_k, P_{k'}] &= N^{-1}\left[\sum_r q_r \exp(-ikra), \sum_s p_s \exp(ik'sa)\right] \\ &= N^{-1} \sum_r \sum_s [q_r, p_s] \exp[-i(kr - k's)a] \quad . \end{aligned} \tag{8}$$

Because the operators q, p are conjugate, they satisfy the commutation relation

$$[q_r, p_s] = i\hbar\delta(r,s) \quad , \tag{9}$$

where $\delta(r,s)$ is the Kronecker delta symbol.

Thus (8) becomes

$$[Q_k, P_{k'}] = N^{-1}\, i\hbar \sum_r \exp[-i(k - k')ra] = i\hbar\delta(k, k') \quad , \tag{10}$$

so that Q_k, P_k also are conjugate variables. Here we have evaluated the summation as

$$\begin{aligned} \sum_r \exp[-i(k - k')ra] &= \sum_r \exp[-i2\pi(n - n')r/N] \\ &= N\delta(n, n') = N\delta(k, k') \quad , \end{aligned} \tag{11}$$

where we have used (6) and a standard result for the finite series in (11).

We carry out the transformations (7) and (4) on the hamiltonian (1), and make use of the summation (11):

$$\begin{aligned}\sum_s p_s^2 &= N^{-1} \sum_s \sum_k \sum_{k'} P_k P_{k'} \exp[-i(k+k')sa] \\ &= \sum_k \sum_{k'} P_k P_{k'} \delta(-k, k') = \sum_k P_k P_{-k} \ ;\end{aligned} \tag{12}$$

$$\begin{aligned}\sum_s (q_{s+1} - q_s)^2 = N^{-1} \sum_s \sum_k \sum_{k'} Q_k Q_{k'} \exp(iksa)[\exp(ika) - 1] \\ \times \exp(ik'sa)[\exp(ik'a) - 1] = 2 \sum_k Q_k Q_{-k}(1 - \cos ka) \ .\end{aligned} \tag{13}$$

Thus the hamiltonian (1) becomes, in phonon coordinates,

$$H = \sum_k \left\{ \frac{1}{2M} P_k P_{-k} + C Q_k Q_{-k} (1 - \cos ka) \right\} \ . \tag{14}$$

If we introduce the symbol ω_k defined by

$$\omega_k \equiv (2C/M)^{1/2} (1 - \cos ka)^{1/2} \ , \tag{15}$$

we have the phonon hamiltonian in the form

$$H = \sum_k \left\{ \frac{1}{2M} P_k P_{-k} + \frac{1}{2} M \omega_k^2 \, Q_k Q_{-k} \right\} \ . \tag{16}$$

The equation of motion of the phonon coordinate operator Q_k is found by the standard prescription of quantum mechanics:

$$i\hbar \dot{Q}_k = [Q_k, H] = i\hbar P_{-k}/M \ , \tag{17}$$

with H given by (14). Further, using the commutator (17),

$$i\hbar \ddot{Q}_k = [\dot{Q}_k, H] = M^{-1}[P_{-k}, H] = i\hbar \omega_k^2 Q_k \ , \tag{18}$$

so that

$$\ddot{Q}_k + \omega_k^2 Q_k = 0 \ . \tag{19}$$

This is the equation of motion of a harmonic oscillator with the frequency ω_k.

The energy eigenvalues of a quantum harmonic oscillator are

$$\epsilon_k = \left(n_k + \frac{1}{2} \right) \hbar \omega_k \ , \tag{20}$$

where the quantum number $n_k = 0, 1, 2, \ldots$. The energy of the entire system of all phonons is

$$U = \sum_k \left(n_k + \frac{1}{2} \right) \hbar \omega_k \ . \tag{21}$$

This result demonstrates the quantization of the energy of elastic waves on a line.

Creation and Annihilation Operators

It is helpful in advanced work to transform the phonon hamiltonian (16) into the form of a set of harmonic oscillators:

$$H = \sum_k \hbar\omega_k \left(a_k^+ a_k + \frac{1}{2} \right) . \tag{22}$$

Here a_k^+, a_k are harmonic oscillator operators, also called creation and destruction operators or boson operators. The transformation is derived below.

The boson creation operator a^+ which "creates a phonon" is defined by the property

$$a^+|n\rangle = (n+1)^{1/2}|n+1\rangle , \tag{23}$$

when acting on a harmonic oscillator state of quantum number n, and the boson annihilation operator a which "destroys a phonon" is defined by the property

$$a|n\rangle = n^{1/2}|n-1\rangle . \tag{24}$$

It follows that

$$a^+a|n\rangle = a^+n^{1/2}|n-1\rangle = n|n\rangle , \tag{25}$$

so that $|n\rangle$ is an eigenstate of the operator a^+a with the integral eigenvalue n, called the quantum number or occupancy of the oscillator. When the phonon mode k is in the eigenstate labeled by n_k, we may say that there are n_k phonons in the mode. The eigenvalues of (22) are $U = \Sigma\,(n_k + \frac{1}{2})\hbar\omega_k$, in agreement with (21).

Because

$$aa^+|n\rangle = a(n+1)^{1/2}|n+1\rangle = (n+1)|n\rangle , \tag{26}$$

the commutator of the boson wave operators a_k^+ and a_k satisfies the relation

$$[a, a^+] \equiv aa^+ - a^+a = 1 . \tag{27}$$

We still have to prove that the hamiltonian (16) can be expressed as (19) in terms of the phonon operators a_k^+, a_k. This can be done by the transformation

$$a_k^+ = (2\hbar)^{-1/2}[(M\omega_k)^{1/2}Q_{-k} - i(M\omega_k)^{-1/2}P_k] ; \tag{28}$$

$$a_k = (2\hbar)^{-1/2}[(M\omega_k)^{1/2}Q_k + i(M\omega_k)^{-1/2}P_{-k}] . \tag{29}$$

The inverse relations are

$$Q_k = (\hbar/2M\omega_k)^{1/2}(a_k + a_{-k}^+) ; \tag{30}$$

$$P_k = i(\hbar M\omega_k/2)^{1/2}(a_k^+ - a_{-k}) . \tag{31}$$

By (4), (5), and (29) the particle position operator becomes

$$q_s = \sum_k (\hbar/2NM\omega_k)^{1/2}[a_k \exp(iks) + a_k^+ \exp(-iks)] . \tag{32}$$

This equation relates the particle displacement operator to the phonon creation and annihilation operators.

To obtain (29) from (28), we use the properties

$$Q_{-k}^{+} = Q_k \ ; \qquad P_k^{+} = P_{-k} \tag{33}$$

which follow from (5) and (7) by use of the quantum mechanical requirement that q_s and p_s be hermitian operators:

$$q_s = q_s^{+} \ ; \qquad p_s = p_s^{+} \ . \tag{34}$$

Then (28) follows from the transformations (4), (5), and (7). We verify that the commutation relation (33) is satisfied by the operators defined by (28) and (29):

$$[a_k, a_k^{+}] = (2\hbar)^{-1}(M\omega_k[Q_k, Q_{-k}] - i[Q_k,P_k] + i[P_{-k},Q_{-k}] + [P_{-k},P_k]/M\omega_k) \ . \tag{35}$$

By use of $[Q_k,P_{k'}] = i\hbar\delta(k,k')$ from (10) we have

$$[a_k, a_{k'}^{+}] = \delta(k,k') \ . \tag{36}$$

It remains to show that the versions of (16) and (22) of the phonon hamiltonian are identical. We note that $\omega_k = \omega_{-k}$ from (15), and we form

$$\hbar\omega_k(a_k^{+}a_k + a_{-k}^{+}a_{-k}) = \frac{1}{2M}(P_kP_{-k} + P_{-k}P_k) + \frac{1}{2}M\omega_k^2(Q_kQ_{-k} + Q_{-k}Q_k) \ .$$

This exhibits the equivalence of the two expressions (14) and (22) for H. We identify $\omega_k = (2C/M)^{1/2}(1 - \cos ka)^{1/2}$ in (15) with the classical frequency of the oscillator mode of wavevector k.

APPENDIX D: FERMI-DIRAC DISTRIBUTION FUNCTION[1]

The Fermi-Dirac distribution function[1] may be derived in several steps by use of a modern approach to statistical mechanics. We outline the argument here. The notation is such that conventional entropy S is related to the fundamental entropy σ by $S = k_B\sigma$, and the Kelvin temperature T is related to the fundamental temperature τ by $\tau = k_BT$, where k_B is the Boltzmann constant with the value 1.38066×10^{-23} J K.

The leading quantities are the entropy, the temperature, the Boltzmann factor, the chemical potential, the Gibbs factor, and the distribution functions. The

[1]This appendix follows closely the introduction to C. Kittel and H. Kroemer, *Thermal Physics*, 2nd ed., Freeman, 1980.