PHZ7428–Modern Condensed Matter Physics

Spring 2019

Take-home final examination

April 19, 2019

Due: April 26, 2019

1-week take-home exam containing three separate problems. **The problems should be worked out alone and may not be discussed, in specifics, with others.**

Problem 1

In the following, we shall consider a one dimensional chain having N sites and mobile electrons which we model by a simple tight-binding model:

$$H_0 = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \tag{1}$$

with dispersion-relation

$$\xi_k = -2t\cos(ak), \qquad \text{for} \qquad k \in [-\pi/a, \pi/a], \tag{2}$$

where t denotes the nearest-neighbor hopping amplitude (in dimensions of energy), k is the wave-vector along the chain and a is the lattice constant. We consider the half-filled band and hence take the chemical potential to be zero.

a:

Sketch the dispersion relation (ξ_k vs. k) and indicate the Fermi level. Show that the density of states, i.e. $N(\omega) = \sum_k \delta(\omega - \xi_k)$, is given by

$$N(\omega) = \frac{N}{\pi}(4t^2 - \omega^2)^{-1/2}\theta(2t - |\omega|). \tag{3}$$

(hint: remember that $\delta(f(x)) = \sum_{x_0} \delta(x - x_0)/|f'(x_0)|$, where x_0 are the zeros of $f(x)$).

b:

Assuming that $T \ll t$, show that the retarded electronic polarization bubble (cf. Fig.1a) in the static limit and at wave-vector $2k_F$, i.e. $\Pi^{(0)R}(q,\omega)$ for $\omega = 0$ and $q = 2k_F$, is given by:

$$\Pi^{(0)R}(2k_F, 0) = \frac{N}{\pi t}\ln\left(\frac{4te^\gamma}{\pi T}\right), \tag{4}$$

and thus diverges as $T \to 0$. Along the way, you may want to make use of the following integral:

$$\alpha\int_0^\alpha dx \frac{\tanh(x)}{x\sqrt{\alpha^2 - x^2}} \approx \ln(\alpha) + \ln(4e^\gamma/\pi), \ \text{for}\ \alpha \gg 1. \tag{5}$$

where $\gamma = 0.577...$ is Eulers constant.

c:

The harmonic vibrations of the underlying ion-lattice can be described by the following (retarded) free *phonon* Green's function:

$$\mathcal{D}^{(0)R}(q,\omega) = \frac{2\omega_q}{(\omega + i0_+)^2 - \omega_q^2}. \tag{6}$$

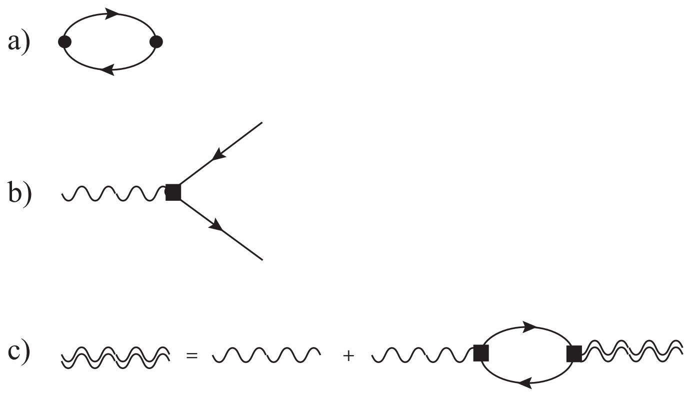


FIG. 1: Feynman diagrams corresponding to respectively: a) the electron polarization bubble $\Pi^{(0)R}$ (dots merely denote the beginning and ending of Greens functions), b) the electron-phonon interaction vertex, here denoted by a black square and corresponding to a factor of g_{el-ph}, and c) the Dyson equation for the renormalized phonon Green's function, taking the polarization bubble as the irreducible phonon self-energy.

Within the so-called Debye model, the energy of an acoustic phonon as a function of its wave-vector is given by the dispersion-relation $\omega_q = v_D|q|$. This phonon mode interacts with the electron system via the vertex shown in Fig.1b, corresponding to the coupling constant

$$g_{el-ph} = \left(\lambda \frac{\omega_q}{2N(0)}\right)^{1/2}, \tag{7}$$

$N(0)$ being the density of states at the Fermi level. The dressed phonon Green's function can be found from the following Dyson equation for the retarded Green's function (cf. Fig.1c)

$$\mathcal{D}^R(q,\omega) = \mathcal{D}^{(0)R}(q,\omega) - \mathcal{D}^{(0)R}(q,\omega) g_{el-ph} \Pi^{(0)R}(q,\omega) g_{el-ph} \mathcal{D}^R(q,\omega), \tag{8}$$

which is quite an accurate approximation for $q \approx 2k_F$ and $\omega \approx 0$, when $T \ll t$. (*Note*: the minus in this Dyson equation comes from particular Feynman rules for phonon propagators which you are not expected to know).

Solve this Dyson equation for the renormalized phonon Green's function, $\mathcal{D}^R(q,\omega)$, and find the renormalized phonon dispersion-relation $\widetilde{\omega}_q$ for $q \approx 2k_F$. You may neglect the (q,ω)-dependence of the polarization bubble and use the constant value for $\Pi^{(0)R}$ found above for $(q,\omega) = (2k_F, 0)$.

d:

Show that for $q \approx 2k_F$ this renormalized dispersion relation, $\widetilde{\omega}_q$, vanishes identically when decreasing the temperature to some critical value T_C, where

$$T_C = \frac{4t}{\pi} e^{\gamma} e^{-1/(2\lambda)}. \tag{9}$$

For $T < T_C$, this $\widetilde{\omega}_q$ (near $q \approx 2k_F$) becomes imaginary and hence physically meaningless. Approaching T_C from above, $\widetilde{\omega}_q$ vanishes as a power-law very close to T_C. Expand $\widetilde{\omega}_q$ in $(T - T_C)/T_C \ll 1$ and find the exponent ν for the transition to $\widetilde{\omega}_q = 0$, i.e. the exponent in the relation:

$$\widetilde{\omega}_q \propto |T - T_C|^{\nu}, \;\text{for}\, T \gtrsim T_C. \tag{10}$$

This demonstrates an instability of one-dimensional electron systems due to a spontaneous deformation of the ion-lattice, here signalled by a *soft* mode in the phonon spectrum. For $T < T_C$, it costs no energy to excite a phonon, and the phonon-system is therefore unstable towards a spontaneous deformation involving two different lattice-spacings. This was first demonstrated (in a different manner!) by Rudolf Peierls (1907-1995) in 1930.

Problem 2

In this problem we remain focussed on electrons in two dimensions (2D). The study of 2D electron gases is relevant for a large field of active research since they can be realized in so-called GaAs heterostructures. The physics of 2D electrons is surprisingly rich and includes e.g. the fractional quantum Hall effect which was the subject of a Nobel prize in 1998. Below, you will study the electron-electron interactions in 2D, and derive the associated screening and plasmons properties. Throughout this problem we take $\hbar = 1$.

a:

The Hamiltonian which we study is

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2\mathcal{A}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{\sigma\sigma'} W^{2D}(\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}, \tag{11}$$

where $\mathcal{A}$ is the area of our sample, $\xi_{\mathbf{k}} = \frac{k^2}{2m} - \mu$, the usual quadratic dispersion of free electrons. By Fourier transforming the real-space potential $W(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{4\pi\epsilon_r\epsilon_0} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$, show that

$$W^{2D}(\mathbf{q}) = \frac{e^2}{2\epsilon_r\epsilon_0 q}. \tag{12}$$

You may want to use that $\int_0^{2\pi} d\theta \exp(i\alpha\cos\theta) = 2\pi J_0(\alpha)$ and $\int_0^\infty dx J_0(bx) = 1/b$, where J_0 is the zero'th order Bessel function of the first kind.

b:

Within RPA, the dielectric function $\epsilon^{2D}_{RPA}(\mathbf{q}, iq_n)$ is given by

$$\epsilon^{2D}_{RPA}(\mathbf{q}, iq_n) = 1 - W^{2D}(\mathbf{q})\chi^{2D}_0(\mathbf{q}, iq_n), \tag{13}$$

with

$$\chi^{2D}_0(\mathbf{q}, iq_n) = 2\int \frac{d^2k}{(2\pi)^2} \frac{n_F(\xi_{\mathbf{k}+\mathbf{q}}) - n_F(\xi_{\mathbf{k}})}{\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}} - iq_n}. \tag{14}$$

Explain how one can derive this expression for $\chi^{2D}_0(\mathbf{q}, iq_n)$.

c:

Write down the renormalized Coulomb interaction $W^{RPA}(\mathbf{q}, iq_n)$, and derive an expression for the static Thomas-Fermi screening wavenumber k^{2D}_s in terms of physical parameters of the electron gas. Using that for GaAs: $\epsilon_r = 13$, $m = 0.067 m_e$ (m_e is the bare electron mass), how does k^{2D}_s compare to k_F when the density is $n = 2 \times 10^{15} m^{-2}$.

d:

For $k_BT/\epsilon_F \ll 1$ and $q \ll k_F$, show that

$$Re\chi^{2D}_0(\mathbf{q}, \omega) = \frac{1}{2\pi^2} \frac{k_F}{\hbar v_F} \int_0^{2\pi} d\theta \frac{v_F q \cos\theta}{\omega - v_F q\cos\theta}. \tag{15}$$

e:

Using Eq. (15) in the long wavelength limit $q \ll \omega/v_F$, show that the 2D plasmon dispersion $\omega(q)$ is given by

$$\omega(q) = v_F\sqrt{\frac{k_s^{2D} q}{2}}. \tag{16}$$

What is the crucial difference compared to the 3D case? Given that visible light corresponds to the $q \to 0$ limit, argue whether a 2D electron gas appears reflective or transparent to the human eye.

f:

Where is the particle-hole continuum in 2D? Sketch the analog of Fig. 14.2 from Bruus & Flensberg. What is the condition that the plasmons are not damped by particle-hole excitations in the small q limit? Are plasmons damped in GaAs in this limit?

Problem 3

In the following problem, we consider a single impurity atom on the surface of a metal. The atom is arranged such that a single atomic orbital, henceforth labeled by subscript d, hybridizes with the conduction-electrons in the metal. This system can be probed by a scanning tunneling microscope (STM) and the question is what one should expect for the tunneling current when the STM-tip is brought in close to the metal a certain distance away from the impurity atom.

As a simple model for this physical system, we shall approximate the metal-surface by a two-dimensional electron-gas having a simple quadratic dispersion $\xi_k = \frac{k^2}{2m} - \mu$, where μ denotes the electron chemical potential. The impurity-atom is modeled by a single resonant level with momentum-independent hybridization, t, to the metal at the position $\mathbf{r} = (x, y) = (0, 0)$. Throughout this problem we shall take $\hbar = 1$ and for simplicity we shall omit the spin of the electrons. The area of the electron-gas we denote by $\mathcal{A}$.

a:

Argue how the Hamiltonian,

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \varepsilon_d c_d^\dagger c_d + \frac{1}{\sqrt{\mathcal{A}}}\sum_{\mathbf{k}}\left(t^* c_{\mathbf{k}}^\dagger c_d + t c_d^\dagger c_{\mathbf{k}}\right) \tag{17}$$

reflects this model, i.e. what is the physical content of the individual terms? Argue why H includes merely a hybridization with conduction-electrons at position $\mathbf{r} = (0, 0)$. Make a simple drawing sketching the system. Finally, list a few additional terms and complications which one might have added to this Hamiltonian in order to make it more realistic.

b:

Assuming that the STM-tip probes the conduction-electron system at a position $\mathbf{r}$, relative to the location of the impurity atom, we need to calculate the retarded Green function describing the propagation from $\mathbf{r}$ to $\mathbf{r}$:

$$G^R(\mathbf{r}, \mathbf{r}; \omega) = -i\theta(t - t')\langle\{\psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}, t')\}\rangle. \tag{18}$$

Show that, in general, we have

$$G^R(\mathbf{r}, \mathbf{r}; \omega) = \frac{1}{\mathcal{A}}\sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} G^R(\mathbf{k}, \mathbf{k}'; \omega), \tag{19}$$

and, for the bare Green function describing propagation from the STM-tip to the impurity atom,

$$G_0^R(\mathbf{r},\mathbf{0};\omega) = \frac{1}{\mathcal{A}}\sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\omega - \xi_k + i\eta}. \tag{20}$$

c:

Write down the equations of motion for the following two retarded Green-functions:

$$G^R(\mathbf{k},\mathbf{k}';t-t') = -\,i\theta(t-t')\langle\{c_{\mathbf{k}}(t), c^\dagger_{\mathbf{k}'}(t')\}\rangle, \tag{21}$$

$$G^R(d,\mathbf{k}';t-t') = -\,i\theta(t-t')\langle\{c_d(t), c^\dagger_{\mathbf{k}'}(t')\}\rangle, \tag{22}$$

and Fourier-transform these equations to frequency-space. Solve the transformed equations to show that

$$G^R(\mathbf{k},\mathbf{k}';\omega) = \frac{1}{\omega - \xi_k + i\eta}\left[\delta_{k,k'} + \left(\frac{|t|^2}{\omega - \varepsilon_d + i\eta}\right)\frac{1}{\mathcal{A}}\sum_{k''} G^R(\mathbf{k}'',\mathbf{k}';\omega)\right]. \tag{23}$$

d:

From equation (23) derived in question **c**, show that

$$G^R(\mathbf{r},\mathbf{r};\omega) = G_0^R(\mathbf{r},\mathbf{r};\omega) + G_0^R(\mathbf{r},\mathbf{0};\omega)T^R(\mathbf{0},\mathbf{0};\omega)G_0^R(\mathbf{0},\mathbf{r};\omega), \tag{24}$$

with the so-called T-matrix given by

$$T^R(\mathbf{0},\mathbf{0};\omega) = \frac{|t|^2}{\omega - \varepsilon_d - \Sigma^R(\omega)}. \tag{25}$$

Give an explicit expression for $\Sigma^R(\omega)$ and argue what it is the self-energy of.

e:

The T-matrix found in question **d** describes the repeated scattering off the impurity atom by an electron at position $\mathbf{r} = \mathbf{0}$. Rederive equation (25) using Feynman diagrams in space representation appropriate to the Hamiltonian (17)? (Hint: You can use the diagrammatic elements in (E.13.3) from exercise 13.3 in the textbook (B&F), with $U = 0$.)

f:

Show that the local density of states at the location of the STM-tip is given by

$$A(\mathbf{r},\mathbf{r};\omega) = 2\pi N(\omega) + 2\left(\mathrm{Im}[G_0^R(\mathbf{r},\mathbf{0};\omega)]\right)^2\left\{2q\mathrm{Re}[T^R(\mathbf{0},\mathbf{0};\omega)] + (1-q^2)\mathrm{Im}[T^R(\mathbf{0},\mathbf{0};\omega)]\right\}, \tag{26}$$

in terms of the bare density of states per area of the homogeneous electron gas, $N(\omega)$, and the dimensionless quantity

$$q = -\frac{\mathrm{Re}[G_0^R(\mathbf{r},\mathbf{0};\omega)]}{\mathrm{Im}[G_0^R(\mathbf{r},\mathbf{0};\omega)]}. \tag{27}$$

g:

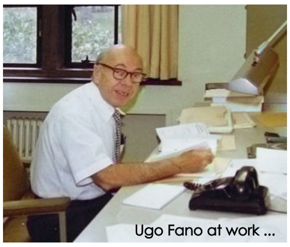
We proceed by making a few simplifying approximations. First of all, we shall neglect the real-part of $\Sigma^R(\omega)$ and assume the imaginary part to be constant, i.e. assume that $\Sigma^R(\omega) \approx -i\Gamma$ (express Γ in terms of t). Furthermore, we assume that $\varepsilon_d, \Gamma \ll \mu$, which allows us to neglect the ω-dependence in $G_0^R(\mathbf{r}, \mathbf{0}; \omega)$ in equation (26) (argue why). Finally, we assume that $\mathrm{Im}[G_0^R(\mathbf{r}, \mathbf{0}; \omega)] \approx \mathrm{Im}[G_0^R(\mathbf{r}, \mathbf{r}; \omega)]$ (what does this require for the distance $|\mathbf{r}|$?).

Under these assumptions, show that equation (26) derived in question **f** can be rewritten as

$$A(\mathbf{r}, \mathbf{r}; x) = 2\pi N(0) \frac{(q+x)^2}{1+x^2}, \tag{28}$$

with $x = (\omega - \varepsilon_d)/\Gamma$. Sketch A as a function of x, for representative values of q, and describe in words the change in the density of states at position $\mathbf{r}$ due to the hybridization with the impurity atom at $\mathbf{r} = (0, 0)$. Finally, make a rough prediction for the I-V (current-voltage) characteristics which will be recorded by the STM tip, i.e. how does I depend on V?

The *Fano profile* formula (28) which you have just derived, was first derived by Ugo Fano in 1935, in a seminal paper on the absorption spectrum of noble gases. Fano later published a generalized version of his calculation in a 1961 paper which, by now, has some 5000 citations. As Fano (and now you) demonstrated, a discrete level can have a profound influence on the density of continuum states. This simple formula has been widely used throughout nuclear, atomic, molecular and condensed-matter physics.


Ugo Fano at work ...