Problem Set 12
Quantum Field Theory and Many Body Physics (SoSe2015)

Due: Monday, July 6, 2015 at the beginning of the lecture

There is currently enormous interest in realizing topological superconductors in experiment. This effort is partly motivated by Alexei Kitaev's insight that these topological superconductors have Majorana excitations − fermions which are their own antiparticles as introduced by Majorana in the 30's − and that these Majorana excitations might be useful in the context of topological quantum computation. Specifically, the entity that experimentalists are hunting are Majorana bound states which have zero energy and obey a novel type of quantum statistics, distinct from fermionic or bosonic statistics, which is referred to as non-abelian statistics. In this problem set, we want to discuss a simple model which exhibits these excitations namely a spinless p-wave superconductor in one dimension (Kitaev chain).

At first sight, it might seem problematic that spinless p-wave superconductors do not exist in nature. However, there are now several proposals in the literature which effecively realize this model (or models which are adiabatically connected to this model and exhibit the same essential physics) and which can be implemented in the laboratory. The underlying idea is to induce effective p-wave correlations in a one-dimensional electron system by proximity coupling to a conventional s-wave superconductor. This can be done by judiciously exploiting spin polarization by applied magnetic fields and spin-orbit coupling of the material. Two of the prominent experiments pursuing these ideas and reporting success (which, however, is still under discussion) are: V. Mourik et al., Science **336**, 1003 (2012) and S. Nadj-Perge et al. Science **3**46, 602 (2014).

Incidentally, you should also notice that the Kitaev chain is closely related to the transverse field Ising model in 1d which we discussed in a previous problem set. In fact, we already showed that the transverse field Ising model maps to the Kitaev chain for specific parameters values. At the time, we only solved specific limiting cases. In this problem set, you will effectively also solve this model for general parameters. It is also worthwhile to understand that the existence of the Jordan-Wigner mapping between the two models does not mean that there are no important differences between the physics of the two models. In fact, the transverse field Ising model exhibits a regular symmetry-breaking quantum phase transition. In contrast, this transition maps to a topological quantum phase transition in the Kitaev chain.

Problem 1: Operator approach to BCS theory (10+15 points)

In class, we discussed the functional integral approach to BCS theory. In this exercise, we derive the same mean field theory in the operator formalism and derive the fermionic excitation spectrum of the superconductor more explicitly.

Consider the Hamiltonian of a uniform electron system with an effectively attractive and local interaction,

$$\mathcal{H} = \int \mathrm{d}\mathbf{r} \sum_\sigma \psi^\dagger_\sigma(\mathbf{r}) \left[\epsilon(-i\hbar\nabla) - \mu\right] \psi_\sigma(\mathbf{r}) - g \int \mathrm{d}\mathbf{r} \psi^\dagger_\uparrow(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}). \tag{1}$$

(a) The mean field approximation consists of writing

$$-g\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) = \Delta(\mathbf{r}) + [-g\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) - \Delta(\mathbf{r})], \tag{2}$$

where $\Delta(\mathbf{r})$ will turn out to be the complex-valued gap function, and neglecting quadratic terms in the fluctuations $[-g\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) - \Delta(\mathbf{r})]$ about the mean field $\Delta(\mathbf{r})$. Make this approximation and derive the mean field Hamiltonian

$$\mathcal{H} \simeq \int \mathrm{d}\mathbf{r} \sum_\sigma \psi^\dagger_\sigma(\mathbf{r}) \left[\epsilon(-i\hbar\nabla) - \mu\right] \psi_\sigma(\mathbf{r}) + \int \mathrm{d}\mathbf{r}\Delta^*(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \Delta(\mathbf{r})\psi^\dagger_\uparrow(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r}) + \int \mathrm{d}\mathbf{r}\frac{1}{g}|\Delta(\mathbf{r})|^2. \tag{3}$$

Write this Hamiltonian more compactly by introducing the Nambu spinor

$$\phi(\mathbf{r}) = [\psi_\uparrow(\mathbf{r}), \psi_\downarrow^\dagger(\mathbf{r})]^T. \tag{4}$$

Show that

$$\mathcal{H} \simeq \int d\mathbf{r}\phi^\dagger(\mathbf{r}) \begin{bmatrix} \xi(-i\hbar\nabla) & \Delta \\ \Delta^* & -\xi(-i\hbar\nabla) \end{bmatrix} \phi(\mathbf{r}) + \int d\mathbf{r}\frac{1}{g}|\Delta(\mathbf{r})|^2 + \sum_{\mathbf{k}} \xi_{\mathbf{k}}, \tag{5}$$

where $\xi(-i\hbar\nabla) = \epsilon(-i\hbar\nabla) - \mu$. The last two terms are merely constants which are important for computing the ground-state energy, but not for diagonalizing the Hamiltonian. We will drop them in the following.

The Hamiltonian

$$H = \begin{bmatrix} \xi(-i\hbar\nabla) & \Delta \\ \Delta^* & -\xi(-i\hbar\nabla) \end{bmatrix} \tag{6}$$

is referred to as Bogoliubov-de Gennes Hamiltonian. The corresponding eigenvalue equation is known as Bogoliubov-de Gennes equation, which describes the energies and wavefunctions of fermionic excitations of the superconductor (see below) and which is widely used in the theory of superconductivity. Note that $\Delta(\mathbf{r})$ need not be uniform in space.

(b) We now need to learn how to diagonalize Hamiltonians with terms of the sort $\psi\psi$ and $\psi^\dagger\psi^\dagger$. This is done by means of a Bogoliubov transformation. Let us assume that the superconductor is translationally invariant, so that

$$\mathcal{H} = \sum_{\mathbf{k}} \phi_{\mathbf{k}}^\dagger \begin{bmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta^* & -\xi_{\mathbf{k}} \end{bmatrix} \phi_{\mathbf{k}}, \tag{7}$$

where $\phi_{\mathbf{k}} = [c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^\dagger]^T$. This Hamiltonian can be diagonalized by a suitable linear combination of annihilation and creation operators, termed Bogoliubov transformation,

$$\begin{bmatrix} \gamma_{\mathbf{k},\uparrow} \\ \gamma_{-\mathbf{k},\downarrow}^\dagger \end{bmatrix} = \begin{bmatrix} \cos\theta_{\mathbf{k}} & \sin\theta_{\mathbf{k}} \\ \sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \end{bmatrix} \phi_{\mathbf{k}}. \tag{8}$$

Show that the newly introduced operators (termed Bogoliubov quasiparticle operators) are fermions. Rewrite the Hamiltonian (for real Δ for simplicity) in terms of the new operators and show that it becomes diagonal when choosing

$$\xi_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} - \Delta \cos 2\theta_{\mathbf{k}} = 0. \tag{9}$$

Show that this implies

$$u_{\mathbf{k}} = \cos\theta_{\mathbf{k}} = \frac{1}{2}\sqrt{1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}} \tag{10}$$

$$v_{\mathbf{k}} = \sin\theta_{\mathbf{k}} = \frac{1}{2}\sqrt{1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}} \tag{11}$$

with the quasiparticle energy $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$ and the standard notation of $u_{\mathbf{k}}$ (electron wavefucntion) and $v_{\mathbf{k}}$ (hole wavefunction). Finally show that when written in terms of the new operators, the Hamiltonian takes the form

$$\mathcal{H} = \sum_{\mathbf{k}} E_k(\gamma_{\mathbf{k}\uparrow}^\dagger \gamma_{\mathbf{k}\uparrow} - \gamma_{-\mathbf{k}\downarrow}\gamma_{-\mathbf{k}\downarrow}^\dagger). \tag{12}$$

Discuss the excitation spectrum described by this Hamiltonian.

(If you are ambitious, you may also want to continue this discussion and derive the gap equation and compute the condensation energy of the superconducting state.)

Problem 2: Spinless p-wave superconductors and Majorana fermions (5+5+5+5+5 points)

In the previous problem, you outlined the mean-field theory of 1d p-wave superconductor. The resulting model is often referred to as Kitaev chain and is discussed in more detail in this problem. Consider the Hamiltonian

$$H = -\mu \sum_{i=1}^{N} c_i^\dagger c_i - t \sum_{i=1}^{N} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) - \Delta \sum_{i=1}^{N} \left(c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger \right) \tag{13}$$

where we assume a chain of N sites with periodic boundary conditions through the identification $c_{N+1} = c_1$. Transforming to momentum space

$$c_j = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{\mathrm{i}kj} a_k \tag{14}$$

and introducing the Nambu spinor

$$\phi_k^T = \left(a_k,\, a_{-k}^\dagger \right) \tag{15}$$

leads to the Hamiltonian

$$H = \sum_{k>0} \phi_k^\dagger \begin{pmatrix} \xi_k & 2\mathrm{i}\Delta \sin k \\ -2\mathrm{i}\Delta \sin k & -\xi_k \end{pmatrix} \phi_k, \tag{16}$$

which we want to study.

(a) Show that the excitation spectrum of the Kitaev chain is

$$E_k = \sqrt{\xi_k^2 + 4\Delta^2 \sin^2 k} \tag{17}$$

(b) In the parameter space spanned by the chemical potential μ and the gap Δ, draw the line(s) where the gap (i.e., the smallest E_k for any k) vanishes. Note, that the gap is nonzero on *both* sides of this line. The two sides correspond to different phases of the model as characterized by different topological indices, and the line marks a *topological* quantum phase transition.

(c) One can distinguish the two different topological phases by considering the model with open boundary conditions. To this end, we consider the same Hamiltonian as in Eq. (16), but for a finite and non-perodic chain with N sites. For this finite-length chain, introduce Majorana fermion operators γ_{Aj} and γ_{Bj} through

$$c_j = \frac{1}{2} \left(\gamma_{Bj} + \mathrm{i}\gamma_{Aj} \right) \qquad \text{with} \qquad \gamma_{\alpha i}^\dagger = \gamma_{\alpha i} \tag{18}$$

(similar to separation a complex number $z = x + \mathrm{i}y$ into real and imaginary part). Show that the fermion anticommutation relations

$$\{c_i, c_j\} = \left\{ c_i^\dagger, c_j^\dagger \right\} = 0 \qquad \left\{ c_i, c_j^\dagger \right\} = \delta_{ij} \tag{19}$$

imply for the real or Majorana fermions

$$\{\gamma_{\alpha i}, \gamma_{\beta j}\} = 2\delta_{\alpha\beta}\delta_{ij}\,. \tag{20}$$

Physically, the relation $\gamma_{\alpha i} = \gamma_{\alpha i}^\dagger$ reflects that Majorana fermions are their own antiparticles.

(d) Now consider the Hamiltonian in Eq. (16) in the special case $\mu = 0$ and $t = \Delta$ and show that it can then be written as

$$H = -\mathrm{i}t \sum_{i=1}^{N-1} \gamma_{Bi}\gamma_{Ai+1}\,. \tag{21}$$

Note that γ_{A1} and γ_{BN} are *not* contained in H!

(e) Now introduce new (conventional) fermion operators

$$d_i = \frac{1}{2} \left(\gamma_{Bi} - \mathrm{i}\gamma_{Ai+1} \right) \qquad i = 1, ..., N-1 \tag{22}$$

(Check that the d_i satisfy the appropriate commutation relations.) Note that there were N c_i-operators, but that there are only $(N-1)$ d_i-operators. Show that in terms of the d operators

$$H = 2t \sum_{i=1}^{N-1} \left(d_i^\dagger d_i - \frac{1}{2} \right) \tag{23}$$

Also express the d_i in terms of the original fermion operators c_i and $c_i^\dagger$.

(f) Discuss the eigenstates and the spectrum of H, paying particular attention to the degeneracy of the ground state. Argue (without explicitly redoing the derivations) why the degeneracy is stable when varying the parameters of the model away from $\mu = 0$, $\Delta = t$.

Problem 3: Proximity effect (25 points)

Consider a 3d superconductor which is coupled to a one-dimensional normal electron system in the sense that electrons can pass between the two systems. For energies below the gap of the superconductor, electrons can enter the superconductor only virtually. These virtual excursions into the superconductor effectively induce superconducting correlations in the normal electron system. In this problem, we want to discuss the physics of this proximity effect in more detail. It turns out that it provides a very nice example of the concept of quasiparticle weight.

Consider the Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\rm sc} + \mathcal{H}_{1d} + \mathcal{H}_t \tag{24}$$

describing a mean-field superconductor

$$\mathcal{H}_{\rm sc} = \int \mathrm{d}\mathbf{r} \psi_\sigma^\dagger(\mathbf{r}) \xi(-i\nabla) \psi_\sigma(\mathbf{r}) + \Delta \psi_\uparrow^\dagger(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) + \Delta^* \psi_\uparrow(\mathbf{r}) \psi_\downarrow(\mathbf{r}), \tag{25}$$

the one-dimensional normal metal (say at $y = z = 0$)

$$\mathcal{H}_{1d} = \int \mathrm{d}x \phi_\sigma^\dagger(\mathbf{r}) \xi(-i\nabla) \phi_\sigma(\mathbf{r}), \tag{26}$$

and the tunnel coupling between the systems,

$$\mathcal{H}_{1d} = t \int \mathrm{d}x [\phi_\sigma^\dagger(x) \psi_\sigma(x,0,0) + \psi_\sigma^\dagger(x,0,0) \phi_\sigma(x)]. \tag{27}$$

Now, introduce two-component Nambu spinors Ψ for the syperconductor and Φ for the 1d system and show that the system is described by the action

$$S = \Phi^\dagger \mathcal{G}_{1d}^{-1} \Phi + \Psi^\dagger \mathcal{G}_{\rm sc}^{-1} \Psi + \Psi^\dagger T \Phi + \Phi^\dagger T \Psi. \tag{28}$$

in matrix notation and an appropriate definition of the operator T. Integrate out the superconductor and obtain the effective action

$$S = \Phi^\dagger (\mathcal{G}_{1d}^{-1} + \Sigma) \Phi \tag{29}$$

in terms of the self energy

$$\Sigma(\mathbf{k}, i\omega_n) = \frac{t^2}{A_\perp} \sum_{\mathbf{k_y},\mathbf{k_z}} \mathcal{G}_{\rm sc}(\mathbf{k}, i\omega_n) \tag{30}$$

when written explicitly in momentum space (with $A_\perp$ the cross-sectional area of the superconductor in the yz-plane). The momentum sum can be converted into an integral and performed explicitly. Do this integral to obtain

$$\Sigma(\mathbf{k}, i\omega_n) \simeq -\frac{\pi \nu_{2d} t^2}{\sqrt{\Delta^2 + \omega^2}} \begin{bmatrix} i\omega & \Delta \\ \Delta & i\omega \end{bmatrix}. \tag{31}$$

Here, we assumed that the self energy depends only weakly on k_x which is valid for sufficiently large μ.

Note that the self energy has off-diagonal contributions which correspond to superconducting correlations induced in the normal metal. How large is the gap induced in the normal metal? What is the correlation length of the proximity-induced superconductivity? Ask your tutor about the quasiparticle weight and its physical interpretation.