University of California at San Diego – Department of Physics – Prof. John McGreevy

Physics 212C QM Spring 2020
Assignment 9 – Solutions

Due 11:00am Wednesday, June 7, 2023

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1. **Peierls' instability.**

On a previous homework, we studied a Hamiltonian describing (spinless) fermions hopping on a chain:

$$H = -t\sum_n (1+u_n)c_n^\dagger c_{n+1} + h.c.$$

where u_n is some modulation of the hopping parameter. (The case we studied was when $u_n = u_{n+2}$, and we regarded c_{2n} and c_{2n-1} as two orbitals on a single site.) Consider an extension of the model to include also *phonon* modes, *i.e.* degrees of freedom encoding the positions of the ions in the solid. (Again we ignore the spins of the electrons for simplicity.)

$$H = -t\sum_n (1+u_n)c_n^\dagger c_{n+1} + h.c. + \sum_n K(u_n - u_{n+1})^2 \equiv H_F + H_E.$$

Here u_n is the deviation of the nth ion from its equilibrium position (in the $+x$ direction), so the second term represents an elastic energy.

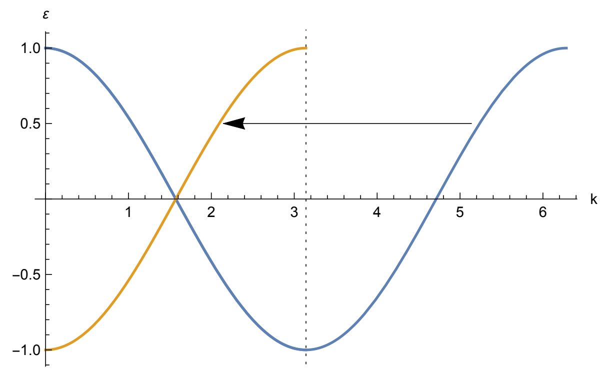
(a) Consider a configuration

$$u_n = \phi(-1)^n \tag{1}$$

where the ions move closer in pairs. Compute the single-particle electronic spectrum. (Hint: this enlarges the unit cell, making a fermionic analog of the problem of phonons in salt. Define $c_{2n} \equiv a_n, c_{2n+1} \equiv b_n$, and solve in Fourier space, $a_n \equiv \oint đk e^{2\mathbf{i}kna} a_k$ *etc*, where a is the lattice spacing.) You should find that when $\phi \neq 0$ there is a gap in the electron spectrum (unlike $\phi = 0$).

When doubling the unit cell, we halve the Brillouin zone. So even when

$\phi = 0$, the spectrum gets folded on itself, like this:

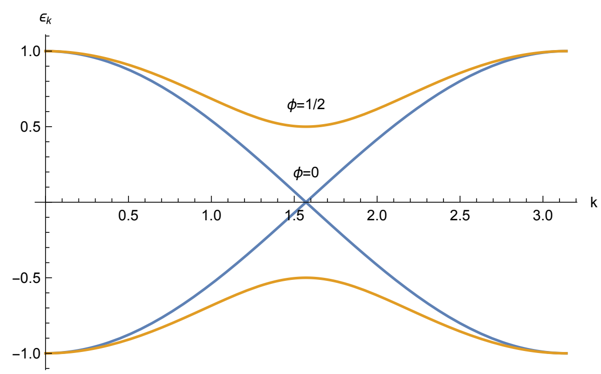


This means that at half-filling, with $\phi = 0$, it looks like there is a Dirac point at $k = \pi/2$.

Now, including ϕ, it allows the two branches of the Dirac point to mix with each other and produces a gap:

$$\epsilon(k) = \pm\sqrt{\cos^2 k + \phi^2 \sin^2 k}$$

which looks like this:



Near the minimum gap at $k = \pi/2$, we can expand to find

$$\epsilon(k = \frac{\pi}{2} + \delta k) = \pm\sqrt{\cos^2 k(1 - \phi^2) + \phi^2} = \pm\sqrt{\delta k^2(1 - \phi^2) + \phi^2}. \tag{2}$$

Comparing to the spectrum of a Dirac fermion with action

$$S[\psi, \phi] = \int d^2x \left(\bar{\psi}\mathbf{i}\partial\!\!\!/\psi - \phi\bar{\psi}\psi\right)$$

which has

$$H = \gamma^0(\mathbf{i}\gamma^1\partial_x - \phi) = \begin{pmatrix} \phi & k \\ k & -\phi \end{pmatrix}$$

and therefore

$$\epsilon_k = \pm\sqrt{k^2 + \phi^2}$$

which agrees with (2) at small k (which is really the deviation from $k = \pi/2$) and small ϕ.

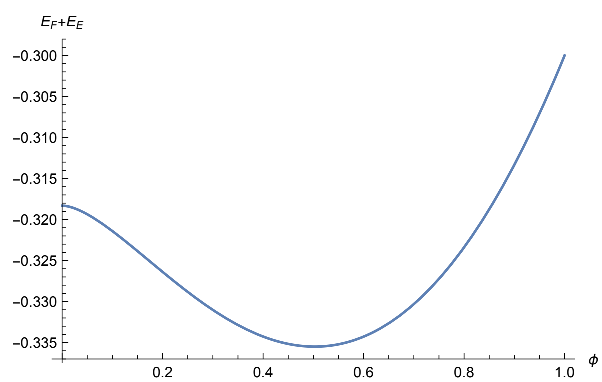
(b) Compute the many-body groundstate energy of H_F in the configuration (1), at half-filling (*i.e.* the number of electrons is half the number of available states).

Compute H_E in this configuration, and minimize (graphically) the sum of the two as a function of ϕ.

At half-filling, in the groundstate the lower band is filled. Note that the Brillouin Zone only extends from 0 to π now. The electronic energy density is

$$E_F(\phi) = -\fint_0^{\pi} dk \sqrt{\cos^2 k + \phi^2 \sin^2 k} = -\frac{1}{\pi}\text{EllipticE}(1-\phi^2).$$

For $8K^2 = .2$ the total energy looks like this:



There is a minimum at $\phi^2 \neq 0$, *i.e.* two minima at $\phi = \pm\phi_0$. Increasing ϕ lowers the total energy because it lowers the energy of the filled states.

(c) [Bonus problem] For large K, the value of ϕ at the minimum is pushed towards small values of ϕ. In that regime, we can approximate the electronic energy by the first few terms of its expansion about $\phi = 0$. Find an analytic expression for the minimum ϕ in this regime.

Actually, it is not quite analytic at $\phi = 0$, in the sense that *e.g.* $E_F''(0) = \int_0^{\pi} \text{đ}k \frac{\sin^2 k}{|\cos k|}$ has a logarithmic divergence at $k = \pi/2$. If we instead keep $\phi \neq 0$ but infinitesimal, the divergence is cut off by ϕ itself:

$$E_F''(\phi \ll 1) = \int \text{đ}k \frac{\sin^2 k}{\sqrt{\cos^2 k + \phi^2 \sin^2 k}} \sim \log\phi.$$

So this means there is a $\phi^2 \log\phi$ term. Mathematica's Series function will tell you (correctly) that

$$-\frac{1}{\pi}\text{EllipticE}(1-\phi^2) = -\frac{1}{\pi} + \frac{1}{4\pi}(1-\log 4\phi^2)\phi^2 + \mathcal{O}(\phi^3)$$

so the total energy is approximately

$$-\frac{1}{\pi} + \frac{1}{4\pi}(1-\log 4\phi^2)\phi^2 + \mathcal{O}(\phi^3) + 2K\phi^2$$

whose minimum occurs when

$$\phi = 4e^{-1-2K\pi}.$$

In retrospect, our approximation that ϕ is small when K is small is quite excellent.

(d) [Bonus problem: emergence of the Dirac equation] We can take a continuum limit of the above results. First, show that the low-energy excitations of $\mathbf{H}_0$ at a generic value of the filling are described the the massless Dirac Hamiltonian in 1+1 dimensions. The single-particle Dirac Hamiltonian in position space is: $h_{\text{Dirac}} = \gamma^0(\mathbf{i}\gamma^1\partial_x + m)$ where m is the mass, and $\gamma^0 = \sigma^1, \gamma^1 = \mathbf{i}\sigma^2$ are 2×2 matrices.

Show that the right-movers are right-handed (meaning eigenvectors of $\gamma^5 \equiv \gamma^0\gamma^1$ with eigenvalue 1) and the left-movers are left-handed (eigenvalue -1).

This system has a conserved charge $N \equiv \sum_n c_n^\dagger c_n$ counting the number of fermions, which we get to pick. The easiest way to do this is to add a chemical potential $H \to H - \mu N$ and choose μ to get the desired number of particles on average. (This is the same as fixing the number of particles in the thermodynamic limit.) In that case we have

$$H = -t\sum_n c_n^\dagger c_{n+1} + h.c. - \mu\sum_n c_n^\dagger c_n = \oint_{\text{BZ}} đk\, c_k^\dagger c_k \epsilon_k$$

with $\epsilon_k = -2t\cos ka - \mu$, and the integral is over the Brillouin zone. $a = 1$ is the lattice spacing. By 'generic filling' I mean choose the number of particles per site to be between 0 and 1. The former and latter correspond to choosing $\mu = \pm 2t$ at the bottom or top of the band, where the dispersion is quadratic, rather than linear.

We can focus on the physics at the two Fermi points $k = \pm k_F$ (where k_F solves $\epsilon_{k_F} = 0$) by plugging in

$$\psi(x) \simeq \int_R đk\, e^{(k_F+k)x}\psi_R + \int_R đk\, e^{(-k_F+k)x}\psi_L$$

where R is a small-enough region in momentum space that the two domains don't overlap. This gives

$$H = \int_R đk \left(v_F k \psi_R^\dagger \psi_R - v_F k \psi_L^\dagger \psi_L \right)$$

where $v_F \equiv \partial_k \epsilon_k|_{k=k_F}$. Translating into an action, setting $v_F = 1$, and pretending R goes on forever (this is how we can fool ourselves that the chiral current is conserved), this is

$$S = \int dxdt \left(\psi_R^\dagger \left(\partial_t - \partial_x\right) \psi_R + \psi_L^\dagger \left(\partial_t + \partial_x\right) \psi_L \right) = \int d^2x \left(\bar{\Psi} \gamma^\mu \partial_\mu \Psi\right)$$

with

$$\Psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$$

and

$$\gamma^0 = \sigma^1, \gamma^1 = \mathbf{i}\sigma^2, \gamma^5 \equiv \gamma^0\gamma^1 = -\sigma^3.$$

This gives

$$\gamma^5 \Psi = -\sigma^3 \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} = \begin{pmatrix} -\psi_L \\ \psi_R \end{pmatrix}$$

so indeed the left-moving particle has left-handed chirality.

(e) [Bonus problem] Next, include the coupling to phonons in the Dirac Hamiltonian. Expand the spectrum near the minimum gap and include the effects of the field ϕ in the continuum theory.

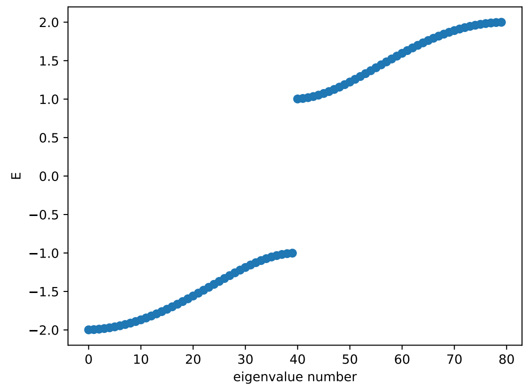
ϕ couples like the mass term.

(f) [Bonus problem] You should find above that the energy is independent of the *sign* of ϕ. This means that there are two groundstates. We can consider a domain wall between a region of $+$ and a region of $-$. Show that this domain wall carries a fermion mode whose energy lies in the bandgap and has fermion number $\pm\frac{1}{2}$.

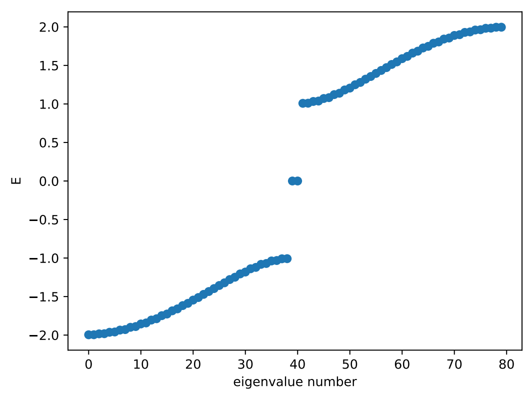
The basic idea is that ϕ must go through zero in between. The existence of a mid-gap fermion mode can be shown by solving the Dirac equation in the background of the domain wall. [This result is due to Jackiw and Rebbi.] In particular, the two states (zero-mode occupied and zero-mode unoccupied) must have a fermion number which differ by 1, but they are related to each other by the symmetry which exchanges particles and holes, so they must have fermion number $\pm\frac{1}{2}$.

(g) [Bonus problem] Diagonalize the relevant tight-binding matrix and find the mid-gap fermion mode.

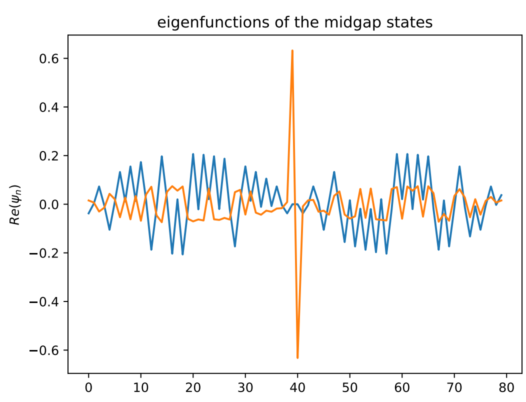
Here is the spectrum of a chain (of length 40) with $\phi = +0.5$ everywhere:



And here is the result when ϕ switches to -0.5 in the middle:



The wavefunctions of the states in the middle look like



(h) [Bonus problem] Time-reversal played an important role here. If we allow complex hopping amplitudes, show that we can make a domain wall without midgap modes.

If the mass is allowed to be complex, then we can interpolate between $-m$ and $+m$ without going through $m = 0$.

2. **Jordan-Wigner solution of the TFIM chain.**

Let's look at the TFIM again:

$$\mathbf{H}_{\text{TFIM}} = -J \sum_j \left(g\mathbf{X}_j + \mathbf{Z}_j \mathbf{Z}_{j+1} \right)$$

has a phase transition between large-g and small-g phases.

(a) Verify the following statements.

(Disordered) large g: excitations are created by $\mathbf{Z}_j$ – they are spin flips. The groundstate is a condensate of domain walls: $\langle \boldsymbol{\tau}^z \rangle \neq 0$. Here $\boldsymbol{\tau}^z_{\bar{j}} \equiv \prod_{j > \bar{j}} \mathbf{X}_j$ is the operator which creates a domain wall between sites j and $j+1$.

(Ordered) small g: excitations are created by the 'disorder' operator $\boldsymbol{\tau}^z_{\bar{j}}$ – they are domain walls. The groundstate is a condensate of spins $\langle \mathbf{Z}_j \rangle \neq 0$, *i.e.* a ferromagnet.

So we understand what are the 'correct variables' (in the sense that they create the elementary excitations above the groundstate) at large and small g. I claim that the Correct Variables *everywhere* in the phase diagram are obtained by "attaching a spin to a domain wall". These words mean the following: let

$$\begin{aligned} \boldsymbol{\chi}_j &\equiv \mathbf{Z}_j \boldsymbol{\tau}^z_{j+\frac{1}{2}} = \mathbf{Z}_j \prod_{j' > j} \mathbf{X}_{j'} \\ \tilde{\boldsymbol{\chi}}_j &\equiv \mathbf{Y}_j \boldsymbol{\tau}^z_{j+\frac{1}{2}} = -\mathbf{i}\mathbf{Z}_j \prod_{j' \geq j} \mathbf{X}_{j'} \end{aligned} \tag{3}$$

The first great virtue of this definition is that these operators agree with the creators of the elementary excitations in both regimes we've studied: When $g \ll 1$, $\langle \mathbf{Z}_j \rangle \simeq 1$ and more strongly, $\mathbf{Z}_j = \langle \mathbf{Z}_j \rangle +$ small, so $\boldsymbol{\chi}_j \simeq \langle \mathbf{Z}_j \rangle \boldsymbol{\tau}^z_{j+\frac{1}{2}} \simeq \boldsymbol{\tau}^z_{j+\frac{1}{2}}$, the domain wall creation operator. Similarly, when $g \gg 1$, $\boldsymbol{\tau}^z_{\bar{j}} \simeq 1+$ small, so $\boldsymbol{\chi}_j \simeq \mathbf{Z}_j \left\langle \boldsymbol{\tau}^z_{j+\frac{1}{2}} \right\rangle \simeq \mathbf{Z}_j$, which is the spin flipper on the paramagnetic vacuum.

(b) Now let us consider the algebra of these $\boldsymbol{\chi}$s. Verify that

- They are *real*: $\boldsymbol{\chi}_j^\dagger = \boldsymbol{\chi}_j, \tilde{\boldsymbol{\chi}}_j^\dagger = \tilde{\boldsymbol{\chi}}_j$.

and

- They are *fermionic*:

$$\text{if } i \neq j, \ \boldsymbol{\chi}_j \boldsymbol{\chi}_i + \boldsymbol{\chi}_i \boldsymbol{\chi}_j \equiv \{\boldsymbol{\chi}_j, \boldsymbol{\chi}_i\} = 0, \quad \{\tilde{\boldsymbol{\chi}}_j, \tilde{\boldsymbol{\chi}}_i\} = 0, \ \{\boldsymbol{\chi}_j, \tilde{\boldsymbol{\chi}}_i\} = 0. \quad (4)$$

This is because the spin flip $\mathbf{Z}_j$ in $\boldsymbol{\chi}_j$ changes sign when it moves through the domain wall created by $\boldsymbol{\chi}_i$.

When they are at the same site:

$$\boldsymbol{\chi}_j^2 = 1 = \tilde{\boldsymbol{\chi}}_j^2. \quad \text{In summary:} \quad \boxed{\{\boldsymbol{\chi}_i, \boldsymbol{\chi}_j\} = 2\delta_{ij}, \ \{\tilde{\boldsymbol{\chi}}_i, \tilde{\boldsymbol{\chi}}_j\} = 2\delta_{ij},}.$$

Notice that (4) means that $\boldsymbol{\chi}_i$ cares about $\boldsymbol{\chi}_j$ even if $|i-j| \gg 1$. Fermions are weird and non-local!

Recall from a previous homework that real fermion operators like this are called *Majorana* fermion operators. We can make more familiar-looking objects by making complex combinations:

$$\mathbf{c}_j \equiv \frac{1}{2}(\boldsymbol{\chi}_j - \mathbf{i}\tilde{\boldsymbol{\chi}}_j) \quad \Longrightarrow \quad \mathbf{c}_j^\dagger = \frac{1}{2}(\boldsymbol{\chi}_j + \mathbf{i}\tilde{\boldsymbol{\chi}}_j)$$

These satisfy the more familiar anticommutation relations:

$$\{\mathbf{c}_i, \mathbf{c}_j^\dagger\} = \delta_{ij}, \quad \{\mathbf{c}_i, \mathbf{c}_j\} = 0, \quad \{\mathbf{c}_i^\dagger, \mathbf{c}_j^\dagger\} = 0,$$

and in particular, $\left(\mathbf{c}_i^\dagger\right)^2 = 0$, like a good fermion creation operator should.

We can write $\mathbf{H}_{\text{TFIM}}$ in terms of the fermion operators. We just need to know how to write $\mathbf{X}_j$ and $\mathbf{Z}_j\mathbf{Z}_{j+1}$.

(c) Show that the operator that *counts* spin flips in the paramagnetic phase is

$$\mathbf{X}_j = -\mathbf{i}\tilde{\boldsymbol{\chi}}_j\boldsymbol{\chi}_j = -2\mathbf{c}_j^\dagger\mathbf{c}_j + 1 = (-1)^{\mathbf{c}_j^\dagger\mathbf{c}_j}.$$

To get this we can use (3) and $\mathbf{YZ} = \mathbf{iX}$ and $(\boldsymbol{\tau}^z)^2 = 1$. Even better: notice that $\tilde{\boldsymbol{\chi}}_j = +\mathbf{i}X_j\boldsymbol{\chi}_j$. Here $\mathbf{c}_j^\dagger\mathbf{c}_j = \mathbf{n}_j$ measures the number of fermions at the site j and is either 0 or 1, since they are fermions. At each site

$$|\rightarrow_j\rangle = |n_j = 0\rangle, \qquad |\leftarrow_j\rangle = |n_j = 1\rangle$$

like in the one-mode case discussed in lecture. The number of spin flips is the number of fermions.

(d) Show that the operator that counts domain walls is

$$\mathbf{Z}_j\mathbf{Z}_{j+1} = \mathbf{i}\tilde{\boldsymbol{\chi}}_{j+1}\boldsymbol{\chi}_j.$$

Check: $\mathbf{i}\tilde{\boldsymbol{\chi}}_{j+1}\boldsymbol{\chi}_j = \mathbf{i}\mathbf{Y}_{j+1}\prod_{k\geq j+2}\mathbf{X}_k\mathbf{Z}_j\prod_{l\geq j+1}\mathbf{X}_l = \left(\underbrace{\mathbf{i}\mathbf{Y}_{j+1}\mathbf{X}_{j+1}}_{=\mathbf{Z}_{j+1}}\right)\mathbf{Z}_j.$

(e) Conclude that

$$\mathbf{H}_{\text{TFIM}} = -J\sum_j\left(\mathbf{i}\tilde{\boldsymbol{\chi}}_{j+1}\boldsymbol{\chi}_j + g\mathbf{i}\boldsymbol{\chi}_j\tilde{\boldsymbol{\chi}}_j\right)$$

is quadratic in these variables, for any g! Free at last!

Comments:

- Notice that the relation

$$\mathbf{X}_j = 1 - 2\mathbf{c}_j^\dagger\mathbf{c}_j$$

is exactly implementing the simple idea that *spinless* fermions on a lattice produce two-states per site which we can regard as spin up or spin down (in this case it's up or down along x): The states $\mathbf{X} = \pm 1$ correspond to $\mathbf{c}^\dagger\mathbf{c} = 0$ and 1 respectively.

- Notice that the description in terms of majoranas is preferred over the complex fermions because the phase rotation symmetry generated by the fermion number $\mathbf{c}^\dagger\mathbf{c}$ is not a symmetry of $\mathbf{H}_{\text{TFIM}}$ – in terms of the $\mathbf{c}$s, it contains terms of the form $\mathbf{c}_j\mathbf{c}_{j+1}$ which change the total number of $\mathbf{c}$ fermions (by ± 2). It is the hamiltonian for a *superconductor*, in which the continuous fermion number symmetry is broken down to a $\mathbb{Z}_2$ subgroup. Fermion number is still conserved mod two, and this is the $\mathbb{Z}_2$ symmetry of the Ising model, which acts by $\mathbf{Z} \to -\mathbf{Z}$.

- A useful thing to remember about majorana operators $\{\chi, \gamma\} = 0$ is that $(\mathbf{i}\chi\gamma)^\dagger = -\mathbf{i}\gamma\chi = +\mathbf{i}\chi\gamma$ is hermitian.

- Another useful fact:

$$\mathbf{c}(-1)^{\mathbf{c}^\dagger\mathbf{c}} = -\mathbf{c} \tag{5}$$

which is true because the BHS only nonzero if the number is nonzero *before* the annihilation operator acts, in which case we get $(-1)^1$. Similarly (the conjugate equation), $(-1)^{\mathbf{c}^\dagger\mathbf{c}}\mathbf{c}^\dagger = -\mathbf{c}^\dagger$, and $(-1)^{\mathbf{c}^\dagger\mathbf{c}}\mathbf{c} = \mathbf{c}$ and so on.

- This procedure of "attaching spin to a domain wall" led to fermions. This maybe isn't so surprising in one dimension. But there are analogs of this procedure in higher dimensions. In 2+1 dimensions, an analog is to attach charge to a vortex (or to attach magnetic flux to charge). This leads to transmutation of statistics from bosons to fermions and more generally to anyons and the fractional quantized Hall effect. In 3+1 dimensions, an analog is attaching charge to a magnetic monopole to produce a 'dyon'; in this case, the angular momentum carried by the EM fields is half-integer.

(f) The hamiltonian is quadratic in the $\mathbf{c}$s, too, since they are linear in the $\boldsymbol{\chi}$s. In terms of complex fermions, show that

$$\mathbf{X}_j = 1-2\mathbf{c}_j^\dagger \mathbf{c}_j, \quad \mathbf{Z}_j = -\prod_{i>j}(1-2\mathbf{c}_i^\dagger \mathbf{c}_i)\left(\mathbf{c}_j + \mathbf{c}_j^\dagger\right) = -\prod_{i>j}(-1)^{\mathbf{c}_i^\dagger \mathbf{c}_i}\left(\mathbf{c}_j + \mathbf{c}_j^\dagger\right).$$

In terms of their Fourier modes $\mathbf{c}_k \equiv \frac{1}{\sqrt{N}}\sum_j \mathbf{c}_j e^{-\mathbf{i}kx_j}$, show that the TFIM hamiltonian is

$$\mathbf{H}_{\text{TFIM}} = J\sum_k \left(2(g-\cos ka)\mathbf{c}_k^\dagger \mathbf{c}_k - \mathbf{i}\sin ka\left(\mathbf{c}_{-k}^\dagger \mathbf{c}_k^\dagger + \mathbf{c}_{-k}\mathbf{c}_k\right) - g\right) .$$

(g) This Hamiltonian is quadratic in $\mathbf{c}_k$s, but not quite diagonal. It involves $c^\dagger c^\dagger$ terms, and is like a mean-field model of a superconductor. The solution for the spectrum involves one more operation the fancy name for which is 'Bogoliubov transformation', which is the introduction of new (complex) mode operators which mix particles and holes:

$$\boldsymbol{\gamma}_k = u_k \mathbf{c}_k - \mathbf{i}v_k \mathbf{c}_{-k}^\dagger$$

Demanding that the new variables satisfy canonical commutators $\{\boldsymbol{\gamma}_k, \boldsymbol{\gamma}_{k'}^\dagger\} = \delta_{k,k'}$ requires $u_k = \cos(\phi_k/2), v_k = \sin(\phi_k/2)$. We fix the angles ϕ_k by demanding that the hamiltonian in terms of $\boldsymbol{\gamma}_k$ be diagonal – no $\boldsymbol{\gamma}_k\boldsymbol{\gamma}_{-k}$ terms. Show that the resulting condition is $\tan\phi_k = \frac{\epsilon_2(k)}{\epsilon_1(k)}$ with $\epsilon_1(k) = 2J(g-\cos ka), \epsilon_2(k) = -2J\sin ka$, and $\mathbf{H} = \sum_k \epsilon_k\left(\boldsymbol{\gamma}_k^\dagger\boldsymbol{\gamma}_k - \frac{1}{2}\right)$, with $\epsilon_k = \sqrt{\epsilon_1^2+\epsilon_2^2}$.

The end result is that the exact single-particle (single $\boldsymbol{\gamma}$) dispersion is

$$\epsilon_k = 2J\sqrt{1+g^2-2g\cos ka} .$$

The argument of the sqrt is positive for $g \geq 0$. This is minimized at $k=0$, which tells us the exact gap at all g:

$$\epsilon_k \geq \epsilon_0 = 2J|1-g| = \Delta(g)$$

which, ridiculously, is just what we got from 1st order perturbation theory on each side of the transition.

3. **Brain-warmer.** Suppose we have a wavefunction Ψ of N bosons on a thin ring of radius R, governed by a Hamiltonian of the form

$$\mathbf{H} = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V(|r_{ij}|).$$

Let θ_i be the angular coordinate of the ith particle. Now suppose we make a new state $\Psi' = e^{-\mathbf{i}\sum_i \theta_i}\Psi$. Show that

$$\langle \Psi' | \mathbf{H} | \Psi' \rangle = \langle \Psi | \mathbf{H} | \Psi \rangle - \omega_c L + \frac{1}{2} I_{cl} \omega_c^2$$

where L is the expected angular momentum of the state $|\Psi\rangle$, $\omega_c \equiv \frac{\hbar}{mR^2}$, $I_{cl} = NmR^2$.

In cylindrical coordinates,

$$p^2 = -\hbar^2 \left(\partial_r^2 + \frac{1}{r^2}\partial_\theta^2 \right)$$

So the key bit is

$$\frac{\hbar^2}{2m} \int \Psi^\star e^{+\mathbf{i}\sum_i \theta_i} \sum_i \frac{1}{R^2} \partial_{\theta_i}^2 \left(e^{-\mathbf{i}\sum_i \theta_i} \Psi \right)$$

and we use the identity $\partial_\theta^2 (f_1 f_2) = f_1'' f_2 + 2 f_1' f_2' + f_2''$. The first term is $N\frac{\hbar^2}{2mR^2} = \frac{1}{2} I_{cl} \omega_c^2$. The cross-term is

$$- \langle \Psi | \mathbf{L} | \Psi \rangle \frac{\hbar}{mR^2} = -\omega_c L$$

where $\mathbf{L} = -\sum_i \mathbf{i}\hbar\partial_{\theta_i}$ is the total angular momentum operator.

4. **Excitations and energy of a weakly-interacting bose fluid.** [Khomski §5.2]

We can see the appearance of the sound mode in the continuum by the following treatment, where we regard the interaction strength as weak.

(a) Write the Hamiltonian

$$\mathbf{H} = \sum_p \mathbf{b}_p^\dagger \mathbf{b}_p \frac{p^2}{2m} + \int d^d r \int d^d r' V(|r - r'|) \mathbf{b}_r^\dagger \mathbf{b}_{r'}^\dagger \mathbf{b}_{r'} \mathbf{b}_r$$

entirely in terms of the momentum-space operators $\mathbf{b}_p, \mathbf{b}_p^\dagger$. After doing this, specialize to the case of contact interactions, *i.e.* $V(r_{ij}) = U\delta^d(r_{ij})$.

Using continuum normalization $\mathbf{b}_r = \frac{1}{\sqrt{V}} \sum_p e^{\mathbf{i} p\cdot r} \mathbf{b}_p$,

$$\mathbf{H} = \sum_p \mathbf{b}_p^\dagger \mathbf{b}_p \frac{p^2}{2m} + \int d^d r \int d^d r' \mathbf{b}_r^\dagger \mathbf{b}_{r'}^\dagger \mathbf{b}_{r'} \mathbf{b}_r V(|r-r'|) \tag{6}$$

$$= \sum_p \mathbf{b}_p^\dagger \mathbf{b}_p \frac{p^2}{2m} + \frac{U}{2V} \sum_{p_1 \cdots p_4} \delta^d(p_1+p_2-p_3-p_4) \tilde{V}(p_1-p_4) \mathbf{b}_{p_1}^\dagger \mathbf{b}_{p_2}^\dagger \mathbf{b}_{p_3} \mathbf{b}_{p_4}. \tag{7}$$

where $\tilde{V}(p) = \int d^d r e^{\mathbf{i} p\cdot r} V(r)$. Specializing to the case of contact interactions means $\tilde{V}$ is a constant.

(b) Here is the trick. In the BEC state, $\mathbf{b}_0^\dagger \mathbf{b}_0 = N_0 \sim N$. We will approximate such a state as a coherent state for $\mathbf{b}_0$ with eigenvalue $b_0 \sim \sqrt{N} \gg 1$, a complex number. Since the commutator $[\mathbf{b}_0^\dagger, \mathbf{b}] = 1 \ll N$ we make a small error by this approximation. We will treat all the other creation and annihilation operators $\mathbf{b}_{p\neq 0}$ as operators, but as *small*. That is, $\mathbf{b}_0 \sim b_0 = \mathcal{O}(\sqrt{N}), \mathbf{b}_p = \mathcal{O}(N^0)$.

Expand the Hamiltonian keeping only the terms of order N and larger, according to this counting.

To eliminate b_0, use the fact that the total number of particles is

$$N = |b_0|^2 + \sum_{p\neq 0} \mathbf{b}_p^\dagger \mathbf{b}_p$$

to write it in terms of $\mathbf{b}_{p\neq 0}, \mathbf{b}_{p\neq 0}^\dagger$.

The terms that survive must have at least two b_0s:

$$\mathbf{H} \simeq \sum_p \mathbf{b}_p^\dagger \mathbf{b}_p \frac{p^2}{2m} + \frac{U}{2V} \left(|b_0|^4 + \sum_p \left(4\mathbf{b}_p^\dagger \mathbf{b}_p |b_0|^2 + |b_0|^2 \mathbf{b}_p^\dagger \mathbf{b}_{-p}^\dagger + |b_0|^2 \mathbf{b}_p \mathbf{b}_{-p} \right) \right).$$

Following the hint, in this approximation, the b_0^4 term is

$$b_0^4 = \left(N - \sum_{p\neq 0} \mathbf{b}_p^\dagger \mathbf{b}_p \right)^2 = N^2 - 2N \sum_{p\neq 0} \mathbf{b}_p^\dagger \mathbf{b}_p + \mathcal{O}(N^0).$$

And to this order, we can replace $|b_0|^2$ with N in the $\mathcal{O}(N)$ terms:

$$\mathbf{H} \simeq \sum_p \mathbf{b}_p^\dagger \mathbf{b}_p \frac{p^2}{2m} + \frac{U}{2V} \left(N^2 - N \sum_p \left(2\mathbf{b}_p^\dagger \mathbf{b}_p + \mathbf{b}_p^\dagger \mathbf{b}_{-p}^\dagger + \mathbf{b}_p \mathbf{b}_{-p} \right) \right).$$

(c) In the previous part you found a hamiltonian that is quadratic in the $\mathbf{b}_{p\neq 0}, \mathbf{b}^\dagger_{p\neq 0}$. This is an Easy Problem (according to our classification). One way to solve it is to substitute

$$\mathbf{b}^\dagger_p = u_p \mathbf{a}_p + v_p \mathbf{a}^\dagger_{-p}, \quad \mathbf{b}_p = u_p \mathbf{a}^\dagger_p + v_p \mathbf{a}_{-p}$$

where the coefficients u_p, v_p are to be determined and can be assumed to be real, and even functions of p. [This is called a Bogoliubov transformation.] Show that demanding that $\mathbf{a}_p, \mathbf{a}^\dagger_p$ satisfy canonical boson commutation relations implies $u_p^2 - v_p^2 = 1$. Find $\mathbf{a}_p$ in terms of $\mathbf{b}_p, \mathbf{b}^\dagger_p$.

Just plug the definition in to $1 = [\mathbf{a}_p, \mathbf{a}^\dagger_p]$. The condition $[\mathbf{a}_p, \mathbf{a}_{p'}] = 0$ is automatic.

Using this relation, consider the combination

$$u_p \mathbf{b}^\dagger_p - v_p \mathbf{b}_{-p} = u_p^2 \mathbf{a}_p + u_p v_p \mathbf{a}^\dagger_{-p} - v_p u_p \mathbf{a}^\dagger_{-p} - v_p^2 \mathbf{a}_p = (u_p^2 - v_p^2)\mathbf{a}_p = \mathbf{a}_p.$$

The expression for $\mathbf{a}^\dagger_p = u_p \mathbf{b}_p - v_p \mathbf{b}^\dagger_{-p}$ is the complex conjugate of the previous equation.

(d) To determine u_p, v_p (or α_p in $u_p = \cosh \alpha_p$) demand that the off-diagonal terms drop out of the Hamiltonian

$$\mathbf{H} = \sum_{p\neq 0} \epsilon_p \mathbf{a}^\dagger_p \mathbf{a}_p + C.$$

[Hint: to solve this condition, I recommend making the substitution $u_p = \frac{1}{\sqrt{A_p^2 - 1}}$, and solving for A_p.]

Find the resulting energy spectrum ϵ_p and [bonus problem] the c-number term C.

The quadratic terms in the hamiltonian are of the form

$$\begin{aligned}
&\sum_{p\neq 0} \left(t_p \left(\mathbf{b}^\dagger_p \mathbf{b}_p + \mathbf{b}^\dagger_{-p} \mathbf{b}_{-p} \right) + \Delta_p \left(\mathbf{b}^\dagger_p \mathbf{b}^\dagger_{-p} + \mathbf{b}_p \mathbf{b}_{-p} \right) \right) \\
&= \sum_{p\neq 0} \left(t_p \left(2v_p^2 + (u_p^2 + v_p^2) \left(\mathbf{a}^\dagger_p \mathbf{a}_p + \mathbf{a}^\dagger_{-p} \mathbf{a}_{-p} \right) + 2u_p v_p \left(\mathbf{a}_p \mathbf{a}_{-p} + h.c. \right) \right) \right. \\
&\left. + \Delta_p \left(2u_p v_p \left(\mathbf{a}^\dagger_p \mathbf{a}_p + \mathbf{a}^\dagger_{-p} \mathbf{a}_{-p} + 1 \right) + (u_p^2 + v_p^2) \left(\mathbf{a}_p \mathbf{a}_{-p} + h.c. \right) \right) \right) \qquad (8) \\
&\stackrel{!}{=} \sum_{p\neq 0} \epsilon_p \mathbf{a}^\dagger_p \mathbf{a}_p + C \qquad (9)
\end{aligned}$$

The coefficient of the off-diagonal term $\mathbf{a}_p \mathbf{a}_{-p}$ is

$$0 \stackrel{!}{=} t_p 2u_p v_p + \Delta_p (u_p^2 + v_p^2) \qquad (10)$$

and

$$\epsilon_p = 2\left(t_p(u_p^2+v_p^2) + 2\Delta_p u_p v_p\right),$$

$$C = 2\sum_{p\neq 0}\left(t_p v_p^2 + \Delta_p u_p v_p\right) = 2\sum_{p\neq 0}\left(t_p\left(-\frac{1}{2}(u_p^2-v_p^2)+\frac{1}{2}(u_p^2+v_p^2)\right)+\Delta_p u_p v_p\right) \tag{11}$$

$$= \frac{1}{2}\sum_{p\neq 0}\left(\epsilon_p - 2t_p\right). \tag{12}$$

Here $2t_p = \frac{p^2}{2m} - \frac{NU}{V} = \frac{p^2}{2m} - nU$ and $\Delta_p = -\frac{NU}{2V} = -nU/2$.

With the suggested substitution, the demand (10) becomes

$$0 = \frac{tA + \Delta(1+A^2)}{1-A^2} \quad \leftrightarrow \quad A = \frac{-t \pm \sqrt{t^2-\Delta^2}}{\Delta}.$$

In terms of A,

$$u^2+v^2 = \frac{1+A^2}{1-A^2} = \frac{\pm t}{\sqrt{t^2-\Delta^2}}, \quad 2uv = \frac{2A}{1-A^2} = \frac{\mp\Delta}{\sqrt{t^2-\Delta^2}}.$$

Therefore

$$\epsilon_p = 2\frac{\pm t_p^2 \mp \Delta_p^2}{\sqrt{t_p^2-\Delta_p^2}} = \pm 2\sqrt{t_p^2-\Delta_p^2}.$$

Clearly we have to pick the upper sign so that the energy is positive.

(e) Expand ϵ_p about $p = 0$ and find a phonon mode. Determine the speed of sound. What does ϵ_p do at large p?

The dispersion is

$$\epsilon_p = 2\sqrt{t_p^2-\Delta_p^2} = \sqrt{\left(\frac{p^2}{2m}-nU\right)^2 - (-nU)^2} = \sqrt{\frac{nUp^2}{m}+\left(\frac{p^2}{2m}\right)^2} \overset{p\to 0}{\simeq} |p|\sqrt{nU/m}$$
$$\overset{p\to\infty}{\simeq} \frac{p^2}{2m}.$$

The speed of sound is then $\sqrt{nU/m}$.

(f) [bonus problem] How does the groundstate energy density E/V depend on the density $n = N/V$ and the scattering length $a \equiv \frac{mU}{4\pi}$?

The groundstate energy is just C above plus the constant term in $\mathbf{H}$. This is a bonus problem because the integral is not finite. We can regulate it by putting a cutoff $\Lambda \gg \sqrt{m^3Un}$ on the momentum.

The integral, in the large-volume limit and in $d = 3$, is then

$$\frac{E_0}{V} = \frac{UN^2}{2V^2} + \frac{1}{2}\int đ^3 p \left(\sqrt{t_p^2 - \Delta_p^2} - t_p\right) \tag{13}$$

$$= \frac{Un^2}{2} + \frac{1}{2}\frac{4\pi}{(2\pi)^3}\int_0^\Lambda dp p^2 \left(\sqrt{\left(\frac{p^2}{2m}\right)^2 + \frac{Unp^2}{m}} - \left(\frac{p^2}{2m} + Un\right)\right). \tag{14}$$

Notice that the integral only depends on U and $n = N/V$ in the combination Un. Here Λ is a UV cutoff, which we take to be bigger than anything. Expanding about $\Lambda \to \infty$ (In Mathematica, Series[f(Λ), {Λ, 0, 2}]), we find

$$\frac{E_0}{V} = \frac{1}{2}Un^2 + \frac{1}{(2\pi)^2}\left(-m(Un)^2\Lambda + \frac{32}{15}(mUn)^{5/2} + \mathcal{O}(\Lambda^{-1})\right)$$

So the bit proportional to n^2 is not so meaningful, since it depends on the cutoff, but the term proportional to $n^{5/2}$ seems to be universal.