Contents

1 Introduction

1.1 Goals in this course

These are my hopes for the course. Let me know if you feel the course is not fulfilling them for you. Be free with your criticism & comments! Thanks.

- Teach basics of collective phenomena in electron systems
- Make frequent reference to real experiment and data
- Use 2nd quantized notation without field-theoretical techniques
- Get all students reading basic CM journals
- Allow students to practice presenting a talk
- Allow students to bootstrap own research if possible

1.2 Statistical mechanics of free Fermi gas

1.2.1 $T = 0$ Fermi sea

Start with simple model of electrons in metal, neglecting $e^- - e^-$ interactions. Hamiltonian is

$$\hat{H} = -\sum_j \frac{\hbar^2 \nabla_j^2}{2m}, \quad j = 1, \ldots N \text{ particles} \tag{1}$$

Eigenstates of each $-(\hbar^2\nabla^2/2m)$ are just plane waves $e^{i\mathbf{k}\cdot\mathbf{r}}$ labelled by $\mathbf{k}$, with $k_i = 2\pi n_i/L_i$ in box with periodic B.C. Recall electrons are fermions, which means we can only put one in each single-particle state. Including spin we can put two particles ($\uparrow\downarrow$) in each $\mathbf{k}$-state. At zero temperature the ground state of N-electron system is then formed by adding particles until we run out of electrons. Energy is $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$, so start with two in lowest state $k = 0$, then add two to next states, with k_x or k_y

or $k_z = 2\pi/L$, etc. as shown. Energy of highest particle called "Fermi energy" ε_F, magnitude of corresponding wave vector called k_F. Typical Fermi energy for metal $\varepsilon_F \simeq 1eV \simeq 10^4 K$. At $T = 0$ only states with $k < k_F$ occupied (Fermi "sea" or Fermi sphere), so we can write density of electrons as 2*# occupied states/Volume (2 is for spin):

$$n = \frac{2}{L^3}\sum_{k=0}^{k_F} \simeq 2\int_{k<k_F} \frac{d^3k}{(2\pi)^3} = \frac{1}{\pi^2}\int_0^{k_F} k^2 dk = \frac{k_F^3}{3\pi^2} \tag{2}$$

so

$$k_F = (3\pi^2 n)^{1/3} \quad \text{or} \quad \varepsilon_F = \frac{\hbar^2(3\pi^2 n)^{2/3}}{2m} \tag{3}$$

in other words, nothing but the density of electrons controls the Fermi energy.

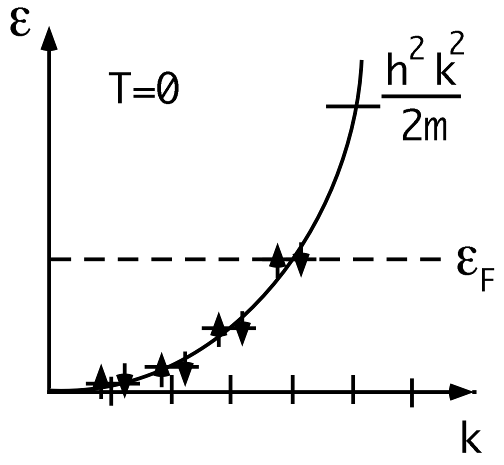

Figure 1: States of Fermi gas with parabolic spectrum, $\varepsilon = k^2/2m$.

The total ground state energy of the Fermi gas must be of order ε_F, since there is no other energy in the problem. If we simply add up the energies of all particles in states up to Fermi level get

$$\frac{E}{L^3} = \frac{1}{\pi^2}\int_0^{k_F} dk\; k^2 \left(\frac{\hbar^2 k^2}{2m}\right) = \frac{\hbar^2 k_F^5}{10\pi^2 m} \tag{4}$$

and the ground state energy per particle ($N = nL^3$ is the total number) is

$$\boxed{\frac{E}{N} = \frac{3}{5}\varepsilon_F}. \tag{5}$$

1.2.2 $T > 0$ Free energy.

Reminder: partition function for free fermions in grnd conical ensemble is

$$
\begin{aligned}
Z &= \text{Tr } e^{-\beta(\hat{H}-\mu\hat{N})} && (6)\\
&= \sum_{n_1,n_2...n_{k_\infty}} \langle n_1, n_2...n_\infty | e^{-\beta(\hat{H}-\mu\hat{N})} | n_1, n_2...n_\infty \rangle && (7)\\
&= \sum_{n_1,n_2...n_\infty} \langle n_1, n_2...n_\infty | e^{-\beta(\Sigma_i[\varepsilon_i n_i - \mu n_i])} | n_1, n_2...n_\infty \rangle && (8)
\end{aligned}
$$

where i labels single-fermion state, e.g. $i = \mathbf{k}, \sigma$, and n_i runs from 0 to 1 for fermions. Since many-fermion state in occ. no. representation is simple product: $|n_1, n_2...n_\infty\rangle = |n_1\rangle|n_2\rangle...|n_\infty\rangle$, can factorize:

$$Z = \left(\sum_{n_1} e^{-\beta[\varepsilon_1 n_1 - \mu n_1]}\right) \cdots \left(\sum_{n_\infty} e^{-\beta[\varepsilon_\infty n_\infty - \mu n_\infty]}\right), \tag{9}$$

so

$$\boxed{Z = \Pi_{i=0}^{\infty} \left(1 + e^{-\beta(\varepsilon_i - \mu)}\right)} \tag{10}$$

Since the free energy (grand canonical potential) is $\Omega = -k_B T \ \log Z$, we get

$$\boxed{\Omega = -k_B T \, \Sigma_{i=1}^{\infty} \log\left(1 + e^{-\beta(\varepsilon_i - \mu)}\right)} \tag{11}$$

1.2.3 Avg. fermion number.

We may want to take statistical averages of quantum operators, for which we need the *statistical operator* $\hat{\rho} = Z^{-1} e^{-\beta(\hat{H}-\mu\hat{N})}$. Then any operator $\hat{\mathcal{O}}$ has an expectation value $\langle\hat{\mathcal{O}}\rangle = \text{Tr}(\hat{\rho}\hat{\mathcal{O}})$. For example, avg. no. of particles

$$
\begin{aligned}
\langle \hat{N} \rangle &= \text{Tr}(\rho \hat{N}) && (12)\\
&= \frac{\text{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})}\hat{N})}{\text{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})})} && (13)
\end{aligned}
$$

Now note this is related to derivative of Ω wrt chem. potential μ:

$$\begin{aligned}\frac{\partial\Omega}{\partial\mu} &= -k_BT\frac{\partial\log Z}{\partial\mu} = \frac{-k_BT}{Z}\frac{\partial Z}{\partial\mu} &(14)\\ &= \frac{-1}{Z}\mathrm{Tr}(\rho\hat{N}) = -\langle\hat{N}\rangle &(15)\end{aligned}$$

and using Eq. 11, we see

$$\langle\hat{N}\rangle = \sum_{i=1}^{\infty}\frac{1}{1+e^{\beta(\varepsilon_i-\mu)}} \equiv \sum_{i=1}^{\infty} n_i^0 \qquad (16)$$

where n_0^i is the avg. number of fermions in a single-particle state i in equilibrium at temperature T. If we recall i was a shorthand for $\mathbf{k},\sigma$, but $\varepsilon_{\mathbf{k}}$ doesn't depend on σ, we get Fermi-Dirac distribution function

$$\boxed{n^0_{\mathbf{k}\sigma} = \frac{1}{1+e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}}} \qquad (17)$$

1.2.4 Fermi gas at low T.

Since the Fermi energy of metals is so high ($\sim 10^4K$), it's important to understand the limit $k_BT \ll \varepsilon_F$, where the Fermi gas is nearly degenerate, and make sure the classical limit $k_BT \gg \varepsilon_F$ comes out right too. Let's calculate, for example, the entropy and specific heat, which can be obtained from the thermodynamic potential Ω via the general thermodynamic relations

$$S = -\left(\frac{\partial\Omega}{\partial T}\right)_{V,\mu}; \quad C_V = T\left(\frac{\partial S}{\partial T}\right)_{V,\mu} \qquad (18)$$

From (11) and (16), and including spin, we have

$$\begin{aligned}\Omega &= -2k_BT\sum_{\mathbf{k}}\log\left(1+e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right)\\ &= 2k_BTL^3\int d\varepsilon N(\varepsilon)\log\left(1+e^{-\beta(\varepsilon-\mu)}\right)\\ &\Rightarrow\\ c_V &\equiv \frac{C_V}{L^3} = 2\,\frac{1}{k_BT}\int_0^\infty d\varepsilon N(\varepsilon)\left(\frac{-\partial f}{\partial\varepsilon}\right)(\varepsilon-\mu)^2\\ &= 2\,\frac{1}{k_BT}\int_{-\mu}^{\infty}d\xi\; N(\xi)\;\left(\frac{-\partial f}{\partial\xi}\right)\xi^2 \qquad (19)\end{aligned}$$

where I introduced the *density of* $\mathbf{k}$*-states* for one spin $N(\varepsilon) = L^{-3}\sum_{\mathbf{k}}\delta(\varepsilon - \varepsilon_{\mathbf{k}})$. The Fermi function is $f(\varepsilon) = 1/(1+\exp\beta(\varepsilon-\mu))$, & I defined shifted energy variable $\xi = \varepsilon - \mu$. In general, the degenerate limit is characterized by $\mathbf{k}$ sums which decay rapidly for energies far from the Fermi surface, so the game is to assume the density of states varies slowly on a scale of the thermal energy, and replace $N(\varepsilon)$ by $N(\varepsilon_F) \equiv N_0$. This type of Sommerfeld expansion[1] assumes the density of states is a smoothly varying fctn., i.e. the thermodynamic limit $V \to \infty$ has been taken (otherwise $N(\varepsilon)$ is too spiky!). For a parabolic band, $\varepsilon_{\mathbf{k}} = \hbar^2k^2/(2m)$ in 3D, the delta-fctn. can be evaluated to find[2]

$$\boxed{N(\varepsilon) = \frac{3}{2}\frac{n}{\varepsilon_F}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \theta(\varepsilon).} \tag{22}$$

This can be expanded around the Fermi level:[3]

$$N(\xi) = N(0) + N'(0)\xi + \frac{1}{2}N''(0)\xi^2 + \dots \tag{24}$$

(In a horrible misuse of notation, $N(0)$, $N(\varepsilon_F)$, and N_0 all mean the

---

[1]If you are integrating a smooth function of ε multiplied by the Fermi function derivative $-\partial f/\partial\varepsilon$, the derivative restricts the range of integration to a region of width k_BT around the Fermi surface. If you are integrating something times $f(\varepsilon)$ itself, it's convenient to do an integration by parts. The result is (see e.g. Ashcroft & Mermin appendix C)

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon)f(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) + \sum_{n=1}^{\infty} a_n(k_BT)^{2n}\frac{d^{2n-1}}{d\varepsilon^{2n-1}}H(\varepsilon)|_{\varepsilon=\mu} \tag{20}$$

where $a_n = \left(2 - 1/2^{2(n-1)}\right)\zeta(2n)$ (ζ is Riemann ζ fctn., $\zeta(2) = \pi^2/6$, $\zeta(4) = \pi^4/90$, etc.).

[2]Here's one way to get this:

$$N(\varepsilon) = L^{-3}\sum_{\mathbf{k}}\delta(\varepsilon - \varepsilon_{\mathbf{k}}) \to \int \frac{d^3k}{(2\pi)^3}|\frac{d\varepsilon}{dk}|^{-1}\delta(k - \frac{\sqrt{2m\varepsilon}}{\hbar}) = \int \frac{k^2dk}{2\pi^2}\left(\frac{m}{\hbar^2k}\right)\delta(k - \frac{\sqrt{2m\varepsilon}}{\hbar}) = \frac{3}{2}\frac{n}{\varepsilon_F}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \tag{21}$$

[3]When does the validity of the expansion break down? When the approximation that the density of states is a smooth function does, i.e. when the thermal energy k_BT is comparable to the splitting between states at the Fermi level,

$$\delta\varepsilon_k|_{\varepsilon_F} \simeq \frac{\hbar^2k_F\delta k}{m} \simeq \varepsilon_F\frac{\delta k}{k_F} \simeq \varepsilon_F\frac{a}{L}, \tag{23}$$

where a is the lattice spacing and L is the box size. At $T = 1K$, requiring $k_BT \sim \delta\varepsilon$, and taking $\varepsilon_F/k_B \simeq 10^4K$ says that systems (boxes) of size less than $1\mu m$ will "show mesoscopic" effects, i.e. results from Sommerfeld-type expansions are no longer valid.

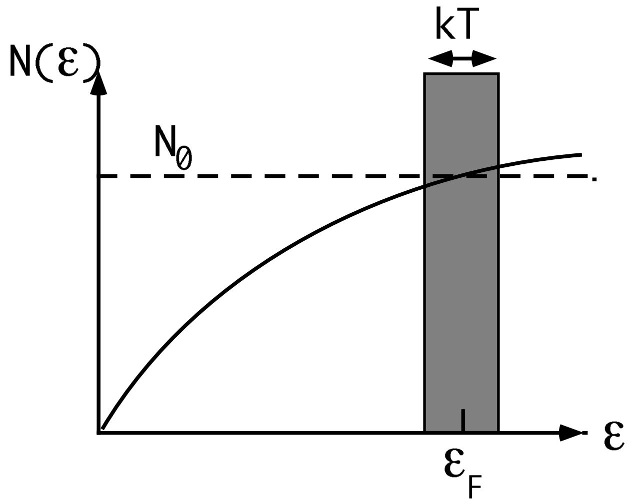

Figure 2: Density of states for parabolic spectrum, $\varepsilon = k^2/2m$

density of states at the Fermi level). The leading order term in the low-T specific heat is therefore found directly by scaling out the factors of T in Eq. (19):

$$c_V \simeq 2k_B \frac{1}{T} N_0 \int_{-\infty}^{\infty} d\xi \left(\frac{-\partial f}{\partial \xi}\right) \xi^2 \;=\; 2k_B T \underbrace{\int_{-\infty}^{\infty} dx \left(\frac{-\partial f}{\partial x}\right) x^2}_{\pi^2/3} \quad (25)$$

So

$$c_V \simeq \frac{2\pi^2}{3} N_0 k_B T + \mathcal{O}(T^3). \quad (26)$$

This is the famous linear in temperature specific heat of a free Fermi gas. [4]

[4]Note in (26), I extended the lower limit $-\mu$ of the integral in Eq. (19) to $-\infty$ since it can be shown that the chemical potential is very close to ε_F at low T. Since we are interested in temperatures $k_B T \ll \varepsilon_F$, and the range in the integral is only several $k_B T$ at most, this introduces neglible error.

Why:

At T=0, the Fermi function $n^0_{\mathbf{k}} \to$ step function $\theta(\mu - \varepsilon_{\mathbf{k}})$, so we know $\mu(T=0)$ must just be the Fermi energy $\varepsilon_F = \hbar^2(3\pi^2 n)^{2/3}/2m$.

$$\begin{aligned} n &= \frac{N}{L^3} = 2L^{-3}\sum_{\mathbf{k}}^{\infty} n^0_{\mathbf{k}} \\ &= 2\int d\varepsilon N(\varepsilon) f(\varepsilon) \\ &\simeq \int_{-\infty}^{\mu} d\varepsilon N(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 N'(\varepsilon)|_{\varepsilon=\mu} \end{aligned}$$

(continued on next page)

1.2.5 Classical limit.

I won't calculate the classical limit. All the standard results for a Boltzman statistics gas, e.g. $c_V(T \gg \varepsilon_F) = (3/2)Nk_B$ follow immediately from noticing that the Fermi function reduces to the Boltzman distribution,

$$f(\varepsilon) \to e^{-\beta(\varepsilon-\mu)}, \qquad T \to \infty. \tag{27}$$

(You will need to convince yourself that the classical result $\mu/(k_BT) \to -\infty$ is recovered to make this argument.)

1.3 Second quantization

The idea behind the term "second quantization" arises from the fact that in the early days of quantum mechanics, forces between particles were treated classically. Momentum, position and other observables were represented by operators which do not in general commute with each other. Particle *number* is assumed to be quantized as one of the tenets of the theory, e.g. Einstein's early work on blackbody radiation.

At some point it was also realized that forces between particles are also quantized because they are *mediated* by the exchange of other particles. In Schrödinger's treatment of the H-atom the force is just the classical static Coulomb force, but a more complete treatment includes the interaction of the H-atom and its constituents with the radiation field, which must itself be quantized ("photons"). This quantization of the fields mediating the interactions between matter particles was referred to as "second" quantization. In the meantime, a second-quantized description has been developed in which *both* "matter fields" and "force fields" are described

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$$\simeq \underbrace{\int_{-\infty}^{\varepsilon_F} d\varepsilon N(\varepsilon)}_{n} + (\mu - \varepsilon_F)N(\varepsilon_F) + \frac{\pi^2}{6}(k_BT)^2 N'(\varepsilon)|_{\varepsilon=\mu}$$

$$\Rightarrow \qquad \boxed{\mu \simeq \varepsilon_F - \frac{\pi^2}{6}(k_BT)^2\frac{N'(\varepsilon_F)}{N(\varepsilon_F)}}$$

Since N'/N is typically of order $1/\varepsilon_F^2$, corrections are small.

by second-quantized field operators. In fact, modern condensed matter physics usually does go backwards and describe particles interacting via classical Coulomb forces again,[5] but these particles are described by field operators. Once the calculational rules are absorbed, calculating with the 2nd-quantized formalism is easier for most people than doing 1st-quantized calculations. They must, of course, yield the same answer, as they are rigorously equivalent. I will not prove this equivalence in class, as it is exceedingly tedious, but merely motivate it for you below. I urge you to read the proof once for your own edification, however.[6]

1.3.1 Symmetry of many-particle wavefunctions

Quantum mechanics allows for the possibility of indistinguishable particles, and nature seems to have taken advantage of this as a way to construct things. No electron can be distinguished from another electron, except by saying where it is, what quantum state it is in, etc. Internal quantum-mechanical consistency requires that when we write down a many-identical-particle state, we make that state noncommittal as to which particle is in which single-particle state. For example, we *say* that we have electron 1 and electron 2, and we put them in states a and b respectively, but exchange symmetry requires (since electrons are fermions) that a satisfactory wave-function has the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = A[(\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) - \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)]. \tag{28}$$

If we have N particles, the wavefunctions must be either symmetric or antisymmetric under exchange:[7]

$$\Psi^B(\mathbf{r}_1 \ldots \mathbf{r}_i \ldots \mathbf{r}_j \ldots \mathbf{r}_N) = \Psi^B(\mathbf{r}_1 \ldots \mathbf{r}_j \ldots \mathbf{r}_i \ldots \mathbf{r}_N) \quad \text{Bosons} \tag{29}$$

$$\Psi^F(\mathbf{r}_1 \ldots \mathbf{r}_i \ldots \mathbf{r}_j \ldots \mathbf{r}_N) = -\Psi^F(\mathbf{r}_1 \ldots \mathbf{r}_j \ldots \mathbf{r}_i \ldots \mathbf{r}_N) \quad \text{Fermions} \tag{30}$$

[5] Q: when does this approximation break down?

[6] See, e.g. Fetter & Wallecka, *Quantum Theory of Many-Particle Systems*

[7] Recently, a generalization of Bose & Fermi statistics to particles called anyons has been intensely discussed. Under exchange an anyon wavefunction behaves as $\Psi^A(\mathbf{r}_1 \ldots \mathbf{r}_i \ldots \mathbf{r}_j \ldots \mathbf{r}_N) = e^{i\theta}\Psi^A(\mathbf{r}_1 \ldots \mathbf{r}_j \ldots \mathbf{r}_i \ldots \mathbf{r}_N)$ for some $0 \le \theta \le 2\pi$.

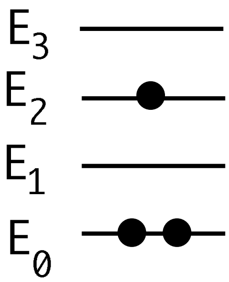
Given a set of single-particle wave functions $\phi_{E_i}(\mathbf{r})$, where E_i is a quantum number, e.g. energy, we can easily construct wave fctns. which satisfy statistics, e.g.

$$\Psi^{\,B}_{\,F\; n_1 \dots n_\infty}(\mathbf{r}_1, \dots \mathbf{r}_N) = \left(\frac{n_1! n_2! \cdots n_\infty!}{N!}\right)^{1/2} \sum_{\mathcal{P} \in \{E_1, E_2 \dots E_N\}} (\pm 1)^{\,\mathrm{sgn}\mathcal{P}}\, \mathcal{P}\, \Pi_{i=1}^{N}\, \phi_{E_i}(\mathbf{r}_i) \quad (31)$$

Remarks on Eq. (31):

- sum all permutations of the E_i's in product $\phi_{E_1}(\mathbf{r}_1)\phi_{E_2}(\mathbf{r}_2)\dots\phi_{E_N}(\mathbf{r}_N)$.[8]
- # distinct E_i's occuring may be less than N, some missing because of multiple occupation in boson case. Example:

particles



$$\Psi^B_{20100\dots0}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) =$$
$$= \frac{1}{\sqrt{3}}\{\phi_{E_1}(\mathbf{r}_1)\phi_{E_1}(\mathbf{r}_2)\phi_{E_3}(\mathbf{r}_3) +$$
$$+\phi_{E_3}(\mathbf{r}_1)\phi_{E_1}(\mathbf{r}_2)\phi_{E_1}(\mathbf{r}_3) +$$
$$+\phi_{E_1}(\mathbf{r}_1)\phi_{E_3}(\mathbf{r}_2)\phi_{E_1}(\mathbf{r}_3)\}$$

Fig. 2. Possible state of 3 noninteracting Bose

- Completely antisymmetric Fermionic wavefunction called Slater determinant:

$$\Psi_{n_1 \dots n_\infty}(\mathbf{r}_1, \dots \mathbf{r}_N) = \left(\frac{1}{N!}\right)^{1/2} \begin{vmatrix} \phi_{E_{min}}(\mathbf{r}_1) & \dots & \phi_{E_{max}}(\mathbf{r}_1) \\ \vdots & & \vdots \\ \phi_{E_{min}}(\mathbf{r}_N) & \dots & \phi_{E_{max}}(\mathbf{r}_N) \end{vmatrix} \quad (32)$$

  where there are N eigenvalues which occur between E_{min} and E_{max}, inclusive, corresponding to N occupied states.

[8]You might think the physical thing to do would be to sum all permutations of the particle labels. This is correct, but actually makes things harder since one can double count if particles are degenerate (see example of 3 bosons below.) The normalization factor is chosen with the sum over all permutation of the E_i's in mind.

1.3.2 Field operators

2nd quantization is alternative way of describing many body states. We describe a particle by a *field operator*

$$\hat{\psi}(\mathbf{r}) = \sum_i a_i \phi_{E_i}(\mathbf{r}) \tag{33}$$

where i runs over the quantum numbers associated with the set of eigenstates ϕ, a_i is a "coefficient" which is an operator (I'm going to neglect the hats ($\hat{}$) which normally denote an operator for the a's and $a^\dagger$'s), and ϕ_{E_i} is a "1st-quantized" wavefunction, i.e. a normal Schrödinger wavefunction of the type we have used up to now, such that (for example) $H\phi_{E_i} = E_i\phi_{E_i}$. Now we *impose* commutation relations

$$\begin{aligned} \left[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right]_\pm &= \delta(\mathbf{r} - \mathbf{r}') && (34) \\ \left[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')\right]_\pm &= \left[\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right]_\pm = 0, && (35) \end{aligned}$$

which implies

$$[a_i, a_j^\dagger]_\pm = \delta_{ij} \quad ; \quad [a_i, a_j]_\pm = [a_i^\dagger, a_j^\dagger]_\pm = 0. \tag{36}$$

The upper sign is for fermions and the lower for bosons in Eqs. (35) and (36).

Now construct many-body states from vacuum (no particles) $|0\rangle$. a called *annihilation* operator, $a^\dagger$ *creation operator* (see below).

Examples & comments (*all properties follow from commutation relations*):

<u>Bosons</u>:

- one particle in state i: $a_i^\dagger|0\rangle \equiv |1\rangle_i$
- annihilate vacuum $a_i|0\rangle = 0$
- (Bosons)[9] $a_i^\dagger a_i^\dagger|0\rangle \equiv |2\rangle_i$

[9] Analogous state for fermions is zero, by commutation relations-check!

- (Bosons) two in i and one in j: $a_i^\dagger a_i^\dagger a_j^\dagger|0\rangle \equiv |2\rangle_i|1\rangle_j$
- $a_i^\dagger a_i \equiv \hat{n}_i$ is *number operator* for state i.

Proof: (bosons)

$$\begin{aligned}(a_i^\dagger a_i)|n\rangle_i &= (a_i^\dagger a_i)(a_i^\dagger)^n|0\rangle \\ &= a_i^\dagger(1 + a_i^\dagger a_i)(a_i^\dagger)^{n-1}|0\rangle = |n\rangle_i + (a_i^\dagger)^2 a_i(a_i^\dagger)^{n-1}|0\rangle \\ &= 2|n\rangle_i + (a_i^\dagger)^3 a_i(a_i^\dagger)^{n-2}|0\rangle \ldots = n|n\rangle_i\end{aligned}$$

Similarly show (bosons):[10]

- $\boxed{a_i^\dagger|n\rangle_i = (n+1)^{1/2}|n+1\rangle_i}$
- $\boxed{a_i|n\rangle_i = n^{1/2}|n-1\rangle_i}$
- many-particle state

$$\left(\frac{1}{n_1!n_2!\ldots n_\infty!}\right)^{1/2}(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots|0\rangle \equiv |n_1, n_2\ldots n_\infty\rangle \qquad (37)$$

$\star$ occupation numbers specify state completely, exchange symmetry included due to commutation relations! (normalization factor left for problem set)

Fermions

- Anticommutation relations complicate matters, in particular note

$$a^2 = (a^\dagger)^2 = 0 \quad \Rightarrow n_i = \begin{matrix}1\\0\end{matrix} \quad \text{(Pauli principle)} \qquad (38)$$

[10]By now it should be clear that the algebra for the bosonic case is identical to the algebra of simple harmonic oscillator *ladder operators*.

- so

$$\boxed{\begin{array}{cc} a^\dagger|0\rangle = |1\rangle & a|1\rangle = |0\rangle \\ a^\dagger|1\rangle = 0 & a|0\rangle = 0 \end{array}} \tag{39}$$

- many-particle state

$$(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots|0\rangle \equiv |n_1, n_2 \ldots n_\infty\rangle \tag{40}$$

$\star$ note normalization factor is 1 here.

- action of creation & annilation operators (suppose $n_s = 1$):

$$\begin{aligned} a_s|\ldots n_s \ldots\rangle &= (-1)^{n_1+n_2+\ldots n_{s-1}}(a_1^\dagger)^{n_1}\cdots a_s a_s^\dagger \cdots (a_\infty^\dagger)^{n_\infty}|0\rangle \\ &= (-1)^{n_1+n_2+\ldots n_{s-1}}(a_1^\dagger)^{n_1}\cdots(1-\underbrace{a_s^\dagger a_s}_{=0})\cdots(a_\infty^\dagger)^{n_\infty}|0\rangle \\ &= (-1)^{n_1+n_2+\ldots n_{s-1}}|\ldots n_s - 1 \ldots\rangle \end{aligned}$$

also

$$a_s|\ldots 0 \ldots\rangle = 0 \tag{41}$$

and similarly

$$a_s^\dagger|\ldots n_s \ldots\rangle = \begin{cases} (-1)^{n_1+n_2+\ldots n_{s-1}}|\ldots n_s + 1 \ldots\rangle & n_s = 0 \\ 0 & n_s = 1 \end{cases} \tag{42}$$

1.3.3 2nd-quantized Hamiltonian

$\star$ <u>Point:</u> Now "it can be shown"[11] that state vector

$$|\Psi(t)\rangle = \sum_{n_1,n_2\ldots n_\infty} f(n_1, n_2 \ldots n_\infty, t)|n_1, n_2 \ldots n_\infty\rangle \tag{43}$$

[11] Normally I hate skipping proofs. However, as mentioned above, this one is so tedious I just can't resist. The bravehearted can look, e.g. in chapter 1 of Fetter and Wallecka.

satisfies the Schrödinger equation (our old friend)

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \tag{44}$$

if we take the "2nd-quantized" form of $\hat{H}$

$$\begin{aligned}
\hat{H} &= \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j + \frac{1}{2}\sum_{ijk\ell} a_i^\dagger a_j^\dagger \langle ij|V|k\ell\rangle a_\ell a_k & (45)\\
&= \int d^3r \hat{\psi}^\dagger(\mathbf{r}) T(\mathbf{r}, \nabla_\mathbf{r}) \hat{\psi}(\mathbf{r}) & (46)\\
&\quad + \frac{1}{2}\int\int d^3r\, d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) & (47)
\end{aligned}$$

where the 1st quantized Hamiltonian was $H = T + V$.

<u>Translationally invariant system</u>

It may be more satisfying if we can at least verify that this formalism "works" for a special case, e.g. translationally invariant systems. For such a system the momentum $\mathbf{k}$ is a good quantum number, so choose single-particle plane wave states

$$\phi_i(\mathbf{r}) = \phi_{\mathbf{k}\sigma}(\mathbf{r}) = L^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}} u_\sigma, \tag{48}$$

where u_σ is a spinor like $u_\downarrow = \binom{0}{1}$, etc. 1st quantized T is $-\nabla^2/(2m)$,[12] so 2nd-quantized kinetic energy is

$$\boxed{\hat{T} \equiv \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j = \sum_{\mathbf{k}\sigma} \left(\frac{\mathbf{k}^2}{2m}\right) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}}. \tag{49}$$

Since we showed $a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$ is just number operator which counts # of particles in state $\mathbf{k}\sigma$, this clearly just adds up the kinetic energy of all the occupied states, as it should. For general two-particle interaction V, let's assume $V(\mathbf{r}, \mathbf{r}') = V(\mathbf{r} - \mathbf{r}')$ only, as must be true if we have transl. invariance. In terms of the Fourier transform

$$V(\mathbf{q}) = \frac{1}{L^3}\int d^3\mathbf{r}\; e^{i\mathbf{q}\cdot\mathbf{r}}\; V(\mathbf{r}) \tag{50}$$

[12] I'll set $\hbar = 1$ from here on out, unless required for an honest physical calculation.

we have (steps left as exercise)

$$\boxed{\hat{V} = \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} a^\dagger_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} V(\mathbf{q}) a_{\mathbf{k}'\sigma} a_{\mathbf{k}+\mathbf{q}\sigma}} \tag{51}$$

1.3.4 Schrödinger, Heisenberg, interaction representations

Here we just give some definitions & reminders on different (equivalent) representations of quantum mechanics. In different reps., *time dependence* is associated with states (Schrödinger), operators (Heisenberg), or combination (interaction).

- **Schrödinger picture**

$$\begin{aligned} \text{state } |\hat{\psi}_S(t)\rangle, &\qquad \text{operators } \hat{\mathcal{O}}_S \neq \hat{\mathcal{O}}_S(t) \\ i\frac{\partial}{\partial t}|\hat{\psi}_S(t)\rangle &= \hat{H}|\hat{\psi}_S(t)\rangle \end{aligned}$$

  has formal solution

$$\boxed{|\hat{\psi}_S(t)\rangle = e^{-i\hat{H}(t-t_0)}|\hat{\psi}_S(t_0)\rangle} \tag{52}$$

  Note $\hat{H}$ hermitian $\Rightarrow$ *time evolution operator* $\boxed{\hat{U} \equiv e^{i\hat{H}(t-t_0)}}$ is unitary.

- **Interaction picture** (useful for pert. thy.)

$$\hat{H} = \hat{H}_0 + \hat{H}' \qquad \text{(where } \hat{H}_0 \text{ usually soluble)}$$

  Def. in terms of Schr. picture:
$$\begin{aligned} |\hat{\psi}_I(t)\rangle &= e^{i\hat{H}_0 t}|\hat{\psi}_S(t)\rangle \\ \hat{\mathcal{O}}_I(t) &= e^{i\hat{H}_0 t}\hat{\mathcal{O}}_S e^{-i\hat{H}_0 t} \end{aligned}$$

$$\Rightarrow i\frac{\partial}{\partial t}|\hat{\psi}_I(t)\rangle = \hat{H}'(t)|\hat{\psi}_I(t)\rangle$$

$$\text{with} \quad \hat{H}'(t) = e^{i\hat{H}_0 t}\hat{H}' e^{-i\hat{H}_0 t}$$

Remarks:

– states and ops. t-dependent in interaction picture, but time dependence of operators very simple, e.g.

$$\begin{aligned} \hat{H}_0 &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \\ i\frac{\partial}{\partial t} a_{\mathbf{k}I}(t) &= e^{i\hat{H}_0 t}[a_{\mathbf{k}}, \hat{H}_0] e^{-i\hat{H}_0 t} \\ &= \varepsilon_{\mathbf{k}} a_{\mathbf{k}I}(t) \end{aligned}$$

$$\Rightarrow a_{\mathbf{k}I}(t) = a_{\mathbf{k}} e^{-i\varepsilon_{\mathbf{k}} t}$$

– Time evolution operator determines state at time t:

$$|\hat{\psi}_I(t)\rangle = \hat{U}(t, t_0)|\hat{\psi}_I(t_0)\rangle$$

From Schrödinger picture we find

$$\boxed{\hat{U}(t, t_0) = e^{i\hat{H}_0 t} e^{-i\hat{H}(t-t_0)} e^{-i\hat{H}_0 t_0}} \tag{53}$$

(Note ($[\hat{H}, \hat{H}_0] \neq 0$!)

- **Heisenberg picture**

$$\begin{aligned} \text{state} \quad |\hat{\psi}_H\rangle & \qquad t\text{-independent}, \\ \text{operators} \quad \hat{\mathcal{O}}_H(t) &= e^{i\hat{H}t}\hat{\mathcal{O}}_S e^{-i\hat{H}t} \end{aligned}$$

so operators evolve according to *Heisenberg eqn. of motion*

$$\boxed{i\frac{\partial}{\partial t}\hat{\mathcal{O}}_H(t) = [\hat{\mathcal{O}}_H(t), H]} \tag{54}$$

⋆ Note–compare three reps. at $t = 0$:

$$|\hat{\psi}_H\rangle = |\hat{\psi}_S(0)\rangle = |\hat{\psi}_I(0)\rangle \tag{55}$$

$$\hat{\mathcal{O}}_S = \hat{\mathcal{O}}_H(0) = \hat{\mathcal{O}}_I(0) \tag{56}$$

1.4 Phonons

1.4.1 Review of simple harmonic oscillator quantization

I will simply write down some results for the standard SHO quantization from elementary QM using "ladder operators". We consider the Hamiltonian

$$H = \frac{p^2}{2M} + \frac{K}{2} q^2 \tag{57}$$

and extract the relevant dimensions by putting

$$\begin{aligned} \omega^2 &= \frac{K}{M} \\ \xi &= q \left(\frac{M\omega}{\hbar} \right)^{1/2} \\ -i\frac{\partial}{\partial \xi} &= p(\hbar M \omega)^{-1/2} \end{aligned} \tag{58}$$

so

$$H = \frac{\hbar\omega}{2} \left(-\frac{\partial^2}{\partial \xi^2} + \xi^2 \right). \tag{59}$$

We recall soln. goes like $e^{-\xi^2/2} H_n(\xi)$, where H_n are Hermite polynomials, and that eigenvalues are

$$E_n = \hbar\omega(n + 1/2) \tag{60}$$

Define *ladder operators* a, $a^\dagger$ as

$$a = \frac{1}{\sqrt{2}} \left(\xi + \frac{\partial}{\partial \xi} \right) \tag{61}$$

$$a^\dagger = \frac{1}{\sqrt{2}} \left(\xi - \frac{\partial}{\partial \xi} \right) \tag{62}$$

Ladder ops. obey commutation relations (check)

$$[a, a^\dagger] = 1 \quad ; \quad [a, a] = 0 \quad ; \quad [a^\dagger, a^\dagger] = 0 \tag{63}$$

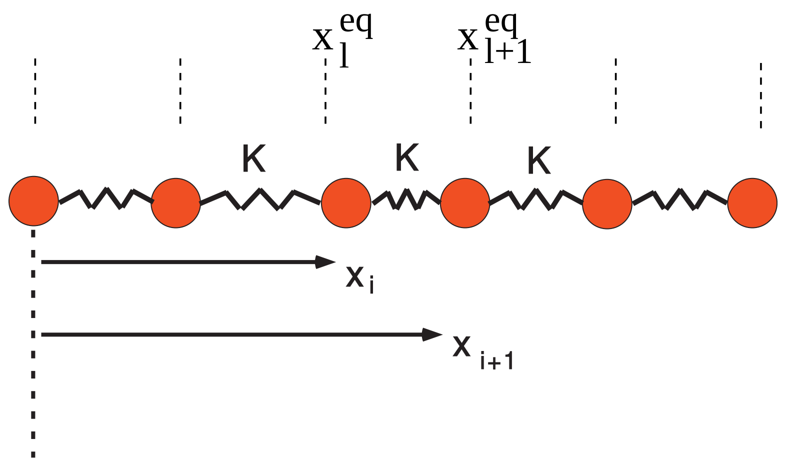


Figure 3: Linear chain with spring couplings K. Dynamical variables are $q_i \equiv x_i - x_i^{eq}$

& then H may be written (check)

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right). \tag{64}$$

$a, a^\dagger$ connect eigenstates of different quantum nos. n, as

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}}|0\rangle, \tag{65}$$

where $|0\rangle$ is state which obeys $a|0\rangle = 0$. Operating on $|n\rangle$ with $a^\dagger$ may be shown with use of commutation relations to give

$$a^\dagger|n\rangle = (n+1/2)^{1/2}|n+1\rangle \quad ; \quad a|n\rangle = n^{1/2}|n-1\rangle \tag{66}$$

so with these defs. the ladder operators for SHO are seen to be *identical* to *boson* creation and annihilation operators defined above in Sec. 1.3.2.

1.4.2 1D harmonic chain

If we now consider N atoms on a linear chain, each attached to its neighbor with a "spring" of spring constant K as shown in figure. First let's consider the problem classically. The Hamiltonian is

$$H = \sum_\ell \frac{p_\ell^2}{2m} + \frac{K}{2}(q_\ell - q_{\ell+1})^2, \tag{67}$$

where the q_ℓ's are the displacements from atomic equilibrium positions. Now Hamilton's eqns. (or Newton's 2nd law!) yield

$$-M\ddot{q}_j = M\omega^2 q_j = K(2q_j - q_{j-1} - q_{j+1}). \tag{68}$$

A standing sinusoidal wave $q_j = A\cos(kaj)$ satisfies this equation *if* the eigenfrequencies have the form

$$\omega_k^2 = \frac{K}{M} 2(1-\cos ka), \tag{69}$$

where if a is the lattice constant, $k = 2\pi/\lambda$. Note that for small k, ω_k is linear, $\omega_k \simeq (K/M)^{1/2} ka$.[13]

This is the *classical* calculation of the normal modes of oscillation on a 1D chain. To quantize the theory, let's *impose* canonical commutation relations on the position and momentum of the ℓth and jth atoms:

$$[q_\ell, p_j] = i\hbar\delta_{\ell m} \tag{70}$$

and construct collective variables which describe the modes themselves (recall k is wave vector, ℓ is position) :

$$\begin{aligned} q_\ell &= \frac{1}{N^{1/2}} \sum_k e^{ika\ell} Q_k \quad ; \quad Q_k = \frac{1}{N^{1/2}} \sum_\ell e^{-ika\ell} q_\ell \\ p_\ell &= \frac{1}{N^{1/2}} \sum_k e^{-ika\ell} p_k \quad ; \quad P_k = \frac{1}{N^{1/2}} \sum_\ell e^{ika\ell} p_\ell, \end{aligned} \tag{71}$$

which leads to canonical commutation relations in wave vector space:

$$\begin{aligned} [Q_k, P_{k'}] &= \frac{1}{N} \sum_{\ell,m} e^{-ikal} e^{ik'am} [q_\ell, p_m] \\ &= \frac{i\hbar}{N} \sum_\ell e^{-ial(k-k')} = i\hbar\delta_{k,k'}. \end{aligned} \tag{72}$$

Let's now express the Hamiltonian (67) in terms of the new variables. We have, with a little algebra and Eq. (69),

$$\begin{aligned} \sum_\ell p_\ell^2 &= \sum_k P_k P_{-k} \\ \frac{K}{2} \sum_\ell (q_\ell - q_{\ell-1})^2 &= \frac{K}{2} \sum_k Q_k Q_{-k} (2 - e^{ika} - e^{-ika}) = \frac{M}{2} \sum_k \omega_k^2 Q_k Q_{-k} \end{aligned} \tag{73}$$

[13]Note since $k = 2\pi n/(Na)$, the ω_k are *independent of system size*

so

$$\boxed{H = \frac{1}{2M}\sum_k p_k p_{-k} + \frac{M}{2}\sum_k \omega_k^2 Q_k Q_{-k}}. \tag{74}$$

Note that the energy is now expressed as the sum of kinetic + potential energy of each *mode* k, and there is no more explicit reference to the motion of the atomic constituents. To *second quantize* the system, we write down creation and annihilation operators for each mode k. Define

$$a_k = \left(\frac{M\omega_k}{2\hbar}\right)^{1/2}\left(Q_k + \frac{i}{M\omega_k}P_{-k}\right) \tag{75}$$

$$a_k^\dagger = \left(\frac{M\omega_k}{2\hbar}\right)^{1/2}\left(Q_{-k} - \frac{i}{M\omega_k}P_k\right) \tag{76}$$

which can be shown, just as in the single SHO case, to obey commutation relations

$$\left[a_k, a_{k'}^\dagger\right] = \delta_{kk'} \tag{77}$$

$$\left[a_k, a_{k'}\right] = 0 \tag{78}$$

$$\left[a_k^\dagger, a_{k'}^\dagger\right] = 0 \tag{79}$$

and the Hamiltonian expressed simply as

$$\sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right) \tag{80}$$

which we could have probably guessed if we had realized that since the normal modes don't interact, we have simply the energy of all allowed harmonic oscillators. Note this is a *quantum* Hamiltonian, but the energy scale in H is the *classical* mode frequency ω_k.

1.4.3 Debye Model

Let us imagine using the Hamiltonian (80) as a starting point to calculate the specific heat of a (3D) solid due to phonons. We take the Debye model for the dispersion to simplify the calculation,

$$\omega_{\mathbf{k}} = \begin{cases} ck & k < k_D \\ 0 & k > k_D \end{cases} \tag{81}$$

where the Debye wave vector $k_D = (6\pi^2 n)^{1/3}$ is obtained by replacing the first Brillouin zone of the solid by a sphere of radius k_D which contains N wave vectors, with N the number of ions in the crystal. The average value of the Hamiltonian is

$$U = \langle H \rangle = 3\sum_k \hbar\omega_{\mathbf{k}} \left(\langle a_k^\dagger a_k \rangle + \frac{1}{2} \right) = 3\sum_k \hbar\omega_{\mathbf{k}} \left(\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} + \frac{1}{2} \right) \tag{82}$$

since the average number of phonons in state $\mathbf{k}$ is simply the expectation value of a boson number operator

$$\langle a_k^\dagger a_k \rangle \equiv \mathrm{Tr}(\rho a_k^\dagger a_k) = b(\hbar\omega_{\mathbf{k}}), \tag{83}$$

where $b(x) = (\exp(\beta x) - 1)^{-1}$ is the free Bose distribution function. The factors of 3 come from the 3 independent phonon polarizations, which we consider to be degenerate here. Taking one derivative wrt temperature, the spec. heat per unit volume is

$$\begin{aligned} c_V &= \left.\frac{\partial u}{\partial T}\right|_n = 3\frac{\partial}{\partial T}\sum_{\mathbf{k}} \frac{\hbar c k}{e^{\beta\hbar c k} - 1} = 3\frac{\partial}{\partial T}\frac{\hbar c}{2\pi^2}\int_0^{k_D} dk \frac{k^3}{e^{\beta\hbar c k} - 1} \\ &\simeq \frac{\partial}{\partial T}\frac{3(k_B T)^4}{2\pi^2(\hbar c)^3} \underbrace{\int_0^\infty \frac{x^3}{e^x - 1}}_{\pi^4/15} = \frac{\partial}{\partial T}\frac{\pi^2}{10}\frac{(k_B T)^4}{(\hbar c)^3} = \frac{2\pi^2}{5} k_b \left(\frac{k_B T}{\hbar c} \right)^3 \end{aligned} \tag{84}$$

So far we have done nothing which couldn't have been done easily by ordinary 1st-quantized methods. I have reviewed some Solid State I material here by way of introduction to problems of interacting particles to which you have not been seriously exposed thus far in the condensed matter grad sequence. The second quantization method becomes manifestly useful for the analysis of *interacting* systems. I will now sketch the formulation (not the solution) of the problem in the case of the phonon-phonon interaction in the anharmonic crystal.

1.4.4 Anharmonicity & its consequences

As you will recall from Solid State I, most thermodynamic properties of insulators, as well as neutron scattering experiments on most materials, can be explained entirely in terms of the harmonic approximation for the ions in the crystal, i.e. by assuming a Hamiltonian of the form (80). There are some problems with the harmonic theory. First, at higher temperatures atoms tend to explore the anharmonic parts of the crystal potential more and more, so deviations from predictions of the equilibrium theory increase. The thermal expansion of solids in the harmonic approximation is rigorously zero.[14] Secondly, some important qualitative aspects of transport cannot be understood: for example, the harmonic theory predicts infinite thermal transport of insulators! (See A&M Ch. 25 for a qualitative discussion of these failures).

The obvious way to go beyond the harmonic approximation is to take into account higher-order corrections to the real-space crystal potential systematically, expanding[15]

$$U = \frac{1}{2!}\sum_{\ell m} D^{(2)}(\ell, m) q_\ell q_m + \frac{1}{3!}\sum_{\ell m n} D^{(3)}(\ell, m, n) q_\ell q_m q_n + \ldots, \tag{86}$$

where

$$D^{(n)}(\ell, m, \ldots n) = \left.\frac{\partial^n U}{\partial q_\ell \partial q_m \ldots \partial q_n}\right|_{u_i=0} \tag{87}$$

[14]This follows from the independence of the phonon energies in harmonic approx. of the system volume. (see above) Since pressure depends on temperature only through the volume derivative of the mode freqs. (see A & M p. 490),

$$\left(\frac{\partial V}{\partial T}\right)_p = \frac{\left(\frac{\partial p}{\partial T}\right)_V}{\left(\frac{\partial p}{\partial V}\right)_T} = 0 \tag{85}$$

[15]I have dropped polarization indices everywhere in this discussion, so one must be careful to go back and put them in for a 2- or 3D crystal.

are the so-called dynamical matrices.[16] Using Eqs. (71,76) we find

$$q_\ell = \frac{1}{\sqrt{N}} \left(\frac{\hbar}{2m\omega} \right)^{1/2} \sum_k Q_k e^{ika\ell} = \sum_k (a_k + a_{-k}^\dagger) e^{ika\ell} \tag{88}$$

Note that the product of 3 displacements can be written

$$q_\ell q_m q_n = \frac{1}{(N)^{3/2}} \sum_{k_1 k_2 k_3} e^{i(k_1 a\ell + k_2 am + k_3 an)} Q_{k_1} Q_{k_2} Q_{k_3} \tag{89}$$

so the cubic term may be written

$$H_3 = \sum_{k_1 k_2 k_3} V^{(3)}(k_1 k_2 k_3) Q_{k_1} Q_{k_2} Q_{k_3} \tag{90}$$

with

$$V^{(3)}(k_1 k_2 k_3) = \sum_{\ell mn} D^{(3)}(\ell, m, n) \exp[i(k_1 \ell + k_2 m + k_3 n)] \tag{91}$$

Note now that the indices ℓ, m, n run over all unit cells of the crystal lattice. Since crystal potential itself is periodic, the momenta k_1, k_2, and k_3 in the sum are not really independent. In fact, if we shift all the sums in (91) by a lattice vector j, we would have

$$\begin{aligned} V^{(3)}(k_1 k_2 k_3) &= \sum_{\ell mn} D^{(3)}(\ell + j, m + j, n + j) e^{i(k_1 a\ell + k_2 am + k_3 an)} e^{i(k_1 + k_2 + k_3)aj} \\ &= \sum_{\ell mn} D^{(3)}(\ell, m, n) e^{i(k_1 a\ell + k_2 am + k_3 an)} e^{i(k_1 + k_2 + k_3)aj} \end{aligned} \tag{92}$$

where in the last step I used the fact that the crystal potential U in every lattice cell is equivalent. Now sum both sides over j and divide by N to find

$$V^{(3)}(k_1 k_2 k_3) = \sum_{\ell mn} D^{(3)}(\ell, m, n) \exp[i(k_1 \ell + k_2 m + k_3 n)] \Delta(k_1 + k_2 + k_3), \tag{93}$$

[16] Recall that the theory with only harmonic and cubic terms is actually formally unstable, since arbitrarily large displacements can lower the energy by an arbitrary amount. If the cubic terms are treated perturbatively, sensible answers normally result. It is usually better to include quartic terms as shown in figure below, however.

where

$$\Delta(k) = \frac{1}{N}\sum_j e^{i(k_1+k_2+k_3)aj} = \frac{1}{N}\sum_k \delta(k+G) \tag{94}$$

and G is any reciprocal lattice vector.

Return now to (90). We have ascertained that $V^{(3)}(\ell, m, n)$ is zero unless $k_1 + k_2 + k_3 = G$, i.e. crystal momentum is conserved. If we expand (90), we will get products of 3 creation or annihilation operators with coefficients $V^{(3)}$. The values of these coefficients depend on the elastic properties of the solid, and are unimportant for us here. The momenta of the three operators must be such that momentum is conserved up to a reciprocal lattice vector, e.g. if we consider the term $a_{k_1}a^\dagger_{-k_2}a^\dagger_{-k_3}$ we have a contribution only from $k_1 + k_2 + k_3 = G$.[17] Note this term should be thought of as corresponding to a physical process wherein a phonon with momentum k_1 is destroyed and two phonons with momenta $-k_2$ and $-k_3$ are created. It can be drawn "diagrammatically" à la Feynman (as the 1st of 2 3rd-order processes in the figure below).

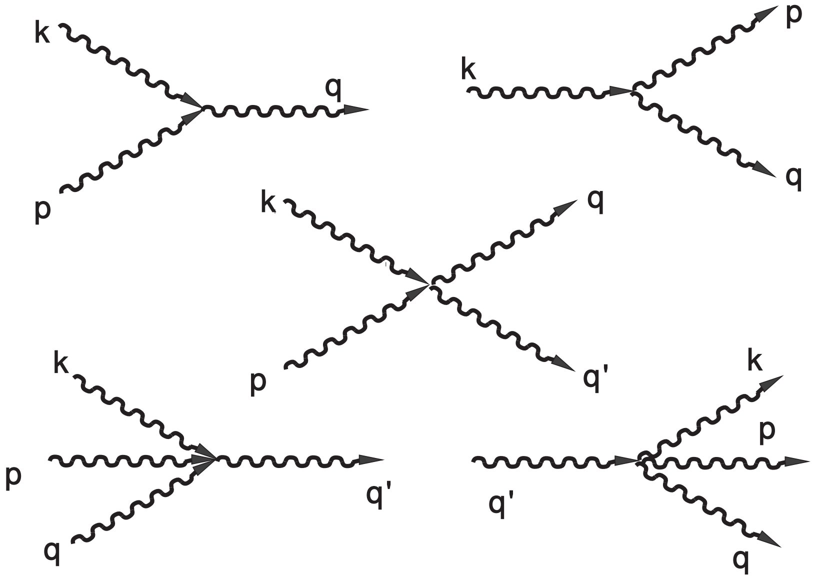


Figure 4: Diagrams representing phonon-phonon collision processes allowed by energy and momentum conservation in 3rd and 4th order.

[17] As usual, processes with $G = 0$ are called *normal* processes, and those with finite G are called *Umklapp* processes.

Questions:

- How does energy conservation enter? What is importance of processes involving destruction or creation of 3 phonons?
- If one does perturbation theory around harmonic solution, does cubic term contribute to thermal averages?
- Can we calculate thermal expansion with cubic Hamiltonian?