Physics 582, Fall Semester 2021
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Problem Set No. 5:

Due Date: Friday November 12, 2021, 9:00 pm US Central Time

1 Fermions in one dimension

In this problem we will consider an application of the Dirac theory to a problem in condensed matter physics: polyacetylene. 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 Su, Schrieffer and Heeger. 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 π-orbital electrons, one 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 as quantum mechanical objects. The Hamiltonian , for a lattice with N (even) sites, is

$$\begin{aligned} H &= -\sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{\sigma=\uparrow,\downarrow} \left[t - \alpha\left(x(n) - x(n+1)\right)\right] \left[c^\dagger_\sigma(n) c_\sigma(n+1) + \text{h.c.}\right] \\ &+ \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left[\frac{P_n^2}{2M} + \frac{D}{2}\left(x(n) - x(n+1)\right)^2\right] \end{aligned} \tag{1}$$

where $c^\dagger_\sigma(n)$ and $c_\sigma(n)$ are *fermion* operators which create and destroy a π-electron with spin σ at the n^{th} site of the chain, the $x(n)$'s are the coordinates of the carbon atoms (measured from their classical equilibrium positions), $P(n)$ are their momenta, M is the carbon mass, D is the elastic constant, 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* system and 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 $E_F = 0$. In this limit, the single particle dispersion law becomes $E(p) \approx v_F(p \pm p_F)$. These states are *right moving* electrons (with $p \approx p_F$) and *left moving* electrons (with $\approx -p_F$). Here v_F is the Fermi velocity. These considerations motivate the following way of writing the electron operators

$$c_\sigma(n) = e^{ip_F n}\, R_\sigma(n) + e^{-ip_F n}\, L_\sigma(n) \tag{2}$$

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

$$x(n) = \delta(n) + e^{2ip_F n}\, \Delta_+(n) + e^{-2ip_F n}\, \Delta_-(n) \tag{3}$$

where $p_F = \frac{\pi}{2a_0}$.

Within this set of approximations, it is natural to write an effective continuum Hamiltonian which only involves the left and right moving fermions and the phonons with $p \approx \frac{\pi}{a_0}$. After Fourier transforming back to position space we get

$$\begin{aligned} H = & \sum_{\sigma=\uparrow,\downarrow} \int dx\; \psi^\dagger_\sigma(x)\; \left(-iv_F \frac{\partial}{\partial x}\right) \sigma_3\; \psi_\sigma(x) \\ & + \int dx\; \left[\frac{\Pi^2(x)}{8Ma_0^2} + \frac{1}{2}\Delta^2(x)\right] + \sum_{\sigma=\uparrow,\downarrow} \int dx\; \sqrt{2g}\Delta(x)\; \bar{\psi}_\sigma(x)\psi_\sigma(x) \end{aligned} \tag{4}$$

where the two-component spinor $\psi_\sigma(x)$

$$\psi_\sigma(x) \equiv \begin{pmatrix} R_\sigma(x) \\ L_\sigma(x) \end{pmatrix} \tag{5}$$

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

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

while all other anticommutators are zero. Here the label $\alpha = 1$ indicates upper (or *right moving*) component and $\alpha = 2$ indicates the lower (or *left moving*) component. These fields differ from the ones we used above by a factor of $1/\sqrt{2a_0}$ which gives these fields units of length$^{-1/2}$. The Bose field $\Delta(x)$ represents lattice vibrations with momentum close to $2p_F$. Thus, $\Delta(x)$ represents small fluctuations around a *staggered* distortion of the position of the atoms, $\Pi(x)$ is the phonon canonical momentum and Δ and Π obey canonical commutation relations

$$[\Delta(x), \Pi(y)] = i\delta(x - y)$$

The matrix σ_3 is the 2×2 Pauli matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ Notice that, in this approximation, the electrons are effectively a relativistic Dirac field with "speed of light" equal to the Fermi velocity. It is useful to define a set of 2×2 "Dirac" matrices,

$$\gamma_0 = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \gamma_1 = i\sigma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad \gamma_5 = \gamma_0\gamma_1 = \sigma_3$$

We will also use the notation $\bar{\psi} = \psi^\dagger\gamma_0 = \psi^\dagger\sigma_2$. The new effective electron-phonon coupling constant is $g = \frac{\alpha}{\sqrt{tD}}$.

1. Consider the limit in which the mass of the carbon atoms is very heavy ($M \to \infty$). In this *adiabatic limit* the phonon kinetic energy term of the effective Hamiltonian of Eq.(2) can be neglected and the phonon coordinates $\Delta(x)$ become classical variables. Find the ground state vector $|\text{gnd}\rangle$ and energy of the system in this limit by calculating the (constant) value of Δ for which the ground state energy is minimized. You will have to cutoff some of the integrals at a relative momenta $\pm E_c/p_F$.
   Note: The *spontaneous* staggered distortion of the lattice is known as *dimerization* and this phenomenon is called the Peierls Instability.

2. Determine the energy spectrum and quantum numbers of the single-particle electronic states in this approximation.

3. Show that the continuum Hamiltonian (and the associated Lagrangian) is invariant under the global *discrete* symmetry transformation

   $$\psi(x) \to \gamma_5\psi(x), \qquad \Delta(x) \to -\Delta(x) \tag{7}$$

   with $\gamma_5 = \sigma_3$. Show that, in terms of the lattice model, this transformation amounts to a shift of all the fields by one lattice site. In that language, the symmetry corresponds to an ambiguity in the way the dimerized structure is placed on the lattice Show that the operator $\bar{\psi}_\sigma(x)\psi_\sigma(x)$ is *odd* under the discrete symmetry and, hence, it is an order parameter.

4. Compute the ground state expectation value for the order parameter of the previous section

   $$\sum_\sigma \langle \text{gnd}|\bar{\psi}_\sigma(x)\psi_\sigma(x)|\text{gnd}\rangle \tag{8}$$

   in the $M \to \infty$ approximation. Show that this order parameter has non-vanishing expectation value *only* is $\Delta \neq 0$ and establish a connection between both quantities.

2 Grassmann Stuff

1. Let a and a^* be a pair of Grassmann variables. Let $g(a^*)$ be an "analytic function" of a single Grassmann variable a^*, i.e.

$$g(a^*) = g_0 + g_1 a^* \tag{9}$$

and let $f(a)$ be another such function. Show that the inner product $\langle f|g\rangle$ defined by

$$\langle f|g\rangle = \int da^* da \; e^{-a^* a} f^*(a) g(a^*) \tag{10}$$

implies that

$$\langle f|g\rangle = \bar{f}_0 g_0 + \bar{f}_1 g_1 \tag{11}$$

where $\bar{x}$ stands for the complex conjugate of x.

2. Show that

$$(Af)(a^*) = \int d\alpha^* d\alpha A(a^*, \alpha) f(\alpha^*) e^{-\alpha^* \alpha} = g(a^*) \tag{12}$$

is equivalent to

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \begin{pmatrix} A_{00} & A_{10} \\ A_{01} & A_{11} \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} \tag{13}$$

and that

$$(A\ B)\,(a^*, a) = \int d\alpha^* d\alpha \;\; e^{-\alpha^* \alpha} \; A(a^*, \alpha)\; B(\alpha^*, a) = C(a^*, a) \tag{14}$$

is equivalent to the standard definition of the product of two 2×2 matrices.

3. Show that the operators $\hat{a}^*$ and $\hat{a}$, defined by

$$\hat{a}^* f(\alpha^*) = a^* f(a^*) \qquad \hat{a} f(a^*) = \frac{d}{da^*} f(a^*) \tag{15}$$

satisfy canonical anticommutation relations,i.e. $\hat{a}^* \;\hat{a}^* = \hat{a} \;\hat{a} = 0$ and $\{\hat{a}^*, \hat{a}\} = 1$.

4. Show that, if $\{\xi_j\}$ is a set of N Grassmann variables ($j = 1, \ldots, N$), then

$$\mathcal{Z} = \int \prod_{j=1}^{N} d\xi_j^* d\xi_j \;\; \exp\{-\sum_{k,l=1}^{N} \xi_k^* M_{kl} \xi_l\} = \det M \tag{16}$$

3 Dirac Fermions

The Lagrangian density $\mathcal{L}$ for the free massive Dirac field in 4-dimensional Minkowski space is

$$\mathcal{L} = \bar{\psi} \left(i\partial\!\!\!/ - m \right) \psi \tag{17}$$

1. Consider the path integral for a free Dirac field in four space-time dimensions, coupled to a set of Grassmann sources $\bar{\eta}_\alpha(x)$ and $\eta_\alpha(x)$. Derive an expression for this generating function in terms of the sources and a Fermion determinant. Do *not* compute the determinant.

2. Use the results of previous question to show that the Feynman propagator of the Dirac theory is given by

$$S_F^{\alpha\beta}(x-y) = \langle x, \alpha | \frac{1}{i\partial\!\!\!/ - m} | y, \beta \rangle \tag{18}$$

3. Use the results of the first part of this problem to derive an expression for the four point function

$$S_F^{(4)}(x_1, x_2, x_3, x_4)_{\alpha,\beta,\gamma,\delta} = \langle 0 | \psi_\alpha(x_1) \psi_\beta(x_2) \bar{\psi}_\gamma(x_3) \bar{\psi}_\delta(x_4) | 0 \rangle \tag{19}$$

   in terms of products of propagators. Beware of the signs!!!!!!

4 Functional Determinants and the Casimir Effect

In this problem we are going to consider a free scalar field $\phi(x,t)$ in $1+1$ space-time dimensions. The Lagrangian density $\mathcal{L}$ is

$$\mathcal{L} = \frac{1}{2}\partial_\mu \phi(x) \partial^\mu \phi(x) - \frac{1}{2} m^2 \phi(x)^2 \tag{20}$$

where $x \equiv (x,t)$. Consider the case in which the total length of the system along the space coordinate is equal to L and assume *periodic boundary conditions*, i.e.

$$\phi(x,t) = \phi(x+L,t) \tag{21}$$

for all times t.

1. Calculate the *classical* value of the ground state energy of the system with the boundary conditions specified above.

2. Use path integral methods to derive a formal expression for the total ground state energy density (i.e. energy per unit length). This formula should contain a determinant which you should not compute for the moment.

3. Use the method of the ζ-function to compute the quantum correction to the ground state energy density. Consider the massless limit $m \to 0$ only. Write your answer down in the form of an *extensive* piece and a *finite-size* term which vanishes as $L \to \infty$ like A/L^η, with $\eta > 0$. Find the value of this exponent η as well as the value of the coefficient A, sign included. Note: You may have to keep a dependence on the mass in one of the two

terms. Keep just the leading behavior in the small mass limit. Note: At some point of the calculation the following result may be useful:
Poisson Summation Formula:

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dx \;\; f(x) \;\; e^{2\pi i m x} \tag{22}$$

4. If you interpret the dependence of the ground state energy on the linear size of the system L as a potential energy for the"walls" that confine the system, what can you say about the force that the zero-point fluctuations exert on these "walls".
Note: In order to speak about walls we should have used vanishing, instead of periodic boundary conditions as we have done. The calculation is somewhat more complicated in that case. This effect, i.e. a force exerted on the walls of a system by the zero point motion of a field is known as the *Casimir effect*.

5 The Weakly-Interacting Bose Gas

Consider a gas of non-relativistic Bose particles at fixed density ρ inside a very large box of linear size L in three space dimensions. Let $\phi^\dagger(\boldsymbol{x})$ and $\phi(\boldsymbol{x})$ be a set of boson creation and annihilation operators. The second quantized Hamiltonian is

$$H = \int d^3x \; \phi^\dagger(\boldsymbol{x}) \left(\frac{\hat{\boldsymbol{p}}^2}{2m} - \mu \right) \phi(\boldsymbol{x}) + \frac{1}{2} \int d^3x \int d^3x' \hat{n}(\boldsymbol{x}) V(\boldsymbol{x} - \boldsymbol{x}') \hat{n}(\boldsymbol{x}'). \tag{23}$$

where μ is the chemical potential, $\hat{n} = \phi^\dagger \phi$ and $V(r)$ is a rotationally invariant short range interaction which we will take to be equal to

$$V(\boldsymbol{x} - \boldsymbol{x}') = \lambda \delta^3(\boldsymbol{x} - \boldsymbol{x}') \tag{24}$$

The positive constant λ is the scattering amplitude and will play the role of a coupling constant for this system.

1. Use the method of Bose coherent states to find a path integral *formula* for the partition function of this system at temperature T. Do not compute the path integral at this stage. Assume *constant* boundary conditions at spacial infinity (i.e. that the field amplitude approaches a constant value at the boundaries). Carefully specify the boundary conditions in the imaginary time dimension. Write your answer down in the form

$$\mathcal{Z} = \int \mathcal{D}\phi^* \; \mathcal{D}\phi \;\; e^{-S_E(\phi^*, \phi)} \tag{25}$$

and give an explicit expression for the Euclidean action S_E.

2. Use the method of semiclassical quantization (i.e. the saddle point expansion) to determine the classical path at temperature T. What condition should be satisfied by $\phi(x)$ in order for it to be such a classical path?. Find the relationship between the ground state of the system at $T = 0$ and this classical path in the limit $T \to 0$. Is the solution unique?. Justify your answer.
   Hint: Think of the symmetries of the Lagrangian. This will give you an idea about the uniqueness of the classical path. You may find it convenient to write the classical path $\phi(x)$ in the form of an amplitude times a phase.

3. Compute the time-ordered Green function

$$G(x-y) = -i \, \langle \hat{T}\hat{\phi}(x)\hat{\phi}^{\dagger}(y)\rangle \tag{26}$$

   at $T = 0$, in the semiclassical limit. What is the asymptotic value of G in the limit of equal times and large space separation?. Give a physical interpretation of this result.

4. Consider small quantum fluctuations around the classical path found in the previous sections. Write an arbitrary (but close) configuration $\phi(x)$ in the form

$$\phi(x) = \sqrt{\rho_0 + \delta\rho(x)} \quad e^{i\theta(x)} \tag{27}$$

   Expand the action in powers of $\delta\rho$ and θ up to second order in both. Check the cancellation of the linear terms. Integrate out the density fluctuations and find an effective action for the phase variable

$$e^{-S_{\rm eff}(\theta(x))} = \int \mathcal{D}\delta\rho \; e^{-S_E} \tag{28}$$

   which is quadratic in θ.

5. Show that, for configurations $\{\theta(x)\}$ which are slowly varying, the effective action has the form

$$S_{\rm eff} = \int d^4x \; \frac{1}{2} K \left[(\partial_\tau \theta)^2 + v^2 \left(\boldsymbol{\nabla}\theta(x) \right)^2 \right] \tag{29}$$

   and calculate the coefficients K and v. Find the analytic continuation of this expression back in real time. Show that v is the velocity of propagation of the excitations. Find the time ordered propagator of the phase field $\theta(x)$. What equation of motion does it satisfy?. Draw an analogy between this equation and the equation of motion for a relativistic massless scalar field.