Physics 561, Fall Semester 2015
Professor Eduardo Fradkin

Problem Set No. 4: One-dimensional conductors
Due Date: Wednesday December 2, 2015

Polyacetylene is a long polymer chain of the type $(CH)_n$. The motion of the conduction electrons in polyacetylene can be described by the following model, due to W.P. Su, J.R. Schrieffer and A. Heeger. [Some general references for this problem are, W. P. Su, J. R. Schrieffer and A. Heeger, Phys. Rev. B **22**, 2099 (1980), R. Jackiw and J. R. Schrieffer, Nucl. Phys. B **190**[FS3], 253 (1981), and E. Fradkin and J. E. Hirsch, Phys. Rev. B **27**, 1680 (1983).]

In this model, one considers a linear chain of carbon atoms, C, with classical equilibrium positions at the regularly spaced sites $\{x(n)|x(n) = n\ a_0\}$ (where a_0 is the lattice constant). The carbon atoms *share* their electrons in their π-orbitals, and there is one such electron per carbon atom. These electrons are allowed to hop from site to site. This hopping process is *modulated* by the lattice vibrations. Since the mass M of the atoms is *much larger* than the mass of the electrons (or, what is the same, the tunneling hopping (kinetic) energy t of the electrons is *much larger* than the kinetic energy of the atoms), we can give an *approximate* description by treating the atoms classically while treating the electrons quantum mechanically. In this problem set we will consider a simplified version of this problem in which the electrons are considered to be *spinless* (*i.e.,* their spins have been fully polarized by a magnetic field).

The Hamiltonian for this system on a one-dimensional lattice (a chain) with N (even) sites, is

$$\begin{aligned} H &= -\sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left[\bar{t} - \alpha\,(u_n - u_{n+1})\right]\ \left[c^\dagger(n)c(n+1) + \text{h.c.}\right] \\ &+ \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left[\frac{P_n^2}{2M} + \frac{K}{2}\,(u_n - u_{n+1})^2\right] \end{aligned} \tag{1}$$

where $c^\dagger(n)$ and $c(n)$ are *fermion* operators which create and destroy a π (spinless) electron at the nth site of the chain, $u_n \equiv u[x(n)]$ are the displacements of the coordinates of the carbon atoms measured from their classical equilibrium positions $x(n)$, $P(n)$ are their momenta, M is the carbon mass, K is the elastic constant, $\bar{t}$ is the electron hopping matrix element for the undistorted lattice, and α is the electron-phonon coupling constant. Polyacetylene has one electron per carbon atom and, hence, it is a *half-filled* band system: there are N electrons in a chain with N atoms.

The study of this problem is greatly simplified by considering a continuum version of the model. If the coupling constant α is not too large, the only

physical processes which are important are those which mix nearly degenerate states, *i.e.,* the only electronic states that will matter are those within a narrow band of width $2E_c$ centered at the Fermi energy $E_F = 0$, where E_c is a high energy cutoff. In this limit, the single particle dispersion law can be linearized, $E(p) \simeq v_F(p \pm p_F)$. These electronic states can be regarded as *right moving* electrons (with $p \simeq p_F$) and *left moving* electrons (with $p \simeq -p_F$). Here v_F is the Fermi velocity. These considerations motivate the following way of writing the electron operators

$$c[x(n)] = \frac{1}{\sqrt{2a_0}} \left[e^{ip_F x(n)} \; R[x(n)] + e^{-ip_F x(n)} \; L[x(n)] \right] \tag{2}$$

Likewise, since the only processes in which phonons mix electrons near $\pm p_F$ have momentum $q \simeq 0$ (forward scattering) or $q \simeq 2p_F = \pi/a_0$ (backward scattering), it is also natural to split the phonon fields into two terms

$$\begin{aligned} u[x(n)] =& u_0[x(n)] + e^{2ip_F x(n)} \; \Delta_+[x(n)] + e^{-2ip_F x(n)} \; \Delta_-[x(n)] \\ \equiv& u_0[x(n)] + \cos(\pi n) \Delta[x(n)] \end{aligned} \tag{3}$$

where $u_0[x(n)]$ represents phonons with wave-vectors close to $q = 0$, while $\Delta_\pm(n)$ represent phonons with wave-vectors close to $q = \pm 2p_F$. For a half-filled band (*i.e.,* one electron per carbon site), $p_F = \frac{\pi}{2a_0}$, there is only one slow phonon field $\Delta_\pm[x(n)] \equiv \Delta[x(n)]$ since in this case $q \simeq 2p_F = \pi/a_0$ and it differs from $-q$ by a reciprocal lattice vector, $2\pi/a_0$.

Within these approximations, the effective continuum Hamiltonian only involves the left and right moving fermions and the phonons with $q \simeq \frac{\pi}{a_0}$:

$$\begin{aligned} H = \sum_{\alpha,\alpha'} = R, L \int dx \; \psi^\dagger_\alpha(x) \begin{pmatrix} -iv_F\partial_x & g\Delta(x) \\ g\Delta(x) & +iv_F\partial_x \end{pmatrix}_{\alpha,\alpha'} \psi_{\alpha'}(x) \\ + \int dx \; \left[\frac{\Pi^2(x)}{2(M/4K)} + \frac{1}{2}\Delta^2(x) \right] \end{aligned} \tag{4}$$

where the two-component spinors $\psi(x)$ and $\psi^\dagger(x)$ are

$$\psi(x) \equiv \begin{pmatrix} R(x) \\ L(x) \end{pmatrix}, \qquad \psi^\dagger(x) = \left(R^\dagger(x), L^\dagger(x) \right) \tag{5}$$

is a Fermi field which represents the right and left moving electrons close to the Fermi energy, which obey equal-time canonical anticommutation relations

$$\left\{ \psi_\alpha(x), \psi^\dagger_{\alpha'}(x') \right\} = \delta_{\alpha\alpha'}\delta(x - x'), \qquad \{\psi_\alpha(x), \psi_{\alpha'}(x')\} = 0 \tag{6}$$

Here, $\alpha = R$ is the *right moving* component of the fermion and $\alpha = L$ is the *left moving* component. The Bose field $\Delta(x)$ represents lattice vibrations with momentum close to $2p_F$, and it represents small fluctuations around a *staggered* distortion of the position of the atoms. $\Pi(x)$ is the canonical momentum conjugate to the $2p_F$ phonon field, and obey equal-time canonical commutation relations

$$[\Delta(x), \Pi(y)] = i\delta(x - y) \tag{7}$$

The effective electron-phonon coupling constant is $g \propto \frac{\alpha}{\sqrt{Dt}}$.

1. Consider first the case of zero electron-phonon coupling, $g = 0$. Compute in this limit the following propagators at $T = 0$

   (a) The propagator for right-moving electrons

   $$S_{RR}(p,\omega) = \int dx \int dt e^{i(p(x-x')-\omega(t-t')} \langle TR(x,t)R^\dagger(x',t')\rangle \quad (8)$$

   (b) The propagator for left-moving electrons

   $$S_{LL}(p,\omega) = \int dx \int dt e^{i(p(x-x')-\omega(t-t')} \langle TL(x,t)L^\dagger(x',t')\rangle \quad (9)$$

   (c) The propagator for the $2p_F$ phonon field Δ,

   $$G_\Delta(p,\omega) = \int dx \int dt e^{i(p(x-x')-\omega(t-t')} \langle T\Delta(x,t)\Delta(x',t')\rangle \quad (10)$$

2. Determine the form of the electron-phonon vertex shown in Fig.1

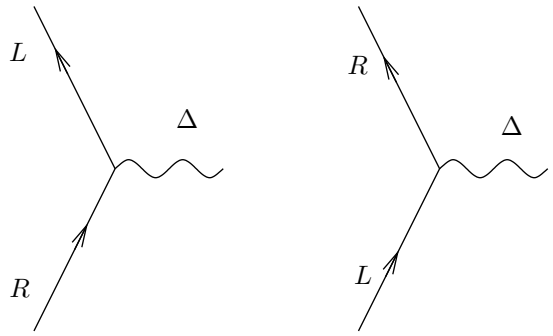

Figure 1: The electron-phonon vertex .

3. Consider the limit in which the mass of the carbon atoms is very heavy, *i.e.,* $M \to \infty$. In this *adiabatic limit*, the phonon kinetic energy term of the effective Hamiltonian of Eq.(4) can be neglected compared to the other terms and the phonon fields (displacements) $\Delta(x)$ become classical variables. Find the ground state vector $|\text{gnd}\rangle$ and energy of the system in this limit by calculating the (constant) value $\pm\Delta_0$ for which the *total* ground state energy (*i.e.* fermions plus vibrations) is minimized. You will have to cutoff some of the integrals at a relative momenta $\pm E_c/p_F$.
   Note: This *spontaneous* staggered distortion of the lattice is called *dimerization.* This phenomenon is known as the *Peierls Instability.* This dimerized ground state is a bond charge-density wave (CDW).

4. Compute the fermion propagator $S_{\alpha\alpha'}(p,\omega)$ in momentum and frequency space within this approximation. Show that for $g \neq 0$ right and left moving fermions are coupled and that as a result there is non-vanishing component for $S_{RL}(p,\omega)$. Find explicit expressions for all the four components of $S_{\alpha\alpha'}(p,\omega)$ in the adiabatic approximation.

5. Determine the energy spectrum and quantum numbers of the single-particle electronic states in this approximation. Show that the spectrum of single particle excitations (*quasiparticles*) has a gap. Find a formula for the gap in terms of the effective coupling constant g and Δ_0. What is the total functional dependence of the gap on the coupling constant g?

6. Show that the Hamiltonian of Eq.(4) is invariant under the global *discrete* symmetry transformation

$$\begin{pmatrix} R(x) \\ L(x) \end{pmatrix} \to \begin{pmatrix} R(x) \\ -L(x) \end{pmatrix}, \qquad \Delta(x) \to -\Delta(x) \tag{11}$$

Show that, in terms of the lattice model, this transformation is equivalent to a translation of all the fields *by one lattice spacing*, *i.e., half* of the period of the dimerization. Show that the local operator

$$\mathcal{O}_{\mathrm{CDW}}(x) = R^\dagger(x)L(x) + L^\dagger(x)R(x) \tag{12}$$

is *odd* (*i.e., changes sign*) under this global discrete symmetry and hence it is the bond CDW order parameter.

7. Compute the ground state expectation value for the *charge density wave* order parameter $\mathcal{O}_{\mathrm{CDW}}$ we just defined in the $M \to \infty$ approximation. Show that this order parameter has non-vanishing expectation value *only* if $\Delta_0 \neq 0$ and establish a connection between both quantities.

8. Use the *bosonization* methods discussed in class to find an expression for the bond CDW order parameter in terms of the (charge) Bose field ϕ of the bosonized fermions.

9. Use the result of item 8 (and the results derived in class for spinless Luttinger liquids) to find the bosonized Hamiltonian for the SSH Hamiltonian of Eq.(4). Show that this bosonized Hamiltonian is invariant under the symmetry $\Delta(x) \mapsto -\Delta(x)$ and $\phi(x) \mapsto \phi(x) + \sqrt{\pi}/2$. Interpret this symmetry in terms of the dimerization pattern.

10. In this last question we will consider a classical configuration of the phonon field $\Delta(x)$ that satisfies the boundary conditions $\lim_{x\to\infty} \Delta(x) = \Delta_0$ $\lim_{x\to-\infty} \Delta(x) = -\Delta_0$ and interpolates smoothly and monotonically between these two limits. This state is known as a *soliton*. Let us consider the one-dimensional Dirac Hamiltonian that we used in Eq.(4)

$$h_{\mathrm{Dirac}} = \begin{pmatrix} -iv_F\partial_x & g\Delta(x) \\ g\Delta(x) & +iv_F\partial_x \end{pmatrix} \tag{13}$$

(a) Show that if $\Delta(x)$ is a soliton configuration, then the Dirac Hamiltonian of Eq.(13) has a square-integrable (*normalizable*) eigenvector *with vanishing eigenvalue* (*i.e.,* a fermion *zero-mode*) of the form

$$\psi(x) = \begin{pmatrix} R \\ L \end{pmatrix} e^{-f(x)} \tag{14}$$

where R and L are constants. Find explicit expressions for the constants R, L and the function $f(x)$ in terms of the coupling constant g, the Fermi velocity v_F and the soliton configuration $\Delta(x)$. In order to obtain simple expressions it is useful to make the "thin-soliton" approximation,

$$\Delta(x) = \Delta_0 \, \mathrm{sign}(x) \tag{15}$$

(b) Use the expression for the total charge in terms of the boson $\phi(x)$ obtained by bosonization to show that the charge of the soliton is $1/2$ (in units of the electric charge e).