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

Physics 212C QM Spring 2020
Assignment 9

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 $\phi = 0$).

   (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.

(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.

(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).

(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.

(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 $\pm\frac{1}{2}$.

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

(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.

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

Let's look at the TFIM again:

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

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

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

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, $\mathbf{Z}_j = \langle \mathbf{Z}_j \rangle + \text{small}$, 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 $g \gg 1$, $\boldsymbol{\tau}^z_j \simeq 1+$ 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*:

$$\text{if } i \neq j,\ \boldsymbol{\chi}_j \boldsymbol{\chi}_i + \boldsymbol{\chi}_i \boldsymbol{\chi}_j \equiv \{\boldsymbol{\chi}_j, \boldsymbol{\chi}_i\} = 0, \quad \{\tilde{\boldsymbol{\chi}}_j, \tilde{\boldsymbol{\chi}}_i\} = 0, \quad \{\boldsymbol{\chi}_j, \tilde{\boldsymbol{\chi}}_i\} = 0. \tag{3}$$

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 (3) 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

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

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

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

(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!

(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 $\epsilon_1(k) = 2J(g - \cos ka)$, $\epsilon_2(k) = -J\sin ka$, 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

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

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 $|\Psi\rangle$, $\omega_c \equiv \frac{\hbar}{mR^2}$, $I_{cl} = NmR^2$.

4. **Excitations and energy of a weakly-interacting bose fluid.**

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.* $V(r_{ij}) = U\delta^d(r_{ij})$.

(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 $\mathbf{b}_{p\neq 0}, \mathbf{b}_{p\neq 0}^\dagger$.

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

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

where the coefficients u_p, v_p are to be determined and can be assumed to be real, and even functions of p.

Show that demanding that $\mathbf{a}_p, \mathbf{a}_p^\dagger$ satisfy canonical boson commutation relations implies $u_p^2 - v_p^2 = 1$. Find $\mathbf{a}_p$ in terms of $\mathbf{b}_p, \mathbf{b}_p^\dagger$.

(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

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

[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.

(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?

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