Physics 130C Lecture Notes
Chapter 3: Applications to condensed matter and to particle physics

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3.1   Harmonic oscillator review, operator solution

[Le Bellac 11.1] The simple harmonic oscillator is ubiquitous in physics, not just because it is exactly solvable both classically and quantum mechanically, but because it arises as the leading approximation to any system near a stable equilibrium. Expanding a potential in one dimension about its minimum, Taylor's theorem says

$$V(x) = V(x_0) + 0 + \frac{1}{2}V''(x_0)(x - x_0)^2 + \ldots$$

and we can often ignore the ... (aka anharmonic terms) for systems that are near their equilibrium configuration.

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2 = \frac{1}{2}\left(\mathbf{P}^2 + \mathbf{Q}^2\right) = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\right)$$

with

$$\mathbf{a} \equiv \frac{1}{\sqrt{2}}\left(\mathbf{Q} + i\mathbf{P}\right), \quad \mathbf{a}^\dagger \equiv \frac{1}{\sqrt{2}}\left(\mathbf{Q} - i\mathbf{P}\right).$$

Here I've defined these new operators to hide the annoying factors:

$$\mathbf{Q} \equiv \left(\frac{\hbar}{m\omega}\right)^{1/2}\mathbf{x}, \quad \mathbf{P} \equiv (m\hbar\omega)^{1/2}\mathbf{p}.$$

$$[\mathbf{x}, \mathbf{p}] = i\hbar\mathbb{1} \quad \implies \quad [\mathbf{a}, \mathbf{a}^\dagger] = \mathbb{1}.$$

The *number operator* $\mathbf{N} \equiv \mathbf{a}^\dagger\mathbf{a}$ satisfies

$$[\mathbf{N}, \mathbf{a}] = -\mathbf{a}, \quad [\mathbf{N}, \mathbf{a}^\dagger] = +\mathbf{a}^\dagger \quad.$$

So $\mathbf{a}$ and $\mathbf{a}^\dagger$ are lowering and raising operators for the number operator. The eigenvalues of the number operator have to be positive, since

$$0 \leq \|\mathbf{a}|n\rangle\|^2 = \langle n|\mathbf{a}^\dagger\mathbf{a}|n\rangle = \langle n|\mathbf{N}|n\rangle = n\langle n|n\rangle$$

which means that $n = 0 \implies \mathbf{a}|n\rangle = 0$. If it isn't zero, $\mathbf{a}|n\rangle$ is also an eigenvector of $\mathbf{N}$ with eigenvalue $n - 1$. It has to stop somewhere! So the eigenstates of $\mathbf{N}$ (and hence of $\mathbf{H} = \hbar\omega\left(\mathbf{N} + \frac{1}{2}\right)$ are

$$|0\rangle, \quad |1\rangle \equiv \mathbf{a}^\dagger|0\rangle, \quad \ldots, |n\rangle = c_n\left(\mathbf{a}^\dagger\right)^n|0\rangle\ldots$$

where we must choose c_n to normalize these states. The answer which gives $\langle n|n\rangle = 1$ is $c_n = \frac{1}{\sqrt{n!}}$.

3.1.1   Coherent states

[Le Bellac 11.2] You get to explore eigenstates of the creation and annihilation operators on HW 8.

3.2 Towards quantized fields

3.2.1 Quantum sound: Phonons

[Le Bellac section 11.3] Let's think about a crystalline solid. The specific heat of solids (how much do you have to heat it up to change its temperature by a given amount) was a mystery before QM. The first decent (QM) model was due to Einstein, where he supposed that each atom is a (independent) quantum harmonic oscillator with frequency ω. This correctly predicts that the specific heat decreases as the temperature is lowered, but is very crude. Obviously the atoms interact: that's why they make a nice crystal pattern, and that's why there are sound waves, as we will see. By treating the elasticity of the solid quantum mechanically, we are going to discover quantum field theory. One immediate benefit of this will be a framework for quantum mechanics where particles can be created and annihilated.

As a more accurate toy model of a one-dimensional crystalline solid, let's consider a linear chain of masses m connected with springs with spring constant κ. When in equilibrium, the masses form a regular one-dimensional crystal lattice (equally spaced mass points). Now let q_n denote the displacement of the jth mass from its equilibrium position x_n and let p_j be the corresponding momentum. Assume there are N masses and impose periodic boundary conditions: $q_{n+N} = q_n$. (This and a number of features below will be familiar from HW 2.) The equilibrium positions themselves are

$$x_n = na, n = 1, 2...N$$

where a is the lattice spacing. The Hamiltonian for the collection of masses is:

$$\mathbf{H} = \sum_{n=1}^{N} \left(\frac{\mathbf{p}_n^2}{2m} + \frac{1}{2}\kappa \left(\mathbf{q}_n - \mathbf{q}_{n-1} \right)^2 \right) + \lambda q q^4. \tag{1}$$

I've include a token anharmonic term $\lambda \mathbf{q}^4$ to remind us that we are leaving stuff out; for example we might worry whether we could use this model to describe *melting*.

Now set $\lambda = 0$. This hamiltonian above describes a collection of coupled oscillators, with a matrix of spring constants $V = k_{ab}\mathbf{q}_a\mathbf{q}_b$. If we diagonalize the matrix of spring constants, we will have a description in terms of decoupled oscillators, called *normal modes*. The purpose of the next few paragraphs is to diagonalize the matrix of spring constants in a smart way.

Notice that the hamiltonian commutes with the operation

$$\mathcal{T} : (q_n, p_n) \rightarrow (q_{n+1}, p_{n+1}) \equiv \left((\mathcal{T}q)_n , (\mathcal{T}p)_n \right)$$

where $\mathcal{T}$ acts on the labels of the masses by

$$\mathcal{T} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

$[\mathbf{H}, \mathcal{T}] = 0$; $\mathcal{T}$ is a symmetry, a discrete translation symmetry.

[End of Lecture 20]

Eigenvectors of $\mathcal{T}$ are Fourier modes

$$q_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{\mathbf{i}kx_n} q_n \equiv \sum_n \mathbf{U}_{kn} q_n \quad , \quad k = j\frac{2\pi}{Na}, j \in \mathbb{Z}.$$

Note that I'm distinguishing the real-space positions q_n and their Fourier modes q_k just by the label. Also notice that I used the equilibrium position x_n in the exponent. In order for the matrix $\mathbf{U}$ to be unitary here, we need $k = j\frac{2\pi}{Na}$ where a is the lattice spacing and j is an integer – Na is the size of the box. The quantization of k is because the number of sites N is finite. This is also familiar from HW 2.

The eigenvalue equation is: $\mathcal{T} q_k = e^{-\mathbf{i}ka} q_k$. Now we must deal with the consequences of our regulators.

Because N is finite, k takes discrete values; this is a long-wavelength "IR" property. Because of the lattice structure, k is periodic: $k \equiv k + 2\pi/a$; this is a short-distance "UV" property. The range of k can be taken to be

$$0 \le k \le \frac{2\pi(N-1)}{Na} \ .$$

Because of the periodicity in k, we an equivalently label the set of wavenumbers by:

$$0 < k \le \frac{2\pi}{a} \quad \text{or} \quad -\frac{\pi}{a} < k \le \frac{\pi}{a}.$$

[Cultural remark: This range of independent values of the wavenumber in a lattice model is called the *Brillouin zone*. There is some convention for choosing a fundamental domain which prefers the last one but it won't matter to us.]

Check that $\mathbf{U}$ is indeed a unitary matrix:

$$\sum_n \mathbf{U}_{kn} \mathbf{U}^{\dagger}_{nk'} = \sum_n \mathbf{U}_{kn} \mathbf{U}^{\star}_{k'n} = \frac{1}{N} \sum_n e^{\mathbf{i}kx_n} e^{-\mathbf{i}k'x_n} = \frac{1}{N} \frac{1 - e^{2\mathbf{i}\pi(j-j')}}{1 - e^{2\mathbf{i}\pi(j-j')/N}} = \delta_{jj'}.$$

It's also worth noting that $\mathbf{U}_{nk}^{\dagger} = \mathbf{U}_{kn}^{\star} = \mathbf{U}_{-kn}$, so unitarity is also

$$\sum_n \mathbf{U}_{kn} \mathbf{U}_{nk'}^{\dagger} = \sum_n \mathbf{U}_{kn} \mathbf{U}_{-k'n} = \delta_{kk'}.$$

The inverse fourier transform is

$$q_n = \frac{1}{\sqrt{N}} \sum_{k>0}^{2\pi/a} e^{-\mathbf{i}kx_n} q_k = \sum_k \mathbf{U}_{nk}^{\dagger} q_k = \sum_k \mathbf{U}_{-kn} q_k.$$

Notice that this $\mathcal{T}$ is an operator acting on the *labels* of the quantum states – it's a classical operator. (Just like in quantum computing, the classical logic gates act on the *labels* $0, 1$ of the qbits $|0\rangle, |1\rangle$.) So don't be surprised that we can also Fourier transform the *momenta* :

$$p_k = \sum_n \mathbf{U}_{kn} p_n.$$

So far we've actually solved a classical problem of finding normal modes of these coupled oscillators. The world is quantum mechanical so let's remember that our variables are quantum operators now, and figure out what the quantum Hamiltonian is for the normal modes. The kinetic term in the Hamiltonian is

$$\sum_n \mathbf{p}_n^2 = \sum_n \sum_{k,k'} \mathbf{U}_{-kn} \mathbf{U}_{-k'n} \mathbf{p}_k \mathbf{p}_{k'} = \delta_{k,-k'} \mathbf{p}_k \mathbf{p}_{k'} = \sum_k \mathbf{p}_k \mathbf{p}_{-k}.$$

The potential energy term is

$$\sum_n (\mathbf{q}_{n+1} - \mathbf{q}_n)^2 = \sum_n ((\mathcal{T} - \mathbb{1})\mathbf{q})_n^2 = \sum_n \sum_{k,k'} \left(e^{-\mathbf{i}ka} - 1\right)\left(e^{-\mathbf{i}k'a} - 1\right) \mathbf{U}_{-kn} \mathbf{U}_{-k'n} \mathbf{q}_k \mathbf{q}_{k'}$$

$$= \sum_k \left(e^{-\mathbf{i}ka} - 1\right)\left(e^{+\mathbf{i}ka} - 1\right) \mathbf{q}_k \mathbf{q}_{-k} = \sum_k 4\sin^2\left(\frac{ka}{2}\right) \mathbf{q}_k \mathbf{q}_{-k}.$$

The whole hamiltonian is a bunch of decoupled oscillators, labelled by these funny wave numbers:

$$\mathbf{H} = \sum_k \left(\frac{\mathbf{p}_k \mathbf{p}_{-k}}{2m} + \frac{1}{2} m \omega_k^2 \mathbf{q}_k \mathbf{q}_{-k}\right)$$

where the frequency of the mode labelled k is

$$\omega_k \equiv 2\frac{\kappa}{m} \sin\frac{|k|a}{2}. \tag{2}$$

This is called the *dispersion relation* – it says how fast a mode of a given wavenumber propagates; it therefore says how quickly a wave packet will disperse.

(The dispersion relation for $N = 40$. ω_k in units of $\omega \equiv \sqrt{\kappa/m}$)
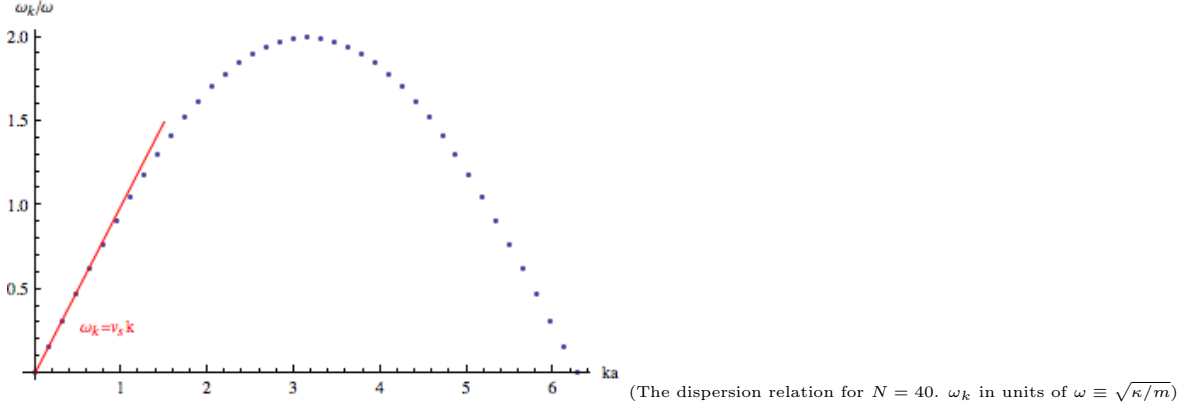
Notice that there are some energies where there aren't any phonon states. In particular, the function (2) has a maximum. More generally, in a system with discrete translation invariance, there are *bands* of allowed energies.

So far the fact that quantumly $[\mathbf{q}_n, \mathbf{p}_{n'}] = \mathbf{i}\hbar\delta_{nn'}\mathbb{1}$ hasn't mattered in our analysis (go back and check). For the Fourier modes, this implies the commutator

$$[\mathbf{q}_k, \mathbf{p}_{k'}] = \sum_{n,n'} \mathbf{U}_{kn}\mathbf{U}_{k'n'}[\mathbf{q}_n, \mathbf{p}'_n] = \mathbf{i}\hbar\mathbb{1}\sum_n \mathbf{U}_{kn}\mathbf{U}_{k'n} = \mathbf{i}\hbar\delta_{k,-k'}\mathbb{1}.$$

To make the final step to decouple the modes with k and $-k$, introduce the annihilation and creation operators

$$\mathbf{q}_k = \sqrt{\frac{\hbar}{2m\omega_k}}\left(\mathbf{a}_k + \mathbf{a}^\dagger_{-k}\right), \quad \mathbf{p}_k = \frac{1}{\mathbf{i}}\sqrt{\frac{\hbar m\omega_k}{2}}\left(\mathbf{a}_k - \mathbf{a}^\dagger_{-k}\right).$$

They satisfy

$$[\mathbf{a}_k, \mathbf{a}^\dagger_{k'}] = \delta_{kk'}\mathbb{1}.$$

In terms of these, the hamiltonian is

$$\mathbf{H} = \sum_{k=0}^{2\pi/a} \hbar\omega_k\left(\mathbf{a}^\dagger_k\mathbf{a}_k + \frac{1}{2}\right),$$

a sum of independent harmonic oscillators with frequencies ω_k. The ground state satisfies $\mathbf{a}_k|0\rangle = 0$ for all k. The excitation above the ground state,

$$\mathbf{a}^\dagger_k|0\rangle = |\text{one phonon with momentum } \hbar k\rangle.$$

is called a *phonon* with momentum $\hbar k$. This is what previously we would have called "$|k\rangle$"; we can make a state with one phonon in a position eigenstate by taking superpositions:

$$|\text{one phonon at position } x\rangle = \sum_k e^{\mathbf{i}kx}|\text{one phonon with momentum } \hbar k\rangle = \sum_k e^{\mathbf{i}kx}\mathbf{a}^\dagger_k|0\rangle.$$

The number operator $\mathbf{N}_k \equiv \mathbf{a}_k^\dagger \mathbf{a}_k$ counts the number of phonons with momentum k. The ground state is the state with no phonons. We can make a state with two phonons:

$$|k, k'\rangle = \mathbf{a}_k^\dagger \mathbf{a}_{k'}^\dagger |0\rangle$$

and so on.

So this construction allows us to describe situations where the number of particles $\mathbf{N} = \sum_k \mathbf{N}_k$ can vary! That is, we can now describe dynamical processes in which the number particles change. In all our previous discussions of quantum mechanics we have described the hilbert space of two particles as a tensor product of the hilbert space of each. How can we act with an operator which enlarges the hilbert space?? We just figured out how to do it.

We can specify basis states for this Hilbert space

$$\left(\mathbf{a}_{k_1}^\dagger\right)^{n_{k_1}} \left(\mathbf{a}_{k_2}^\dagger\right)^{n_{k_2}} \cdots |0\rangle = |\{n_{k_1}, n_{k_2}\}\rangle$$

by a collection of *occupation numbers* n_k, eigenvalues of the number operator.

Notice that in this description it is manifest that phonons have no identity. We only keep track of how many of them there are and what is their momentum. They cannot be distinguished. Also notice that we can have as many we want in the same state – n_k can be any non-negative integer. These are an example of *bosons*.

Sound waves

Let's pretend that the system is classical for a moment. Recall that in a classical mechanics course, the step we did above is called finding the normal modes. The equations of motion in real-space are

$$m\ddot{q}_n = -\kappa\left((q_n - q_{n-1}) - (q_n - q_{n+1})\right) = -\kappa\left(2q_n - q_{n-1} - q_{n+1}\right).$$

Another point from HW 2 is that this equation can be written as

$$m\ddot{q}_n = -\kappa\left(2\mathbb{1} - \mathcal{T} - \mathcal{T}^\dagger\right)_{nn'} q_{n'}.$$

Plugging in the fourier ansatz (*i.e.* diagonalizing $\mathcal{T}$), we get

$$m\ddot{q}_k = -\kappa\left(2 - 2\cos ka\right) q_k .$$

Plugging in a fourier ansatz in time $q_k(t) = \sum_\omega e^{-\mathbf{i}\omega t} q_{k,\omega}$ turns this into an algebraic equation which says $\omega^2 = \omega_k^2 = \left(\frac{2\kappa}{m}\right)^2 \sin^2\frac{|k|a}{2}$ for the allowed modes. We see that (the classical version of) this system describes waves:

$$0 = \left(\omega^2 - \omega_k^2\right) q_{k,\omega} \stackrel{k \ll 1/a}{\simeq} \left(\omega^2 - v_s^2 k^2\right) q_{k,\omega}.$$
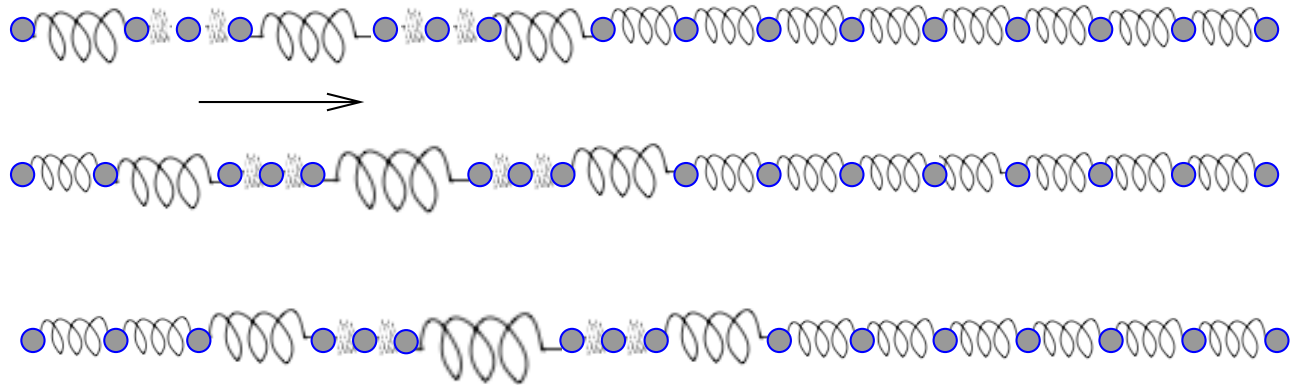
The result for small k is the fourier transform of the wave equation:

$$\left(\partial_t^2 - v_s^2 \partial_x^2\right) q(x,t) = 0 . \tag{3}$$

v_s is the speed of propagation of the waves, in this case the speed of sound. Comparing to the dispersion relation (2), we have found

$$v_s = \frac{\partial \omega_k}{\partial k}\Big|_{k \to 0} = \frac{\kappa a}{m}.$$

The description above is a quantization of sound waves. Below we will quantize EM waves.

Heat capacity of (insulating) solids: phonons are real

The simplest demonstration that phonons are real is the dramatic decrease at low temperatures of the heat capacity of insulating solids. At high temperatures, the equipartition theorem of classical thermodynamics correctly predicts that the energy of the solid from the lattice vibrations should be T times the number of atoms, so the pacity, $C_V = \partial_T E$ should be independent of T. At low temperatures $T < \Theta_D$, this is wrong. Θ_D is the temperature scale associated with the frequencies of the lattice vibrations (say the maximum of the curve ω_k above). The resolution lies in the thermal energy of a quantum harmonic oscillator which you calculated on HW 5, problem 2: for $T < \omega$, the energy goes to a constant $\frac{1}{2}\hbar\omega$:
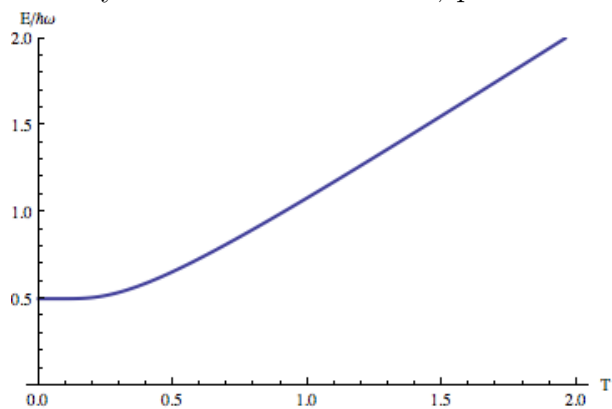

so the heat capacity (the slope of this curve) goes to zero as $T \to 0$.

The Mössbauer effect: phonons are real

Here is another dramatic consequence of the quantization of the lattice vibrations of solids, known as the *Mössbauer effect*, first described in words. The nuclei of the atoms in a solid have various energy levels; by sending in a γ-ray photon, these nuclei can experience transitions from the groundstate to some excited energy level. If an excited nucleus somewhere in the lattice gets hit by a very energetic photon (a γ-ray) of some very specific energy $E_\gamma = \Delta E \equiv E_{\text{excited}} - E_0$, the nucleus can absorb that photon. The resulting sharp resonant absorption lines at $E_\gamma = \Delta E$ are indeed observed.

This sounds simple, but here is a mystery about this: Consider a nucleus alone in space in the excited state, when it gets hit by a photon. The photon carries a momentum $p_\gamma = E_\gamma/c$. Momentum is conserved, and it must be made up by some *recoil* of the emitting nucleus. But if some of its energy $\Delta E = E_{\text{excited}} - E_0$ goes to kinetic energy of recoil, not all of that energy can go to the photon, and the emitted photon energy will be *less* than E_γ by $E_{\text{recoil}} = \frac{p_\gamma^2}{2M} = \frac{E_\gamma^2}{2Mc^2}$.

The solution of the puzzle is phonons: for a nucleus in a lattice, its recoil means that the springs are stretched – it must excite a lattice vibration, it must create some phonons. But there is a nonzero probability for it to create *zero* phonons. In this case, the momentum conservation is made up by an acceleration of *the whole solid*, which is very massive, and therefore does not recoil very much at all (it loses only energy $\frac{p_\gamma^2}{2NM}$). This allows for very sharp resonance lines. In turn, this effect has allowed for some very high-precision measurements.
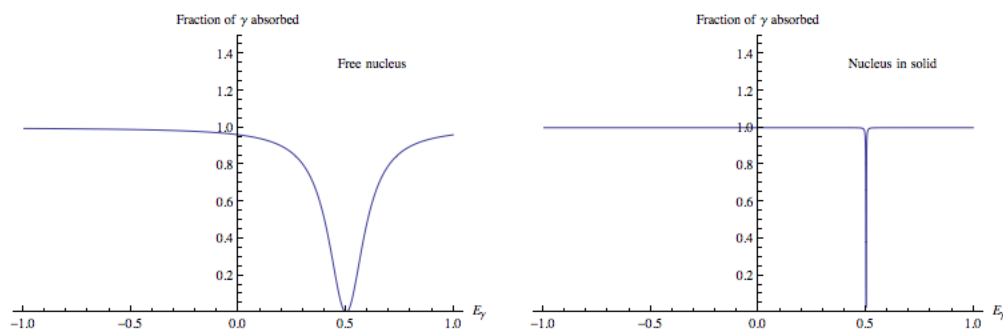
The different widths in these cartoon absorption spectra don't do justice to relative the factor of N.

An essentially similar effect makes it possible to get precise peaks from scattering of X-rays off of a solid (Bragg scattering) – there is a finite amplitude for the scattering to occur without exciting any phonons.

This is actually a remarkable thing: although solids seem ordinary to us because we encounter them frequently, the rigidity of solids is a quantum mechanical emergent phe-

nomenon. You can *elastically* scatter photons off of a solid only because the atoms making up the solid participate in this collective behavior wherein the whole solid acts like a single quantum object!

Just for fun, here is a sketch of the quantitative calculation of the probability of a nucleus at x_n emitting a γ-ray photon without creating any phonons. Recall from your discussion of time-dependent perturbation theory that the transition amplitude is

$$W(N_i \to N_f; L_i \to L_f) \propto |\langle f|\mathbf{H}_{\text{int}}|i\rangle|^2, \qquad \mathbf{Prob} = |W|^2$$

where $N_{i,f}$ and $L_{i,f}$ are initial and final states of the nucleus and lattice, respectively. $\mathbf{H}_{\text{int}}$ is the perturbing hamiltonian by which the transition can occur. This is Fermi's golden rule. Because the nuclear forces are such high-energy things, we can ignore the density of states of the final states, and we can assume that the transition matrix element factorizes:

$$W(N_i \to N_f; L_i \to L_f) \propto |\langle L_f|\mathbf{H}_{\text{L}}|L_i\rangle|^2,$$

where we've factored out some nuclear stuff that we don't care about right now into the $\propto$.

The requirements of translation invariance and Galilean invariance (*i.e.* momentum is conserved, and the transition for a moving observer shouldn't depend on the velocity of the observer) require that

$$\mathbf{H}_{\text{L}} = ae^{i\vec{K}\cdot\vec{\mathbf{x}}}$$

where $\hbar\vec{K}$ is the momentum of the emitted gamma ray (a c-number), and $\vec{\mathbf{x}}$ is the center-of-mass position of the nucleus in question. [1] But, in the 1d case, we have an expression for $\mathbf{x}$ in terms of the phonon creation operators:

$$\mathbf{x}_n = na + \mathbf{q}_n = na + \sum_k \mathcal{N}_k \left(e^{ikna}\mathbf{a}_k + e^{-ikna}\mathbf{a}_k^\dagger \right),$$

where a is the lattice spacing and $\mathcal{N}_k = \sqrt{\frac{\hbar}{2mN\omega_k}}$.

Now the amplitude for emitting no phonons is the 'vacuum-persistence amplitude', i.e. the amplitude for $|L_i\rangle = |0\rangle$ to stay that way:

$$P_{\text{Mössbauer}} \propto |\langle 0|e^{iK(na+\mathbf{q}_n)}|0\rangle|^2 \ .$$

Now it is an exercise in harmonic oscillator physics to get a function out of this. A useful general fact is that for harmonic oscillators (and any gaussian theory)

$$\langle e^{iK\mathbf{q}} \rangle = e^{-K^2\langle \mathbf{q}^2\rangle} \ .$$

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[1] It is possible to show that the interactions with the EM field, to be discussed next, I promise, meet these requirements and reproduce this form of the answer. The relevant term is from $\mathbf{H}_{\text{int}} = \frac{1}{2m}(\mathbf{p}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{p}) \in \frac{1}{2m}(\mathbf{p}+\mathbf{A})^2$. Then we use the fact that the Maxwell field representing a photon is a wave $\mathbf{A} \propto e^{i\vec{K}\cdot\vec{\mathbf{x}}}$, evaluated at the position of the nucleus.

Applying this here,

$$P_{\text{Mössbauer}} \propto e^{-K^2 \sum_k \frac{\hbar}{2m\omega_k}} \sim e^{-K^2 \frac{\hbar}{2m} \frac{1}{Na} \ln(Na)} .$$

Here Na is the system size, and the (IR) divergence is a 1d artifact. For future reference, these effects of fluctuations of the lattice on photon scattering are called *Debye-Waller factors*.

Scalar field theory in one dimension

Notice that if we use the path integral description, some of these things (in particular the continuum, sound-wave limit) are more obvious-seeming. The path integral for our collection of oscillators is

$$Z = \int [dq_1 \cdots dq_N] e^{iS[q]}$$

with $S[q] = \int dt \left(\sum_n \frac{1}{2} m_n \dot{q}_n^2 - V(\{q\}) \right)$. $V(\{q\}) = \sum_n \frac{1}{2} \kappa (q_{n+1} - q_n)^2$. Now let's try to take the continuum limit $a \to 0, N \to \infty$ (now N is the number of points in space, not in time like in the last chapter). Basically the only thing we need is to think of $q_n = q(x = na)$

ϕ_n Continuum Limit $\phi(x)$

$(n-1)a$ na $(n+1)a$
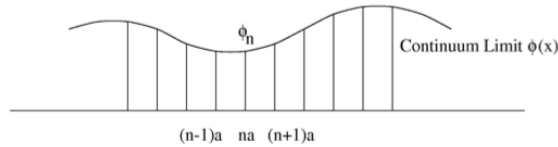
as defining a smooth function: [Note that the continuum field is often called $\phi(x)$ instead of $q(x)$ for some reason. At least the letters $q(x)$ and $\phi(x)$ look similar.]

We now have

$$(q_a - q_b)^2 \simeq a^2 (\partial_x q)^2$$

Now the path integral becomes:

$$Z = \int [Dq] e^{iS[q]}$$

with Dq now representing an integral over all configurations $q(t,x)$ (*defined* by this limit) and

$$S[q] = \int dt \int dx \frac{1}{2} \left(\mu (\partial_t q)^2 - \mu v_s^2 (\partial_x q)^2 - rq^2 - uq^4 - \ldots \right) \equiv \int dt \int dx \mathcal{L}$$

where I've introduced some parameters μ, v_s, r, u determined from m, κ... in some ways that we needn't worry about. $\mathcal{L}$ is the Lagrangian *density* whose integral over space is the Lagrangian $L = \int dx \mathcal{L}$.

The equation of motion (stationary phase condition) is

$$0 = \frac{\delta S}{\delta q(x,t)} = -\mu \ddot{q} - \mu v_s^2 \partial_x^2 q - rq - 2uq^3 - \ldots$$

From the phonon problem, we automatically found $r = u = 0$, and the equation of motion is just the wave equation (3). This happened because of the symmetry $q_n \to q_n + \epsilon$. This

is the operation that *translates* the whole crystal, It guarantees zero-energy phonons when $k = 0$ because it means $q(x)$ can only appear in S via its derivatives.

The following will be quite useful for our subsequent discussion of quantum light. Notice that we can construct a hamiltonian from this action by defining a canonical field-momentum $\pi(x) = \frac{\partial \mathcal{L}}{\partial_t q} = \mu \partial_t q$ and doing the Legendre transformation:

$$H = \sum_n (p_n \dot{q}_n - L_n) = \int dx \, (\pi(x)\dot{q}(x) - \mathcal{L}) = \int dx \left(\frac{\pi(x)^2}{2\mu} + \mu v_s^2 \left(\partial_x q(x) \right)^2 + rq^2 + uq^4 + ... \right) .$$

(4)

(Note that I suppress the dependence of all the fields on t just so it doesn't get ugly, not because it isn't there.)

If we were feeling fancy, we could now talk more about the *field operator*

$$\mathbf{q}(x) = \sqrt{\frac{\hbar}{2\mu}} \sum_k \frac{1}{\sqrt{\omega_k}} \left(e^{\mathbf{i}kx} \mathbf{a}_k + e^{-\mathbf{i}kx} \mathbf{a}_k^\dagger \right)$$

and its canonical conjugate momentum

$$\mathbf{p}(x) = \mathbf{i}\sqrt{\frac{\hbar\mu}{2}} \sum_k \sqrt{\omega_k} \left(e^{\mathbf{i}kx} \mathbf{a}_k - e^{-\mathbf{i}kx} \mathbf{a}_k^\dagger \right) .$$

($\mathbf{p}(x)$ is the quantum operator associated with the field-momentum π above.) Notice that the position along the chain x here is just a *label* on the fields, not a quantum operator.

The field q is called a *scalar field* because it doesn't have any indices decorating it. This is to be distinguished from the Maxwell field, which is a vector field, and which is our next subject. (Note that vibrations of a crystal in three dimensions actually do involve vector indices. We will omit this complication from our discussion.)

The lattice spacing a and the size of the box Na in the discussion above are playing very specific roles in *regularizing* our 1-dimensional scalar field theory. The lattice spacing a implies a maximum wavenumber or shortest wavelength and so is called an "ultraviolet (UV) cutoff", because the UV is the short-wavelength end of the visible light spectrum. The size of the box Na implies a maximum wavelength mode which fits in the box and so is called an "infrared (IR) cutoff".

[End of Lecture 22]

Continuum (free) scalar field theory in $d+1$ dimensions

Notice that these continuum expressions are easy to generalize to scalar field theory in any number of dimensions:

$$\mathbf{H} = \int d^d x \left(\frac{\boldsymbol{\pi}(x)^2}{2\mu} + \frac{1}{2}\mu v_s^2 \left(\vec{\nabla}\phi \cdot \vec{\nabla}\phi \right)^2 \right).$$

Again, think of $q_n(t) \equiv \boldsymbol{\phi}(x_n, t), p_n(t) \equiv \boldsymbol{\pi}(x_n, t)$ as defining the fields via their values at the grid points. A translation invariant problem is solved by Fourier transforms: $\phi(x) = \frac{1}{\sqrt{L^d}} \sum_k e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \phi_k, \boldsymbol{\pi}(x) = \frac{1}{\sqrt{L^d}} \sum_k e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \boldsymbol{\pi}_k$, this is

$$\mathbf{H} = \sum_k \left(\frac{1}{2\mu} \boldsymbol{\pi}_k \boldsymbol{\pi}_{-k} + \frac{1}{2}\mu v_s^2 k^2 \phi_k \phi_{-k} \right)$$

where $k^2 = (-\mathbf{i}\vec{k}) \cdot (\mathbf{i}\vec{k}) = \vec{k} \cdot \vec{k}$. Using

$$\phi_k \equiv \sqrt{\frac{\hbar}{2\mu\omega_k}} \left(\mathbf{a}_k + \mathbf{a}_{-k}^\dagger \right), \boldsymbol{\pi}_k \equiv \frac{1}{\mathbf{i}} \sqrt{\frac{\hbar\mu\omega_k}{2}} \left(\mathbf{a}_k - \mathbf{a}_{-k}^\dagger \right),$$

this is

$$\mathbf{H} = \sum_k \hbar\omega_k \left(\mathbf{a}_k^\dagger \mathbf{a}_k + \frac{1}{2} \right).$$

The field operators

$$
\begin{aligned}
\phi(x) &= \sum_k \sqrt{\frac{\hbar}{2\mu\omega_k}} \left(e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k + e^{\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k^\dagger \right), \\
\boldsymbol{\pi}(x) &= \frac{1}{\mathbf{i}} \sum_k \sqrt{\frac{\hbar\mu\omega_k}{2}} \left(e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k - e^{\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k^\dagger \right),
\end{aligned}
$$

satisfy the canonical commutation relation

$$[\phi(\vec{x}), \boldsymbol{\pi}(\vec{x}')] = \mathbf{i}\hbar \mathbb{1}\delta^d(\vec{x} - \vec{x}').$$

This is really the same equation as our starting point for each ball on springs:

$$[\mathbf{q}_n, \mathbf{p}_{n'}] = \mathbf{i}\hbar \mathbb{1}\delta_{nn'}.$$

3.2.2 Quantum light: Photons

The quantization of the Maxwell field is logically very similar to the preceding discussion. There are just a few complications from its several polarizations, and from the fact that quantum mechanics means that the vector potential is real and necessary (whereas classically it is just a convenience).

Maxwell's equations are :

$$\vec{\nabla} \cdot \vec{B} = 0, \quad \vec{\nabla} \times \vec{E} = -\partial_t \vec{B}, \tag{5}$$

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho, \quad \nabla \times \vec{B} = \partial_t \vec{E} + \frac{4\pi}{c}\vec{j}. \tag{6}$$

The first two equations (5) are constraints on $\vec{E}$ and $\vec{B}$ which mean that their components are not independent. This is annoying for trying to treat them quantumly. To get around this we introduce *potentials* which determine the fields by taking derivatives and which automatically solve the constraints (5):

$$\vec{E} = -\vec{\nabla}\Phi - \partial_t \vec{A}, \quad \vec{B} = \vec{\nabla} \times \vec{A}.$$

Potentials related by a *gauge transformation*

$$\vec{A} \to \vec{A}^\lambda = \vec{A} - \vec{\nabla}\lambda, \quad \Phi \to \Phi^\lambda = \Phi + \partial_t \lambda$$

for any function $\lambda(\vec{r}, t)$, give the same $\vec{E}, \vec{B}$. The Bohm-Aharonov effect (below) is proof that (some of the information in) the potential is real and useful, despite this redundancy. We can partially remove this redundancy be choosing our potentials to satisfy *Coulomb gauge*

$$\vec{\nabla} \cdot \vec{A} = 0 \ .$$

In the absence of sources $\rho = 0 = \vec{j}$, we can also set $\Phi = 0$. In this gauge, Ampere's law becomes

$$c^2 \vec{\nabla} \times \left(\vec{\nabla} \times \vec{A}\right) = c^2 \vec{\nabla} \cdot \left(\vec{\nabla} \cdot \vec{A}\right) - c^2 \nabla^2 \vec{A} = -\partial_t^2 \vec{A} \quad i.e. \ \boxed{\partial_t^2 \vec{A} - c^2 \nabla^2 \vec{A} = 0}.$$

This wave equation is different from our scalar wave equation (3) in three ways:

- we're in three spatial dimensions,

- the speed of sound v_s has been replaced by the speed of light c,

- the field $\vec{A}$ is a vector field obeying the constraint $\vec{\nabla} \cdot \vec{A} = 0$. In fourier space $\vec{A}(x) = \sum_k e^{i\vec{k}\cdot\vec{x}}\vec{A}(k)$ this condition is

$$0 = \vec{k} \cdot \vec{A}(k)$$

  – the vector field is *transverse*.

Recall that the energy density of a configuration of Maxwell fields is $u = \frac{\epsilon_0}{2}\left(\vec{E}^2 + \vec{B}^2\right)$. So the quantum Hamlitonian is

$$\mathbf{H} = \frac{\epsilon_0}{2}\int d^3r\left(\vec{E}^2 + c^2\vec{B}^2\right) \quad . \tag{7}$$

Here $\vec{E} = -\partial_t\vec{A}$ plays the role of field momentum $\pi(x)$ in (4), and $\vec{B} = \vec{\nabla}\times\vec{A}$ plays the role of the spatial derivative $\partial_x q$. We immediately see that we can quantize this system just like for the scalar case, with the canonical commutator

$$[\phi(x), \pi(x')] = \mathbf{i}\hbar\delta(x-x') \qquad \leadsto \qquad [\mathbf{A}_i(\vec{r}), \mathbf{E}_j(\vec{r}')] = -\mathbf{i}\hbar\delta^3(\vec{r}-\vec{r}')\delta_{ij}$$

where $i, j = 1..3$ are spatial indices. [2] So we can immediately write down an expression for the quantum Maxwell field in terms of independent creation and annihilation operators:

$$\vec{A}(\vec{r}) = \sum_{\vec{k}}\sqrt{\frac{\hbar}{2\epsilon_0\omega_k L^3}}\sum_{s=1,2}\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}} + \mathbf{a}_{\vec{k},s}^\dagger\vec{e}_s^\star(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}}\right)$$

The field momentum is $\vec{\mathbf{E}} = -\partial_t\vec{A}$:

$$\vec{\mathbf{E}}(\vec{r}) = \mathbf{i}\sum_{\vec{k}}\sqrt{\frac{\hbar\omega_k}{2\epsilon_0 L^3}}\sum_{s=1,2}\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}} - \mathbf{a}_{\vec{k},s}^\dagger\vec{e}_s^\star(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}}\right)$$

[3] Also, the magnetic field operator is

$$\vec{\mathbf{B}} = \vec{\nabla}\times\vec{A} = \sum_{\vec{k}}\sum_s\sqrt{\frac{\hbar}{2\epsilon_0\omega_k L^3}}\mathbf{i}\vec{k}\times\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}} - \mathbf{a}_{\vec{k},s}^\dagger\vec{e}_s^\star(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}}\right)$$

Plugging these expressions into the Hamiltonian (7), we can write it in terms of these oscillator modes (which create and annihilate *photons*). As for the scalar field, the definitions of these modes were designed to make this simple: It is:

$$\mathbf{H} = \sum_{\vec{k},s}\hbar\omega_k\left(\mathbf{a}_{\vec{k},s}^\dagger\mathbf{a}_{\vec{k},s} + \frac{1}{2}\right).$$

---

[2] As a check, note that using this Hamiltonian and the canonical commutator, we can reproduce Maxwell's equations using Ehrenfest's theorem:

$$\langle\partial_t^2\vec{A}\rangle = \partial_t\langle\vec{E}\rangle = -\frac{\mathbf{i}}{\hbar}\langle[\mathbf{H}, \vec{E}]\rangle = \langle c^2\vec{\nabla}^2\vec{A}\rangle.$$

[3] I am short-changing you a little bit here on an explanation of the *polarization vectors*, $\vec{e}_s$. They conspire to make it so that there are only two independent states for each $\vec{k}$ and they are transverse $\vec{k}\cdot\vec{e}_s(\hat{k}) = 0$, so $s = 1, 2$. Le Bellac discusses this more carefully than we have time for. The bit that I'm leaving out is the completeness relation satisfied by the polarization vectors of a given k:

$$\sum_s e_{si}(\hat{k})e_{sj}^\star(\hat{k}) = \delta_{ij} - \hat{k}_i\hat{k}_j \quad .$$

This says that they span the plane perpendicular to $\hat{k}$.

Notice that the vacuum energy is

$$E_0 = \frac{1}{2} \sum_{\vec{k},s} \hbar\omega_k = \frac{L^3}{(2\pi)^3} \int d^3k\, \hbar ck.$$

The fact that $\sum_k$ is no longer a finite sum might be something to worry about. We will see below in 3.3 that this vacuum energy has physical consequences.

Consolidation of understanding

So far in this chapter, we have studied systems of increasing complexity: the simple harmonic oscillator, a scalar field, and the EM field. They all have the same structure, in the following sense.

In the following, Here $\operatorname{Re}\mathbf{A} \equiv \frac{1}{2}\left(\mathbf{A} + \mathbf{A}^\dagger\right)$ as usual. The normalization constant is $\mathcal{N} = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}$.

$$\mathbf{H}_{SHO} = \frac{1}{2m}\mathbf{p}^2 + \frac{1}{2}m\omega^2\mathbf{x}^2 = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\right)$$

$$[\mathbf{x},\mathbf{p}] = \mathrm{i}\hbar \implies [\mathbf{a},\mathbf{a}^\dagger] = \mathbb{1}.$$

$$\mathbf{x} = \operatorname{Re}\mathcal{N}\mathbf{a}, \quad \mathbf{p} = m\operatorname{Im}\omega\mathcal{N}\mathbf{a}.$$

$$\mathbf{H}_{scalar} = \int dx\left(\frac{1}{2\mu}\boldsymbol{\pi}^2 + \frac{1}{2}\mu c^2\boldsymbol{\phi}^2\right) = \sum_k \hbar\omega_k\left(\mathbf{a}_k^\dagger\mathbf{a}_k + \frac{1}{2}\right)$$

$$[\boldsymbol{\phi}(x),\boldsymbol{\pi}(x')] = \mathrm{i}\hbar\delta(x - x') \implies [\mathbf{a}_k,\mathbf{a}_{k'}^\dagger] = \mathrm{i}\hbar\delta_{kk'}.$$

$$\boldsymbol{\phi}(x) = \operatorname{Re}\left(\sum_k \mathcal{N}_k e^{\mathrm{i}kx}\mathbf{a}_k\right), \quad \boldsymbol{\pi}(x) = \mu\operatorname{Im}\left(\sum_k \omega_k\mathcal{N}_k e^{\mathrm{i}kx}\mathbf{a}_k\right).$$

$$\mathbf{H}_{EM} = \int d^3x\left(\frac{\epsilon_0}{2}\vec{\mathbf{E}}^2 + \frac{\epsilon_0 c^2}{2}\vec{\mathbf{B}}^2\right) = \sum_{k,s=1,2} \hbar\omega_k\left(\mathbf{a}_{ks}^\dagger\mathbf{a}_{ks} + \frac{1}{2}\right)$$

$$[\mathbf{A}_i(x),\mathbf{E}_j(x')] = \mathrm{i}\hbar\delta^3(x - x')\delta_{ij} \implies [\mathbf{a}_{ks},\mathbf{a}_{k's'}^\dagger] = \mathrm{i}\hbar\delta_{kk'}\delta_{ss'}.$$

$$\vec{\mathbf{A}}(x) = \operatorname{Re}\left(\sum_k \mathcal{N}_k e^{\mathrm{i}\vec{k}\cdot\vec{x}}\mathbf{a}_{ks}\vec{e}_s(\hat{k})\right), \quad \vec{\mathbf{E}}(x) = \mu\operatorname{Im}\left(\sum_k \omega_k\mathcal{N}_k e^{\mathrm{i}\vec{k}\cdot\vec{x}}\mathbf{a}_{ks}\vec{e}_s(\hat{k})\right).$$

Note that $\vec{\mathbf{E}}$ is the canonical momentum of $\vec{\mathbf{A}}$ since (in Coulomb gauge) $\vec{E} = -\partial_t\vec{A}$.

Mössbauer more microscopically

Again for recreational purposes, so you can see the photon machinery in action, we return to our discussion of the Mössbauer effect. Now we can answer in more detail the question: where did that $\mathbf{H}_{\text{int}}$ that we used in the Mössbauer effect come from? This requires information from all of the previous subsections: it involves both phonons and photons. A more microscopic description of the transition rate would include the radiation field, too:

$$W(N_i, L_i, R_i \to N_f, L_f, R_f) \propto |\langle f|\mathbf{H}_{\text{int}}|i\rangle|^2,$$

where now $N_{i,f}, L_{i,f}, R_{i,f}$ denote initial and final states of the nucleus, lattice and radiation field, respectively. We are working in a big hilbert space $\mathcal{H} = \mathcal{H}_N \otimes \mathcal{H}_L \otimes \mathcal{H}_R$.

Again we ignore the nuclear stuff:

$$W(N_i, L_i, R_i \to N_f, L_f, R_f) \propto |\langle L_f| \otimes \langle R_f|\mathbf{H}_{LR}|L_i\rangle \otimes |R_i\rangle|^2.$$

The final state of the radiation field is the vacuum, no photons:

$$\langle R_f| = {}_R\langle 0|$$

which is annihilated by the phonon annihilation operators: ${}_R\langle 0|\mathbf{a}_K^\dagger = 0$. The initial state is one photon of momentum K (whose polarization I will not specify but really we should):

$$|R_i\rangle = |K\rangle_R = \mathbf{a}^\dagger|0\rangle_R \ .$$

What is the interaction hamiltonian $\mathbf{H}_{\text{int}}$? You have figured this out on HW 7. The hamiltonian for a charged particle (such as an ion in the solid) in an EM field is

$$\mathbf{H}_1 = \frac{1}{2m}\left(\vec{\mathbf{p}} + e\vec{\mathbf{A}}(\mathbf{x})\right)^2 = \frac{1}{2m}\left(\mathbf{p}^2 + e\mathbf{p}\mathbf{A} + e\mathbf{A}\mathbf{p} + e^2\mathbf{A}^2\right) = \frac{\mathbf{p}^2}{2m} + \mathbf{H}_{\text{int}}.$$

Think of e as small, so that we may treat $\mathbf{H}_{\text{int}}$ as a perturbation. Here we should use our expression above for the quantized photon field:

$$\mathbf{A}(x) \sim \sum_K \left(\mathbf{a}_K e^{iKx} + \mathbf{a}_K^\dagger e^{-iKx}\right).$$

The catch here is that we have to evaluate this *at the location of the ion*, which means that the x appearing in the argument is an operator, $\mathbf{x}$!

The final term in $\mathbf{H}_1$ proportional to $\mathbf{A}^2$ annihilates two photons or zero photons and so doesn't participate in the process we are talking about where one photon is absorbed. So we just need to think about the middle terms with one $\mathbf{A}$. The $\mathbf{p}$ is pretty innocuous:

$$\mathbf{p}e^{iK\mathbf{x}} + e^{iK\mathbf{x}}\mathbf{p} = (\mathbf{p} + K)\,e^{iK\mathbf{x}}$$

and we'll just focus on the second term. So the matrix element is:

$$
\begin{aligned}
W \quad \propto \quad & |\langle L_f| \otimes {}_R\langle 0|e^{i\mathbf{K}\mathbf{x}}\mathbf{a}_K|L_i\rangle \otimes \mathbf{a}_K^\dagger|0\rangle_R|^2 \\
= \quad & |\langle L_f|e^{i\mathbf{K}\mathbf{x}}|L_i\rangle|^2 \, |{}_R\langle 0|\mathbf{a}_K\mathbf{a}_K^\dagger|0\rangle_R|^2 = |\langle L_f|e^{i\mathbf{K}\mathbf{x}}|L_i\rangle|^2
\end{aligned}
$$

which is our previous expression.

3.3   Casimir effect: vacuum energy is real

[Le Bellac, 11.5.12 page 399; A. Zee, *Quantum Field Theory in a Nutshell*] This subsection has two purposes. One is to show that the $\frac{1}{2}\hbar\omega$ energy of the vacuum of the quantum harmonic oscillator is real. Sometimes we can get rid of it by choosing the zero of energy (which doesn't matter unless we are studying dynamical gravity). But it is meaningful if we can *vary* ω (or the collection of ωs if we have many oscillators as for the radiation field) and compare the difference.

The other purpose is to give an object lesson in asking the right questions. In physics, the right question is often a question which can be answered by an experiment, at least in principle. The answers to such questions are less sensitive to our silly theoretical prejudices, *e.g.* about what happens to physics at very short distances.

In the context of the bunch of oscillators making up the radiation field, we can change the spectrum of frequencies of these oscillators $\{\omega_k\}$ by putting it in a box and varying the size of the box. In particular, two parallel conducting plates separated by some distance d experience an attractive force from the change in the vacuum energy of the EM field resulting from their presence. The plates put boundary conditions on the field, and therefore on which normal modes are present.

To avoid some complications of E&M which are not essential for our point here, we're going to make two simplifications:

- we're going to solve the problem in 1+1 dimensions

- and we're going to solve it for a scalar field.

To avoid the problem of changing the boundary conditions *outside* the plates we use the following device with *three* plates:

$$| \leftarrow d \rightarrow | \longleftarrow \qquad L - d \qquad \longrightarrow |$$

(We will consider $L \gg d$, so we don't really care about the far right plate.) The 'perfectly conducting' plates impose the boundary condition that our scalar field $q(x)$ vanishes there. The normal modes of the scalar field $q(x)$ in the left cavity are then

$$q_j = \sin\left(j\pi x/d\right), \quad j = 1, 2, \ldots$$

with frequencies $\omega_j = \frac{\pi|j|}{d}c$. There is a similar expression for the modes in the right cavity which we won't need. We're going to add up all the $\frac{1}{2}\hbar\omega$s for all the modes in both cavities to get the vacuum energy $E_0(d)$; the force on the middle plate is then $-\partial_d E_0$.

The vacuum energy between the outer plates is the sum of the vacuum energies of the two cavities

$$E_0(d) = f(d) + f(L - d)$$

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where
$$f(d) = \frac{1}{2}\hbar c \sum_{j=1}^{\infty} \omega_j = \hbar c \frac{\pi}{2d} \sum_{j=1}^{\infty} j \overset{?!?!!}{=} \infty.$$

We have done something wrong. Our crime is hubris: we assumed that we knew what the modes of arbitrarily large mode number k (arbitrarily short wavelength, arbitrarily high frequency) are doing, and in particular we assumed that they cared about our silly plates. In fact, no metal in existence can put boundary conditions on the modes of large enough frequency – those modes don't care about d. The reason a conductor puts boundary conditions on the EM field is that the electrons move around to compensate for an applied field, but there is a limit on how fast the electrons can move (*e.g.* the speed of light). The resulting cutoff frequency is called the *plasma frequency* but we don't actually need to know about all these details. To parametrize our ignorance of what the high-frequency modes do, we must *cut off* (or *regularize*) the contribution of the high-frequency modes. Let's call modes with $\omega_j \gg \pi/a$ high frequency where a is some short time[4]. Replace

$$
\begin{aligned}
f(d) \rightsquigarrow f(a,d) &= \hbar \frac{\pi}{2d} \sum_{j=1}^{\infty} e^{-a\omega_j/\pi} j \\
&= -\frac{\pi\hbar}{2} \partial_a \underbrace{\left(\sum_{j=1}^{\infty} e^{-aj/d} \right)}_{= \frac{1}{1-e^{-a/d}} - 1} \\
&= +\frac{\pi\hbar}{2d} \frac{e^{a/d}}{\left(e^{a/d} - 1\right)^2} \\
&\overset{a \ll d}{\simeq} \hbar \left(\underbrace{\frac{\pi d}{2a^2}}_{\rightarrow \infty \text{ as } a \to 0} - \frac{\pi}{24d} + \frac{\pi a^2}{480d^3} + \dots \right)
\end{aligned}
\tag{8}
$$

Answers which don't depend on a have a chance of being meaningful. The thing we can measure is the force:

$$
\begin{aligned}
F &= -\partial_d E_0 = -\left(f'(d) - f'(L-d) \right) \\
&= -\hbar \left(\left(\frac{\pi}{2a^2} + \frac{\pi}{24d^2} + \mathcal{O}(a^2) \right) - \left(\frac{\pi}{2a^2} + \frac{\pi}{24\left(L-d\right)^2} + \mathcal{O}(a^2) \right) \right) \\
&\overset{a \to 0}{=} -\frac{\pi\hbar}{24} \left(\frac{1}{d^2} - \frac{1}{(L-d)^2} \right) \\
&\overset{L \gg d}{=} -\frac{\pi\hbar c}{24d^2} \left(1 + \mathcal{O}(d/L) \right) .
\end{aligned}
\tag{9}
$$

This is an attractive force between the plates. (I put the c back in the last line.)

---

[4]You can think of a as the time it takes the waves to move by one lattice spacing. If we work in units where the velocity is $c = 1$, this is just the lattice spacing. I will do so for the rest of this discussion.

The analogous force between real conducting plates, caused by the change of boundary conditions on the electromagnetic field has been measured.

The string theorists will tell you that $\sum_{j=1}^{\infty} j = -\frac{1}{12}$, and our calculation above agrees with them in some sense. But what this foolishness means is that if we compute something which is not dependent on the cutoff we have to get the same answer no matter what cutoff we use. Notice that it is crucial to ask the right questions.

An important question is to what extent could we have picked a different cutoff function (instead of $e^{-\pi\omega/a}$) and gotten the same answer for the physics. This interesting question is answered affirmatively in Zee's wonderful book, 2d edition, section I.9 (available electronically here!).

A comment about possible physical applications of the calculation we actually did: you could ask me whether there is such a thing as a Casimir force due to the vacuum fluctuations of *phonons*. Certainly it's true that the boundary of a chunk of solid puts boundary conditions on the phonon modes, which change when we change the size of the solid. The problem with the idea that this might produce a measurable force (which would lead the solid to want to shrink) is that it is hard to distinguish the 'phonon vacuum energy' from the rest of the *energy of formation* of the solid, that is, the energy difference between the crystalline configuration of the atoms and the configuration when they are all infinitely separated. Certainly the latter is not well-described in the harmonic approximation ($\lambda = 0$ in (1)).

A few comments about the 3+1 dimensional case of E&M.

Assume the size of the plates is much larger than their separation L. Dimensional analysis shows that the force per unit area from vacuum fluctuations must be of the form

$$P = A\frac{\hbar c}{L^4}$$

where A is a numerical number. A is not zero!

Use periodic boundary conditions in the xy planes (along the plates). The allowed wave vectors are then
$$\vec{k} = \left(\frac{2\pi n_x}{L_x}, \frac{2\pi n_y}{L_y}\right)$$
with n_x, n_y integers.

We have to do a bit of E&M here. Assume the plates are perfect conductors (this where the hubris about the high-frequency modes enters). This means that the transverse component of the electric field must vanish at the surface. Instead of plane waves in z, we get standing waves: $\phi(z) \propto \sin(n\pi z/L)$.

The frequencies of the associated standing waves are then

$$\omega_n(\vec{k}) = c\sqrt{\frac{\pi^2 n^2}{L^2} + \vec{k}^2}, n = 0, 1, 2$$

Also, there is only one polarization state for $n = 0$.

So the zero-point energy is

$$E_0(L) = \frac{\hbar}{2}\left(2\sum_{n,\vec{k}}' \omega_n(\vec{k})\right)$$

where it's useful to define

$$\sum_{n,\vec{k}}' \equiv \frac{1}{2}\sum_{n=0,\vec{k}} + \sum_{n\geq1,\vec{k}}$$

Now you can imagine introducing a regulator like the one we used above, and replacing

$$\sum_{n,\vec{k}}' \cdot \leadsto \sum_{n,\vec{k}}' e^{-a\omega_n(\vec{k})/\pi}.$$

and doing the sums and integrals and extracting the small-a behavior.

3.4 Identical particles: Bosons and fermions

[Griffiths chapter 5, Le Bellac chapter 13, Weinberg 4.5]

Every photon is the same as every other photon, except for their position (or momentum) and polarization state. For photons this is an immediate consequence of how we discovered them by quantizing the Maxwell field: the state with n photons of the same momentum and polarization is

$$|n \text{ photons with } \vec{k}, \alpha\rangle = \frac{\left(\mathbf{a}_{\vec{k},\alpha}^{\dagger}\right)^n}{\sqrt{n!}}|0\rangle.$$

The same is true of all the other kinds of particles we know about, including electrons (for which we haven't seen a similar classical field description).

This means that we can write the state of N such *indistinguishable particles* merely by specifying a collection of positions and of spin states – we don't need to say which is which (and in fact, we cannot).

A wavefunction for N such particles is of the form

$$\Psi(k_1, \alpha_1; ...; k_N, \alpha_N) \equiv \langle k_1\alpha_1; \cdots ; k_N, \alpha_N|\Psi\rangle = \langle 0|\mathbf{a}_{k_1\alpha_1}\mathbf{a}_{k_2\alpha_2}\cdots\mathbf{a}_{k_N\alpha_N}|\Psi\rangle.$$

But the same state is described if we switch the labels of any two of the particles:

$$\Psi(k_2, \alpha_2; k_1, \alpha_1; ....) = a\Psi(k_1, \alpha_1; k_2, \alpha_2; ....)$$

where a is some phase (recall: multiplying the whole wavefunction by a phase does not change the state). Switching them back gives back the first state:

$$\Psi(k_1, \alpha_1; k_2, \alpha_2; ....) = a^2\Psi(k_1, \alpha_1; k_2, \alpha_2; ....)$$

so $a^2 = 1$. There are two solutions: $a = +1$ and $a = -1$ and the two classes of particles associated with these two choices are called respectively *bosons* and *fermions*.

Note that the Hilbert space of N indistinguishable particles is therefore not quite a tensor product of the Hilbert spaces of the individual particles.

An immediate consequence of the minus sign under exchange of fermion labels is the *Pauli exclusion principle*:

$$\Psi_{\text{Fermions}}(k_1, \alpha_1; k_1, \alpha_1; ...) = 0.$$

No two fermions can occupy the same single-particle state. The ground state of a collection of (non-interacting) fermions is therefore quite interesting, since we must find a different single-particle state in which to put each of our fermions. This has many dramatic consequences, including the periodic table of elements, and the distinction between metals and insulators that we discuss next.

3.4.1 Band structure: metals and insulators

Now we will say some words about fermions in periodic potentials. This will allow us to quickly understand a way to distinguish metals and insulators.

Consider a collection of fermions which care about each other only because of the Pauli principle – the hamiltonian is a sum of terms involving the fermions one at a time. Suppose that each fermion (call them electrons) can live at one of N sites in a one dimensional crystal, and can hop from one to the next by some tunneling process. Further suppose that each site involves several (we'll say two for simplicity) atomic orbitals (or spin states), so the one-particle hilbert space is $\mathcal{H}_1 = \text{span}\{|n\rangle \otimes |\alpha\rangle, n = 1...N, \alpha = 0, 1\}$. We'll suppose that each electron is governed by the hamiltonian

$$\mathbf{H}_1 = -t \sum_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n| \right) \otimes \mathbb{1} + \sum_n |n\rangle\langle n| \otimes \epsilon |1\rangle\langle 1| \equiv \mathbf{H}_t + \mathbf{H}_\epsilon.$$

The first term allows the electrons to hop. The second term says that one of the orbitals has lower energy than the other ($|0\rangle$ is the ground state and $|1\rangle$ has energy $\epsilon > 0$).

What is the spectrum of $\mathbf{H}_1$, the hamiltonian of *one* electron hopping in this solid? The two terms commute $[\mathbf{H}_t, \mathbf{H}_\epsilon] = 0$, so we can simultaneously diagonalize them. Notice that the problem has a discrete translation invariance, which should be familiar by now. Moreover, it's just two copies of the problem on HW 2; the eigenstates are eigenstates of the momentum

$$|k\rangle \otimes |\alpha\rangle = \sum_n e^{ikna} |n\rangle \otimes |\alpha\rangle \qquad \alpha = 0, 1$$

with eigenvalues

$$\varepsilon_\alpha(k) = (2 - 2\cos ka) + \epsilon \delta_{\alpha,1}. \tag{10}$$

[5] For finite N, the allowed independent wave numbers are $\{k_j = \frac{2\pi}{Na} j, j = 1..N\}$. Here is the spectrum for $\epsilon/t = 6$, with $N = 60$ sites. There are $120 = 2N$ dots because this is
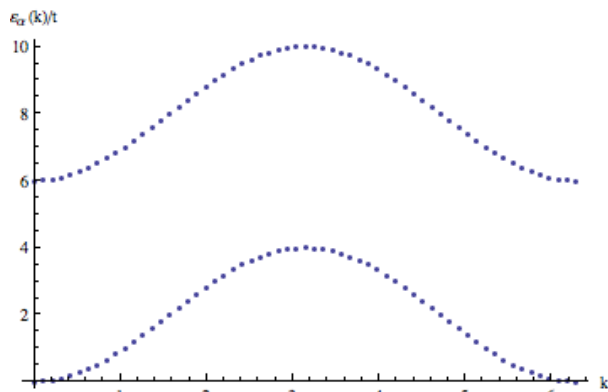

the size of our hilbert space. The two curves

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[5]I picked this example for simplicity so we don't waste time diagonalizing lots of matrices. More generally, it's interesting to consider a more interesting action of $\mathbf{H}_1$ on the orbital degree of freedom. This would give us more interesting bands.

are sometimes called 'bands'. This is because they describe *bands* of allowed energies. The *bandwidth* here is $4t$. In this plot there is a gap between the bands, which depends on ϵ.
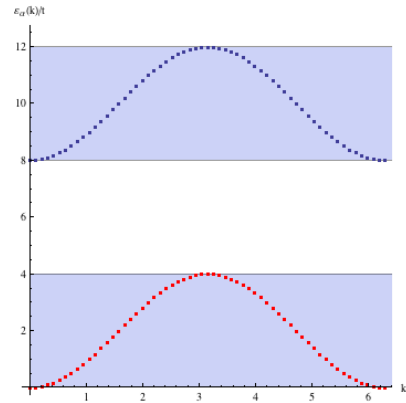

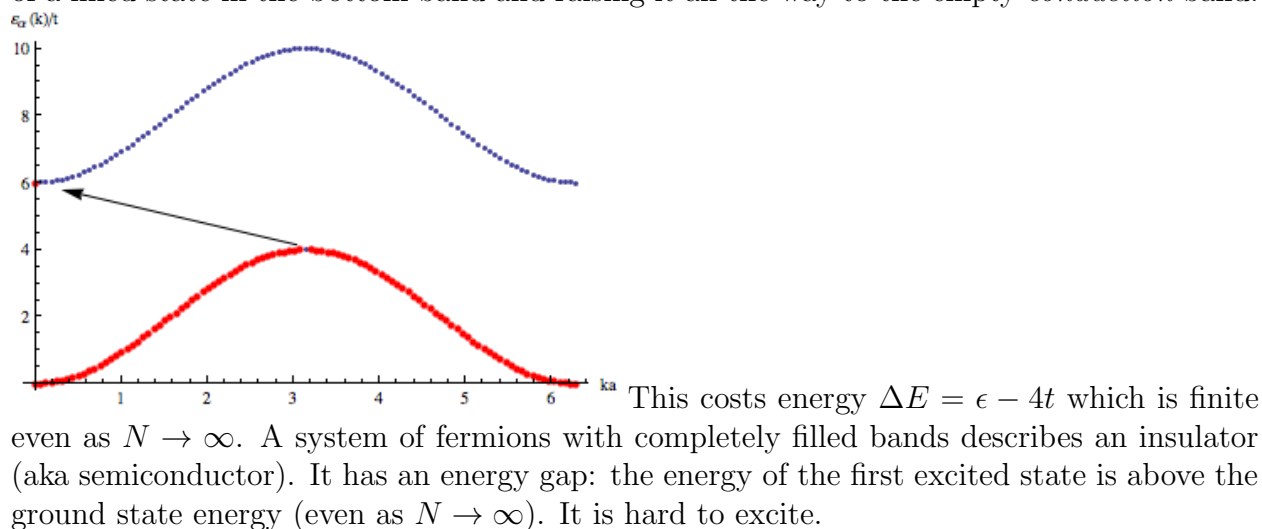Here the allowed bands of energies are highlighted:
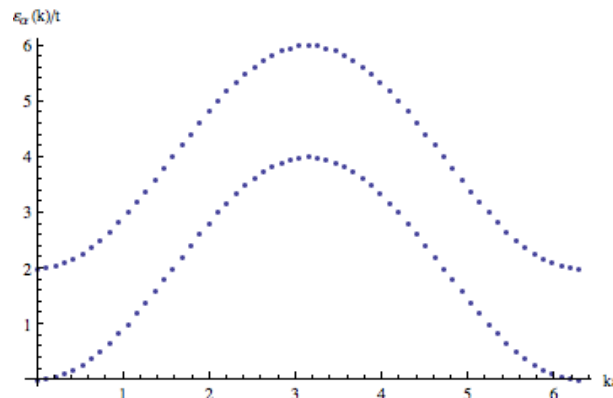
Here is the spectrum for $\epsilon/t = 2$:
Now the bands overlap.

To understand the important consequence of this distinction, now consider what happens if we have many fermions. If we have one fermion, the ground state is found by putting it in the lowest energy state, here $k = 0, \alpha = 0$. If we have two, the Pauli principle forces us to put them in different states; we should put the second (note that they don't really have an order) in the second lowest energy state; here it is $\alpha = 0, k = \frac{2\pi}{Na}$. Each fermion we add fills the next-lowest-energy state. So each dot in these figures is a possible cubbyhole in which to stash our electrons. In the ground state, the electrons pile up in the lowest holes.

Suppose we have N fermions – one per ion site. This is natural if we think of the ions as carrying positive charge; with N electrons the whole thing will be neutral and happy. The ground state is constructed by filling the lowest *half* of the one-electron states – we have $2N$ states altogether. If the bands don't overlap (if $\epsilon \gg t$, this means we just fill the bottom

band: Filled states are indicated in red.
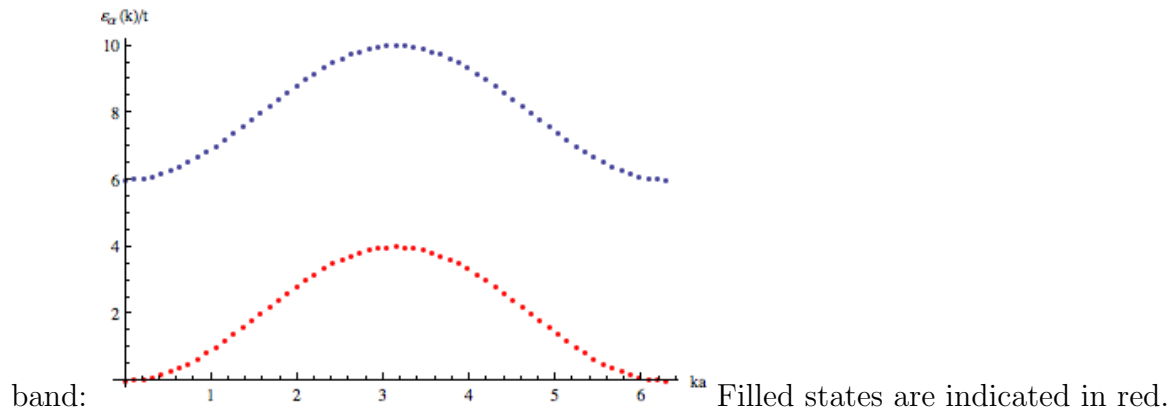
The lowest energy excitation of this system is achieved by taking one of the electrons out of a filled state in the bottom band and raising it all the way to the empty *conduction* band:

This costs energy $\Delta E = \epsilon - 4t$ which is finite even as $N \to \infty$. A system of fermions with completely filled bands describes an insulator (aka semiconductor). It has an energy gap: the energy of the first excited state is above the ground state energy (even as $N \to \infty$). It is hard to excite.

As we decrease the orbital energy difference ϵ, the excited atomic states start to matter and
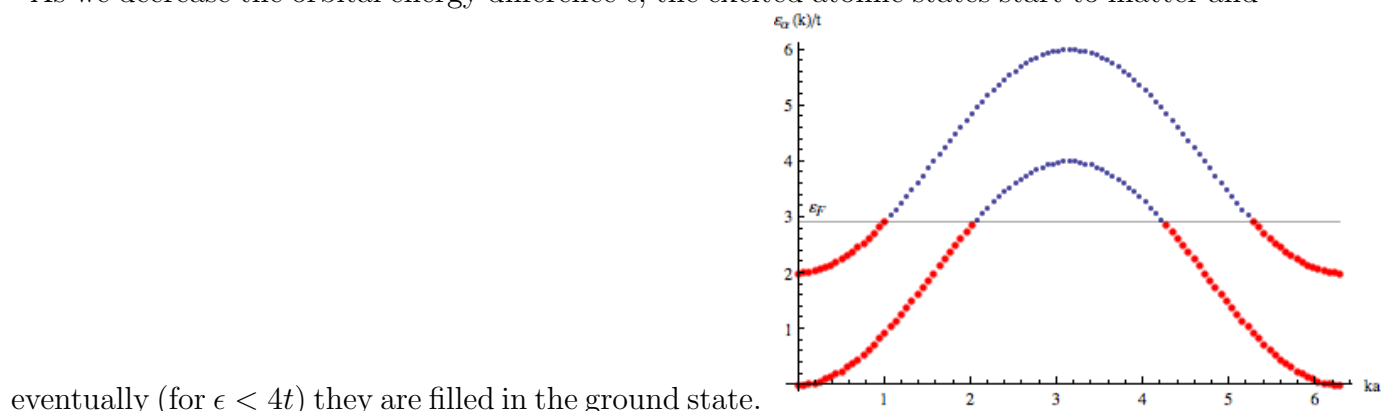
eventually (for $\epsilon < 4t$) they are filled in the ground state.
The name for the energy of the last filled level is the *Fermi energy* ε_F. (and the name of its momentum is the *Fermi momentum, k_F*). [6] Now the first excited state of the N-electron system is achieved by a very small change – we can stay in the same band. The energy cost

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[6]Partly because we chose such a simple example for our Hamiltonian, we find several (4) places where the bands cross the Fermi energy – several Fermi momenta.

to excite the system from the ground state is of order $\Delta k \partial_k \varepsilon|_{\varepsilon_F} \sim \frac{1}{N}$ (where $\Delta k = \frac{2\pi}{Na}$) which goes to zero as $N \to \infty$. There is no energy gap. When the Fermi energy is in the middle of a band, the system is a *metal*.

Groundstates of such macroscopic ($N \to \infty$) systems can be called *states of matter*. This sort of sharp distinction between possible behaviors of states of matter – like whether there is an energy gap – is the central preoccupation of condensed matter physics.

By the way, what we have really shown here is that when the Fermi energy is in the middle of the band, the system has very low-energy excitations. The fact that it actually conducts electricity is also a consequence of quantum mechanics. It happens because the wavefunctions of these low-energy excitations are *extended* across the material – they are (quasi-)momentum (k) eigenstates. This means that they can carry a current across the sample, $\mathrm{Im}\, \psi_k^{\star} \partial_x \psi_k \neq 0$. Notice that this picture departs dramatically from the classical (Drude) picture of charge transport by a charged particle bouncing around in the lattice. Notice that the form of the lattice is already built into the wavefunctions ψ_k!. (At this point we actually have the opposite problem that the answer we would compute for the resistance of such a metal is zero. To get the right finite answer we would need to include some form of *disorder* in the lattice, or interactions between the electrons.)

A quick comment about field theory of fermions, ignore it if you want. What is the analog of the description of the many-body system in terms of mode operators $\mathbf{a}_k$ that we had for phonons and photons? We can introduce operators that *create* and *annihilate* electrons just like we did before:

$$\mathbf{c}_{n\alpha}|0\rangle = 0, \quad \mathbf{c}_{n\alpha}^\dagger|0\rangle = |n\rangle \otimes |\alpha\rangle.$$

Notice that they are labelled by a position n and an orbital label $\alpha = 0, 1$. Our boson creation operators satisfied the algebra $1 = [\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a}$ (for each mode) and this led to boson statistics. We need somehow to prevent two electrons from being in the same state. We can accomplish this simply by demanding that

$$\boxed{\mathbf{c}^2 = 0}$$

for each mode, *i.e.* $\mathbf{c}_{n\alpha}^2 = 0 = \mathbf{c}_{n\alpha}^\dagger$. It's just zero. We also need to change a key sign:

$$1 = \{\mathbf{c}, \mathbf{c}^\dagger\} \equiv \mathbf{c}\mathbf{c}^\dagger + \mathbf{c}^\dagger\mathbf{c}.$$

This is called an *anticommutator*. With the labels the algebra should be:

$$\{\mathbf{c}_{n\alpha}, \mathbf{c}_{n'\alpha'}^\dagger\} = \delta_{\alpha\alpha'}\delta_{nn'}.$$

[7]

Now we can write the many-fermion Hamiltonian as

$$\mathbf{H}_{\text{many}} = -t\sum_n \left(\mathbf{c}_{n\alpha}^\dagger\mathbf{c}_{n+1,\alpha} + \mathbf{c}_{n+1,\alpha}^\dagger\mathbf{c}_{n\alpha}\right) + \sum_n \epsilon_{\alpha\beta}\mathbf{c}_{n\alpha}^\dagger\mathbf{c}_{n\beta}.$$

Above we have chosen the very simple case where $\epsilon_{\alpha\beta} = \begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix}$. This hamiltonian is diagonal by choosing a more favorable linear combination of the creation operators, namely momentum eigenstates:

$$\mathbf{c}_{\alpha k} \equiv \sum_n e^{ikx_n}\mathbf{c}_{n\alpha}$$

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[7]Note that each fermionic operator $\mathbf{c}$ satisfying

$$\mathbf{c}^2 = 0, \quad \{\mathbf{c}, \mathbf{c}^\dagger\} = 1$$

constructs the Hilbert space of a qbit as follows:

$$\mathbf{c}|\downarrow\rangle = 0, \quad \mathbf{c}^\dagger|\downarrow\rangle = |\uparrow\rangle.$$

The two states of the qbit just describe the presence or absence of the fermion in this state. Exercise: we can rewrite the Pauli operators as

$$\boldsymbol{\sigma}^x = \mathbf{c} + \mathbf{c}^\dagger, \quad \boldsymbol{\sigma}^y = \frac{1}{\mathbf{i}}\left(\mathbf{c} - \mathbf{c}^\dagger\right), \quad \boldsymbol{\sigma}^z = 2\mathbf{c}^\dagger\mathbf{c} - \mathbb{1}.$$

Also note that $\boldsymbol{\sigma}^+ = c^\dagger, \boldsymbol{\sigma}^- = c$ and the number operator $\mathbf{c}^\dagger\mathbf{c}$ (whose eigenvalues are 0 and 1) is $\mathbf{c}^\dagger\mathbf{c} = \boldsymbol{\sigma}^z + \mathbb{1}$.

in terms of which

$$\mathbf{H}_{\mathrm{many}} = \sum_{k,\alpha} \mathbf{c}_{\alpha k}^{\dagger} \mathbf{c}_{\alpha k} \varepsilon_\alpha(k)$$

with $\varepsilon_\alpha(k)$ given above in (10). The ground state is

$$|\text{ground state}\rangle = \prod_{N \ k, \alpha \text{ with the smallest } \epsilon_\alpha(k)} \mathbf{c}_{\alpha k}^{\dagger}|0\rangle.$$

3.5 Particles in electromagnetic fields

[Le Bellac 11.4, Shankar chapter 21]

3.5.1 Landau levels

You will have the opportunity to explore the huge degeneracy of the spectrum of a charged particle in a magnetic field on HW 8. The resulting physics is very rich and includes the *quantum Hall effects*. I highly recommend the discussion in Shankar chapter 21 on quantum Hall states.

3.5.2 Aharonov-Bohm effect

Consider the following situation. A infinite solenoid extends in the z direction.
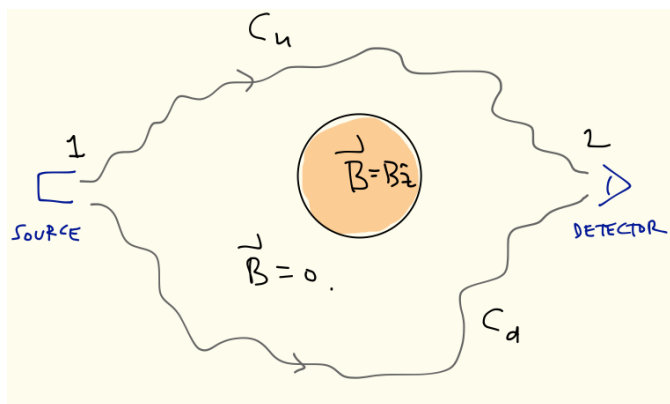
The figure depicts the xy-plane. The $\vec{B}$ field is only nonzero inside the solenoid and points out of the page $\vec{B} = \hat{z}B$. We treat it here as a fixed background field.

We send quantum mechanical charged particles from the source at left to the detector at right. They cannot enter the solenoid, but are otherwise free to proceed as they like. So they never move in a region where $\vec{B} \neq 0$. But we will show that the field affects them.

The path integral is very helpful here: We can group the possible paths (over which we integrate to find *e.g.* the amplitude Z for the particle to hit the detector) into two disconnected components: they either go above the solenoid or below it:

$$Z = \int [dx]... = \int [dx]_u... + \int [dx]_d...$$

The ... here is $e^{\frac{i}{\hbar}S[x]}$ with $S[x]$ the action for a charged particle that you found on HW7. In particular it has a term

$$S_A = \int_1^2 A \equiv e \int_1^2 \vec{A}(x) \cdot d\vec{x} = e \int_{t_1}^{t_2} A_i \frac{dx^i}{dt} dt$$

The vector potential is curl-free $\vec{\nabla} \times \vec{A} = 0$ in the region outside the solenoid – this is what it means that $\vec{B} = 0$. This means that the line integral S_A is *path-independent*. [8] For all the paths which go above the solenoid, the phase factor resulting from the $\int A$ term in the action is the same:

$$e^{\mathbf{i}e \int_{C_u} A}$$

for some fixed reference path C_u (in the figure). Similarly, all the paths below give a phase factor $e^{\mathbf{i}e \int_{C_d} A}$. But these phase factors from above and below are not the same: if we deform the path through the solenoid, we have to go through the region with $\vec{B} \neq 0$.

The probability of a particle hitting the detector is then

$$P = |Z_u e^{\mathbf{i}e \int_{C_u} A} + Z_d e^{\mathbf{i}e \int_{C_d} A}|^2 = |Z_u|^2 + |Z_d|^2 + \left(Z_u Z_d^\star e^{\mathbf{i}e \left(\int_{C_u} A - \int_{C_d} A \right)} + c.c. \right)$$

where $Z_{u,d}$ don't depend on the EM field at all.

But now

$$\left(\int_{C_u} A - \int_{C_d} A \right) = \int_{C_u - C_d} A = \int_{\text{inside}} \vec{B} \cdot d\vec{a} = B_z A \equiv \Phi \ .$$

So, for a simple example, if we arrange things symmetrically so that $Z_d = Z_u \equiv Z$, then

$$P = 2|Z|^2 \left(1 + \cos e\Phi \right) \ .$$

By varying B_z and hence the flux Φ, we can vary the intensity of particles hitting the detector! For example, we could choose $e\Phi = \pi$ to do total destructive interference.

But the particles never went near the region where the magnetic field was nonzero! They only know about it because of the vector potential. Score one more for quantum mechanics.

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[8]Recall from your E&M class that the difference between two paths is

$$\int_{C_1} \vec{A} \cdot d\vec{x} - \int_{C_2} \vec{A} \cdot d\vec{x} = \int_{C_1 - C_2} A = \int_D \vec{\nabla} \times \vec{A} \cdot d\vec{a} = \int_D \vec{B} \cdot d\vec{a}$$

by Stokes' theorem, where D is the region bounded by the paths. So as long as the $\vec{B}$-field vanishes in D, we can change the path without changing the phase.

Since we began the course with a quote from Sidney Coleman, it seems appropriate to end with one. Here is gedanken prank that he proposed. It's a really mean thing you can do to an experimentalist. A magnetic monopole is a *source* of magnetic flux, in the sense of a region of space around which $\oint \vec{B} \cdot d\vec{a} \neq 0$. No one has ever seen one[9].

Thread a very thin solenoid into the laboratory of the victim. If you set $e\Phi = 2\pi n, n \in \mathbb{Z}$, no Bohm-Aharonov experiment can detect the field, but flux will spill out the end of the solenoid and it will look like a magnetic monopole with a magnetic charge n. Just this kind of argument was used by Dirac to show that if magnetic monopoles exist, the electric charge must be quantized.

Concluding remarks

We've come quite far during this brief quarter. Starting from a clear statement of what quantum mechanics *is*, in Chapter 1, I hope to have convinced you that QM differs in many precise ways from classical physics. In particular, we saw a number of simple examples (mostly involving small collections of two-state systems) where QM could do classically-impossible things. Then in Chapter 2 we saw that QM nevertheless gives back classical mechanics when it should. And we understood something about why the peculiarities of QM are so unfamiliar to us, surrounded as we are by a large environment that we don't measure carefully. And finally in Chapter 3, we started to see what can happen when we put together large numbers of quantum degrees of freedom. In this way, we discovered a way (namely, quantum field theory) to describe systems where the number of particles can vary dynamically – where particles can be created and annihilated. We applied these ideas to sound and light and to metals and insulators. This technology is a basic tool in many parts of physics, in particular in high-energy particle physics and in quantum condensed matter physics (and for many of us is the basic object of study). There is a lot more to say about it. To learn more, I highly recommend the book by A. Zee.

Special thanks to those of you who helped improve the lecture notes and the problem sets with your feedback.

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[9]Actually, no one has ever seen *two*. One was probably detected at Stanford in the 1980s.