

PHZ7428–Modern Condensed Matter Physics

Spring 2019

Take-home final examination – solutions

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:

$$H_0 = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (1)$$

with dispersion relation

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

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

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

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

Note if $f(k) = \omega + 2t \cos ak$, then $f'(k) = -2at \sin(ak) = 2at \sqrt{1 - (\xi_k/2t)^2}$

$$N(\omega) = \frac{1}{Na} \sum_k \delta(\omega - \xi_k) = \sum_{s=\pm 1} \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \frac{\delta(k - s \frac{1}{a} \cos^{-1}(\omega/2t))}{a \sqrt{4t^2 - \omega^2}} = \theta(2t - |\omega|) \frac{1}{\pi a \sqrt{4t^2 - \omega^2}}.$$

Note there are two roots, $\pm k_0$, so the DOS acquires a factor of 2. Sorry I did not give quite the correct definition of the DOS in the stated problem.

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:

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

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

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

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

Polarization bubble

$$\Pi_0(q, q_n) = -2T \sum_{k_n} G(k+q, ik_n + iq_n) G(k, ik_n) = -2 \int \frac{dk}{2\pi} \left[\frac{f(\xi_{k+q}) - f(\xi_k)}{\xi_{k+q} - \xi_k - iq_n} \right]$$

as usual. So

$$\Pi_0^R(2k_F, 0) = - \int \frac{dk}{\pi} \left[\frac{f(\xi_{k+2k_F}) - f(\xi_k)}{\xi_{k+2k_F} - \xi_k - i0^+} \right].$$

Nesting for half-filled band: $\xi_{k+2k_F} = -2t \cos(ak + a2(\frac{\pi}{2a})) = 2t \cos(ak) = -\xi_k$. Also note $f(-x) = 1 - f(x)$. So

$$\begin{aligned} \Pi_0^R &= -\frac{1}{\pi} \int_{BZ} \frac{1 - 2f(\xi_k)}{-2\xi_k - i0^+} \\ &= -\frac{1}{\pi} \int d\omega N(\omega) \frac{\tanh \frac{\omega}{2T}}{-2\omega - i0^+}. \end{aligned}$$

Note we will drop the $i0^+$ now since the imaginary part is clearly zero since \tanh vanishes when $\omega = 0$. So we have to do the integral (put $x = \omega/2T$ and $\alpha = t/T$)

$$\begin{aligned} \Pi_0^R(2k_F, 0) &= \frac{1}{\pi} \int_{-2t}^{2t} d\omega \frac{\tanh \frac{\omega}{2T}}{\omega \sqrt{4t^2 - \omega^2}} = \frac{1\alpha}{2\pi t} \int_0^\alpha \frac{dx}{x} \frac{\tanh x}{\sqrt{\alpha^2 - x^2}} \\ &= \frac{\alpha}{\pi t} \left[\frac{1}{\alpha} \int_0^\alpha \frac{\log(\alpha + \sqrt{\alpha^2 - x^2}) - \log x}{\cosh^2 x} - \underbrace{\frac{1}{\alpha} \log \left(\frac{\alpha + \sqrt{\alpha^2 - x^2}}{x} \right) \tanh x |_0^\alpha}_0 \right] \\ &\stackrel{\alpha \gg 1}{\approx} \frac{1}{\pi t} \left[\underbrace{\log 2\alpha \int_0^\infty \frac{dx}{\cosh^2 x}}_1 - \underbrace{\int_0^\infty \frac{dx \log x}{\cosh^2 x}}_{-\log(\frac{4e^\gamma}{\pi})} \right] \quad \gamma = \text{Euler's const.} = 0.577 \\ &= \frac{1}{\pi t} \log \frac{8e^\gamma t}{\pi T} \end{aligned}$$

This is a bit different from the "correct" answer given in the problem, but it has the required log divergence at $T \rightarrow 0$.

c:

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

$$\mathcal{D}^{(0)R}(q, \omega) = \frac{2\omega_q}{(\omega + i0^+)^2 - \omega_q^2}. \quad (6)$$

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

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

$N(0)$ 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)

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

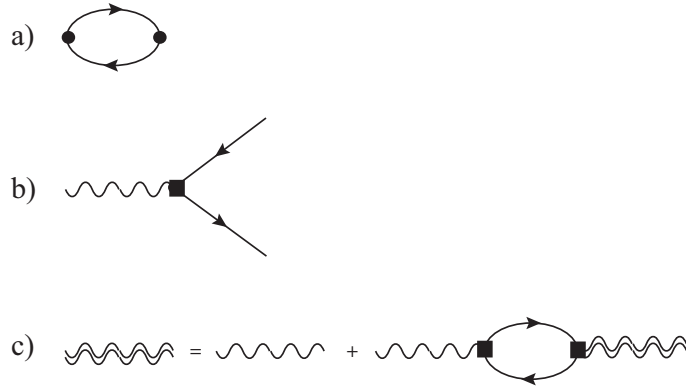


FIG. 1: Feynman diagrams corresponding to respectively: a) the electron polarization bubble $\Pi^{(0)R}$ (dots merely denote the beginning and ending of Greens functions), b) the electron-phonon interaction vertex, here denoted by a black square and corresponding to a factor of g_{el-ph} , and c) the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

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, $D^R(q, \omega)$, and find the renormalized phonon dispersion-relation $\tilde{\omega}_q$ 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 $(q, \omega) = (2k_F, 0)$.

So first of all the electronic DOS at the Fermi level is $N(0) = N/(2\pi t)$. Then the el-ph coupling const. is $g_{el-ph}^2 = \lambda\omega_q/(2N(0)) = \lambda(\omega_q\pi t/N)$. We are told to approximate the polarization operator in the phonon self energy by its static value at $2k_F$, so from Dyson we know that the inverse propagator is

$$\begin{aligned} D^{R-1}(q, \omega) &\simeq D^{(0)R-1}(q, \omega) + g_{el-ph}^2 \Pi^{(0)}(2k_F, 0) \\ &= \frac{\omega^2 - \omega_q^2}{2\omega_q} + \lambda \frac{\omega_q \pi t}{N} \frac{N}{\pi t} \log\left(\frac{8te^\gamma}{\pi T}\right) \\ &= \frac{\omega^2 - \omega_q^2}{2\omega_q} + \lambda\omega_q \log\left(\frac{8te^\gamma}{\pi T}\right). \end{aligned}$$

The renormalized phonon frequencies are just the poles of the inverse Green's function. So we set the above equal to zero, to find

$$\omega^2 = \omega_q^2 \left[1 - 2\lambda \log\left(\frac{8te^\gamma}{\pi T}\right) \right].$$

d:

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

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

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

$$\tilde{\omega}_q \propto |T - T_C|^\nu, \text{ for } T \gtrsim T_C. \quad (10)$$

As $T \rightarrow 0$, the 2nd term in the renormalized phonon dispersion increases, and the phonon will soften (indicating an instability) when $8te^\gamma/(\pi T) = e^{1/(2\lambda)}$, i.e. at a temperature

$$T_C = \frac{8t}{\pi} e^\gamma e^{-1/(2\lambda)}.$$

This is different by the same factor of two from the ‘‘correct’’ answer as the previous result.

Now put $T = T_C + \delta T$ and expand in $\tau = \delta T/T_C = (T - T_C)/T_C$. Near the transition, the frequencies behave as

$$\tilde{\omega}_q^2 = \omega_q^2 2\lambda \log(1 + \tau) \simeq \omega_q^2 2\lambda \tau.$$

so $\tilde{\omega}_q \propto |T - T_C|^{1/2}$ near the transition, $\nu = 1/2$.

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

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

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

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

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.

$$W_{2D}(\mathbf{q}) = \int d^2r e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{1}{4\pi\epsilon_r\epsilon_0} \frac{e^2}{r} = \frac{e^2}{4\pi\epsilon_r\epsilon_0} \int d\theta dr e^{iqr \cos \theta} = \frac{e^2}{2\epsilon_r\epsilon_0} \int dr J_0(qr) = \frac{e^2}{2\epsilon_r\epsilon_0 q}$$

b:

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

$$\epsilon_{RPA}^{2D}(\mathbf{q}, iq_n) = 1 - W^{2D}(\mathbf{q}) \chi_0^{2D}(\mathbf{q}, iq_n), \quad (13)$$

with

$$\chi_0^{2D}(\mathbf{q}, iq_n) = 2 \int \frac{d^2k}{(2\pi)^2} \frac{n_F(\xi_{\mathbf{k}+\mathbf{q}}) - n_F(\xi_{\mathbf{k}})}{\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}} - iq_n}. \quad (14)$$

Explain how one can derive this expression for $\chi_0^{2D}(\mathbf{q}, iq_n)$.

$$\begin{aligned} -T \sum_n \sum_{\mathbf{k}} G^0(\mathbf{k}, i\omega_n) G^0(\mathbf{k} + \mathbf{q}, i\omega_n + i\mathbf{q}_m) &= - \sum_{\mathbf{k}} \int_C \frac{dz}{2\pi i} n_F(z) \frac{1}{i\omega_n - \xi_{\mathbf{k}}} \frac{1}{i\omega_n + i\mathbf{q}_m - \xi_{\mathbf{k}+\mathbf{q}}} \\ &= - \sum_{\mathbf{k}} \int_{C'} \frac{dz}{2\pi i} n_F(z) \frac{1}{z - \xi_{\mathbf{k}}} \frac{1}{z + i\mathbf{q}_m - \xi_{\mathbf{k}+\mathbf{q}}} = \sum_{\mathbf{k}} \left(\frac{n_F(\xi_{\mathbf{k}})}{\xi_{\mathbf{k}} + i\mathbf{q}_m - \xi_{\mathbf{k}+\mathbf{q}}} + \frac{n_F(\xi_{\mathbf{k}+\mathbf{q}} - i\Omega_m)}{\xi_{\mathbf{k}+\mathbf{q}} - i\mathbf{q}_m - \xi_{\mathbf{k}}} \right), \end{aligned}$$

where as usual C is the contour encircling the Matsubara points on the imaginary z axis, and C' is the deformed contour encircling the poles on the real axis. The - sign arises because C' circles the poles in a clockwise fashion. Since Ω_m is a bosonic frequency, $e^{i\beta q_m} = 1$ and $n_F(\xi_{\mathbf{k}+\mathbf{q}} - i\mathbf{q}_m) = n_F(\xi_{\mathbf{k}+\mathbf{q}})$, so the final result is (with spin sum and volume=1)

$$\chi_0^{2D}(\mathbf{q}, iq_m) = 2 \sum_{\mathbf{k}} \left(\frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{\xi_{\mathbf{k}} + i\mathbf{q}_m - \xi_{\mathbf{k}+\mathbf{q}}} \right) = 2 \int \frac{d^2k}{(2\pi)^2} \frac{n_F(\xi_{\mathbf{k}+\mathbf{q}}) - n_F(\xi_{\mathbf{k}})}{\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}} - iq_n}. \quad (15)$$

So the only difference from 3 dimensions is the dimension of the \mathbf{k} -integration.

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_s^{2D} in terms of physical parameters of the electron gas. Using that for GaAs: $\epsilon_r = 13$, $m = 0.067m_e$ (m_e is the bare electron mass), how does k_s^{2D} compare to k_F when the density is $n = 2 \times 10^{15} m^{-2}$?

Within RPA, the dielectric function is

$$\epsilon(\mathbf{k}, \omega_n)|_{\text{RPA}} = 1 - W^{2D}(\mathbf{q}) \chi_0^{2D}(\mathbf{q}, \omega_n).$$

Taking the static homogeneous limit for Thomas-Fermi theory, the limit $q \rightarrow 0$ we find

$$\chi_0^{2D}(0, 0) \rightarrow -2 \sum_{\mathbf{k}} \frac{-\partial f}{\partial \xi_{\mathbf{k}}} \simeq -2N_0 \int d\xi_{\mathbf{k}} \frac{-\partial f}{\partial \xi_{\mathbf{k}}} = -2N_0 = \frac{m}{\pi}.$$

Note the form of the expression is independent of dimension, but of course in the 2D electron gas the expression for $N(0)$ is constant. The dielectric function then becomes

$$\epsilon^{2D}(0, 0) = 1 - \frac{e^2}{2\epsilon_r \epsilon_0 q} \frac{m}{\pi} \equiv 1 - \frac{k_s^{2D}}{q}.$$

In dimensionful units (put back \hbar),

$$k_x^{2D} = \frac{me^2}{2\epsilon_r \epsilon_0 \pi \hbar^2} = a_0^{-1} \frac{(m/m_e)}{2\epsilon_r} = (0.5 \text{Å})^{-1} \frac{0.067}{2 \cdot 13} = 0.0049 \text{Å}^{-1},$$

where a_0 is the Bohr radius. Fermi wave vector is

$$k_F = (2\pi n)^{1/2} = (2\pi [2 \times 10^{-5} \text{Å}^{-2}])^{1/2} = 0.11 \text{Å}^{-1}$$

so two are quite similar.

d:

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

$$\text{Re} \chi_0^{2D}(\mathbf{q}, \omega) = \frac{1}{2\pi^2} \frac{k_F}{\hbar v_F} \int_0^{2\pi} d\theta \frac{v_F q \cos \theta}{\omega - v_F q \cos \theta}. \quad (16)$$

At low T and $q \ll k_F$, we may write $\xi_{\mathbf{k}+\mathbf{q}} \simeq \xi_{\mathbf{k}} + v_{\mathbf{k}} \cdot \mathbf{q}$, $n_F(\xi_{\mathbf{k}+\mathbf{q}}) \simeq n_F(\xi_{\mathbf{k}}) + (v_{\mathbf{k}} \cdot \mathbf{q}) \frac{\partial n_F(\xi_{\mathbf{k}})}{\partial \xi_{\mathbf{k}}}$, so that the numerator of the integrand in χ_0^{2D} is $v_{\mathbf{k}} \cdot \mathbf{q} \frac{\partial n_F}{\partial \xi_{\mathbf{k}}}$. Since the Fermi function derivative restricts the relevant $\xi_{\mathbf{k}}$'s to a range of order T , we may replace $v_{\mathbf{k}}$ by v_F . Then the energy integration $\int d\xi \frac{\partial n_F}{\partial \xi} = -1$ may be performed, leaving

$$\text{Re} \chi_0^{2D}(\mathbf{q}, \omega) = \frac{1}{2\pi} N_0 \int_0^{2\pi} d\theta \frac{v_F q \cos \theta}{\omega - v_F q \cos \theta} = \frac{k_F}{2\pi^2 v_F} \int_0^{2\pi} d\theta \frac{v_F q \cos \theta}{\omega - v_F q \cos \theta}$$

e:

Using Eq. (16) in the long wavelength limit $q \ll \omega/v_F$, show that the 2D plasmon dispersion $\omega(q)$ is given by

$$\omega(q) = v_F \sqrt{\frac{k_s^{2D} q}{2}}. \quad (17)$$

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

In small q limit we can Taylor expand integrand and keep leading term

$$\text{Re} \chi_0^{2D}(\mathbf{q}, \omega) \simeq \frac{k_F}{2\pi^2 v_F} \int_0^{2\pi} d\theta (v_F q)^2 \frac{\cos^2 \theta}{\omega^2} = \frac{k_F}{2\pi v_F} \frac{(v_F q)^2}{\omega^2}$$

so product entering RPA dielectric constant is

$$W_0^{2D}(\mathbf{q}) \chi_0^{2D}(\mathbf{q}, \omega) \simeq \frac{e^2}{2\epsilon_r \epsilon_0 q} \frac{k_F}{2\pi v_F} \frac{(v_F q)^2}{\omega^2} = \frac{(v_F k_s^{2D})(v_F q)}{2\omega^2}.$$

Plasma pole will occur in this limit when the inverse dielectric constant has a pole, or when the dielectric const. has a zero, meaning $1 - \frac{(v_F k_s^{2D})(v_F q)}{2\omega^2} = 0$, or

$$\omega = v_F \sqrt{\frac{k_s^{2D} q}{2}}.$$

A 3D metal is transparent above its plasma frequency, but reflective below it. Now in 2D the plasma frequency effectively extends to zero, so we would expect a perfectly 2D electron gas to be transparent. However in practice the answer depends on the details of the actual thickness of the "2D" gas. See optical properties of solids books e.g. one by D. Tanner, to appear.

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?

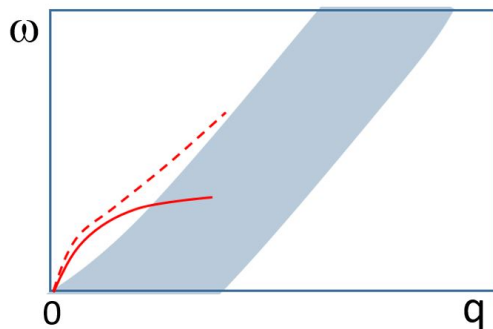


FIG. 2: shaded blue region is schematic p-h continuum, red line is 2D plasmon. Note while there must be a range of q for which the plasmon is undamped, it is not clear if the mode enters the continuum or not. Depends on ϵ_r .

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,

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \epsilon_d c_d^{\dagger} c_d + \frac{1}{\sqrt{\mathcal{A}}} \sum_{\mathbf{k}} \left(t^* c_{\mathbf{k}}^{\dagger} c_d + t c_d^{\dagger} c_{\mathbf{k}} \right) \quad (18)$$

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.

$\xi_{\mathbf{k}}$ represents a band of conduction electrons, while ϵ_d is the energy of the localized fermionic level. The hybridization term describes hopping onto the level from the conduction band and back again. This is the so-called Anderson model, except that there is no Hubbard-type U term penalizing double occupation of the impurity site. Thus there can be no true moment formation.

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} :

$$G^R(\mathbf{r}, \mathbf{r}; \omega) = -i\theta(t - t') \langle \{ \psi(\mathbf{r}, t), \psi^{\dagger}(\mathbf{r}, t') \} \rangle. \quad (19)$$

Show that, in general, we have

$$G^R(\mathbf{r}, \mathbf{r}; \omega) = \frac{1}{\mathcal{A}} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} G^R(\mathbf{k}, \mathbf{k}'; \omega), \quad (20)$$

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

$$G_0^R(\mathbf{r}, \mathbf{0}; \omega) = \frac{1}{\mathcal{A}} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\omega - \xi_{\mathbf{k}} + i\eta}. \quad (21)$$

The impurity breaks translational invariance, so the Green's function must be a function of \mathbf{k} and \mathbf{k}' independently, as discussed in class and in the notes for a potential scattering-type term $V_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}}^\dagger c_{\mathbf{k}'}$ added to the Hamiltonian. The second term results from a Fourier transform with respect to the difference variable $\mathbf{r} - \mathbf{0}$ of the unperturbed $G^0(\mathbf{k}, \omega)$ Green's function for the homogeneous system of conduction electrons, back to real space.

c:

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

$$G^R(\mathbf{k}, \mathbf{k}'; t - t') = -i\theta(t - t') \langle \{c_{\mathbf{k}}(t), c_{\mathbf{k}'}^\dagger(t')\} \rangle, \quad (22)$$

$$G^R(d, \mathbf{k}'; t - t') = -i\theta(t - t') \langle \{c_d(t), c_{\mathbf{k}'}^\dagger(t')\} \rangle, \quad (23)$$

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

$$G^R(\mathbf{k}, \mathbf{k}'; \omega) = \frac{1}{\omega - \xi_{\mathbf{k}} + i\eta} \left[\delta_{\mathbf{k}, \mathbf{k}'} + \left(\frac{|t|^2}{\omega - \epsilon_d + i\eta} \right) \frac{1}{\mathcal{A}} \sum_{\mathbf{k}''} G^R(\mathbf{k}'', \mathbf{k}'; \omega) \right]. \quad (24)$$

$$\begin{aligned} \dot{c}_{\mathbf{k}} &= -i[c_{\mathbf{k}}, H] = -i\epsilon_{\mathbf{k}} - it^* c_d \\ \dot{c}_d &= -i[c_d, H] = -i\epsilon_d - t \sum_{\mathbf{k}} c_{\mathbf{k}} \end{aligned}$$

from which you can derive the eqns. of motion for the G 's:

$$\begin{aligned} \frac{d}{dt} G^R(\mathbf{k}, \mathbf{k}'; t) &= -i\delta(t) \delta_{\mathbf{k}\mathbf{k}'} - i\theta(t) \langle [\dot{c}_{\mathbf{k}}(t), c_{\mathbf{k}'}^\dagger]_+ \rangle \\ \frac{d}{dt} G_d^R(d, \mathbf{k}'; t) &= -i\theta(t) \langle [\dot{c}_d(t), c_{\mathbf{k}'}^\dagger]_+ \rangle \end{aligned}$$

Fourier transforming and using the representation of the θ function we find,

$$\begin{aligned} (\omega - \epsilon_{\mathbf{k}} + i\eta) G^R(\mathbf{k}, \mathbf{k}'; \omega) &= \delta_{\mathbf{k}\mathbf{k}'} + t^* G^R(d, \mathbf{k}'; \omega) \\ (\omega - \epsilon_d + i\eta) G^R(d, \mathbf{k}'; \omega) &= t \sum_{\mathbf{k}'} G^R(\mathbf{k}, \mathbf{k}'; \omega) \end{aligned}$$

or

$$\begin{aligned} G^R(\mathbf{k}, \mathbf{k}'; \omega) &= G_0^R(\mathbf{k}, \omega) \delta_{\mathbf{k}\mathbf{k}'} + t^* G_0^R(\mathbf{k}, \omega) G^R(d, \mathbf{k}'; \omega) \\ G^R(d, \mathbf{k}'; \omega) &= t \sum_{\mathbf{k}} G_0^R(d, \omega) G^R(\mathbf{k}, \mathbf{k}'; \omega), \end{aligned}$$

where $G_0^R(\mathbf{k}, \omega) = (\omega - \epsilon_{\mathbf{k}} + i\eta)^{-1}$. Combine the two equations to get

$$G^R(\mathbf{k}, \mathbf{k}'; \omega) = G_0^R(\mathbf{k}, \omega) \delta_{\mathbf{k}\mathbf{k}'} + |t|^2 G_0^R(\mathbf{k}, \omega) G_0^R(d, \omega) \sum_{\mathbf{k}''} G^R(\mathbf{k}'', \mathbf{k}'; \omega)$$

d:

From equation (24) derived in question **c**, show that

$$G^R(\mathbf{r}, \mathbf{r}; \omega) = G_0^R(\mathbf{r}, \mathbf{r}; \omega) + G_0^R(\mathbf{r}, \mathbf{0}; \omega) T^R(\mathbf{0}, \mathbf{0}; \omega) G_0^R(\mathbf{0}, \mathbf{r}; \omega), \quad (25)$$

with the so-called T-matrix given by

$$T^R(\mathbf{0}, \mathbf{0}; \omega) = \frac{|t|^2}{\omega - \epsilon_d - \Sigma^R(\omega)}. \quad (26)$$

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

Fourier transforming the answer to (c) (note $G(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{k}, \mathbf{k}'} e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}'\cdot\mathbf{r}'}$) gives

$$G^R(\mathbf{r}, \mathbf{r}', \omega) = G_0^R(\mathbf{r} - \mathbf{r}', \omega) + |t|^2 G_0^R(\mathbf{r}, \omega) G_0^R(d, \omega) G^R(\mathbf{0}, \mathbf{r}', \omega)$$

Now let's write down 2 special cases: put $\mathbf{r} = \mathbf{r}'$:

$$G^R(\mathbf{r}, \mathbf{r}, \omega) = G_0^R(0, \omega) + |t|^2 G_0^R(\mathbf{r}, \omega) G_0^R(d, \omega) G^R(\mathbf{0}, \mathbf{r}, \omega)$$

And now put $\mathbf{r}, \mathbf{r}' = 0, \mathbf{r}$:

$$\begin{aligned} G^R(\mathbf{0}, \mathbf{r}) &= G_0^R(-\mathbf{r}) + |t|^2 G_0^R(\mathbf{0}, \omega) G_0^R(d, \omega) G^R(\mathbf{0}, \mathbf{r}, \omega) \\ \Rightarrow G^R(\mathbf{0}, \mathbf{r}) &= \frac{G_0^R(-\mathbf{r}, \omega)}{1 - |t|^2 G_0^R(\mathbf{0}, \omega) G_0^R(d, \omega)} \end{aligned}$$

$$\begin{aligned} \Rightarrow G(\mathbf{r}, \mathbf{r}, \omega) &= G_0^R(0, \omega) + |t|^2 G_0^R(\mathbf{r}, \omega) G_0^R(d, \omega) \left[\frac{G_0^R(-\mathbf{r}, \omega)}{1 - |t|^2 G_0^R(\mathbf{0}, \omega) G_0^R(d, \omega)} \right] \\ \Rightarrow T(0, 0, \omega) &= \frac{|t|^2 G_0^R(d, \omega)}{1 - |t|^2 G_0^R(\mathbf{0}, \omega) G_0^R(d, \omega)} = \frac{|t|^2}{\omega - \epsilon_d + i\eta - |t|^2 G_0^R(\mathbf{0}, \omega)} \end{aligned}$$

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 (26) using Feynman diagrams in space representation appropriate to the Hamiltonian (18)? (Hint: You can use the diagrammatic elements in (E.13.3) from exercise 13.3 in the textbook (B&F), with $U = 0$.)

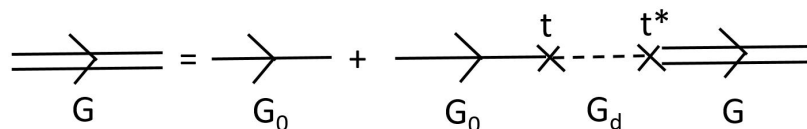


FIG. 3: Diagrammatic equation for conduction electron Green's function.

f:

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

$$A(\mathbf{r}, \mathbf{r}; \omega) = 2\pi N(\omega) + 2 \left(\text{Im}[G_0^R(\mathbf{r}, \mathbf{0}; \omega)] \right)^2 \left\{ 2q \text{Re}[T^R(\mathbf{0}, \mathbf{0}; \omega)] + (1 - q^2) \text{Im}[T^R(\mathbf{0}, \mathbf{0}; \omega)] \right\}, \quad (27)$$

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

$$q = -\frac{\text{Re}[G_0^R(\mathbf{r}, \mathbf{0}; \omega)]}{\text{Im}[G_0^R(\mathbf{r}, \mathbf{0}; \omega)]}. \quad (28)$$

In terms of our definition of the spectral function in class,

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}, \omega) &= -\frac{1}{\pi} \text{Im} G^R(\mathbf{r}, \mathbf{r}, \omega) = -\frac{1}{\pi} \text{Im} [G_0^R(0, \omega) + G_0^R(\mathbf{r}, \omega) T(0, \omega) G_0^R(-\mathbf{r}, \omega)] \\ &= -\frac{1}{\pi} \left[G_0^{R''}(0) - G_0^{R''}(\mathbf{r}) G_0^{R''}(-\mathbf{r}) T'' + G_0^{R'}(\mathbf{r}) G_0^{R'}(-\mathbf{r}) T'' + G_0^{R''}(\mathbf{r}) G_0^{R'}(-\mathbf{r}) T' + G_0^{R'}(\mathbf{r}) G_0^{R''}(-\mathbf{r}) T' \right] \\ &= A_0(0, \omega) - \frac{1}{\pi} [-G_0^{R''}(\mathbf{r})^2 T'' + G_0^{R'}(\mathbf{r})^2 T'' + 2G_0^{R''}(\mathbf{r}) G_0^{R'}(\mathbf{r}) T'], \end{aligned}$$

where ' and '' mean real and imaginary parts, respectively, and I've used the fact that the Hamiltonian is symmetric under reflection about the impurity site. I also dropped the "R" and the ω argument since it is the same for all functions. The change in the spectral function due to the impurity is now

$$\begin{aligned} \delta A(\mathbf{r}, \mathbf{r}, \omega) &= -\frac{1}{\pi} G_0^{R''}(\mathbf{r})^2 \left[-T'' + 2\frac{G_0^{R'}}{G_0^{R''}} T' + \left(\frac{G_0^{R'}}{G_0^{R''}} \right)^2 T'' \right] \\ &= \frac{1}{\pi} G_0^{R''}(\mathbf{r})^2 [(1 - q^2) T'' + 2q T'] \end{aligned}$$

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 (27) (argue why). Finally, we assume that $\text{Im}[G_0^R(\mathbf{r}, \mathbf{0}; \omega)] \approx \text{Im}[G_0^R(\mathbf{r}, \mathbf{r}; \omega)]$ (what does this require for the distance $|\mathbf{r}|$?).

Under these assumptions, show that equation (27) derived in question f can be rewritten as

$$A(\mathbf{r}, \mathbf{r}; x) = 2\pi N(0) \frac{(q + x)^2}{1 + x^2}, \quad (29)$$

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 ?

Conduction electron Green's function varies on scale of Fermi energy μ , but we are interested in energies having to do with the impurity, $\varepsilon_d, \Gamma \ll \mu$. Γ is Im part of self-energy

$$\Gamma = -\text{Im}|t|^2 G_0^R(0, \omega) \simeq \pi N_0 |t|^2 = \mathcal{O}(t^2/\mu).$$

so that

$$T \simeq \frac{|t|^2}{\omega - \epsilon_d + i\Gamma}$$

$$\Rightarrow T' = \frac{|t|^2}{\Gamma} \frac{x}{x^2 + 1} = \frac{1}{\pi N_0} \frac{x}{x^2 + 1}; \quad T'' = -\frac{|t|^2}{\Gamma} \frac{1}{x^2 + 1} = \frac{1}{\pi N_0} \frac{1}{x^2 + 1}$$

with $x = (\omega - \epsilon_d)/\Gamma$. Now note that $G_0^{R''}(0, \omega) \simeq \sum_{\mathbf{k}} (\omega - \epsilon_{\mathbf{k}} + i\eta)^{-1} \simeq -\pi N_0$, plus we will assume that the Green's function does not fall off too fast, so its value on the nearest neighbor site \mathbf{r} will be not too different. So from part (f):

$$A(\mathbf{r}, \mathbf{r}, \omega) = -\frac{1}{\pi} G_0^{R''}(0, \omega) + \frac{1}{\pi} G_0^{R''}(\mathbf{r})^2 [(1 - q^2)T'' + 2qT']$$

$$= N_0 \left[1 + \frac{1 - q^2 + 2qx}{1 + x^2} \right] = N_0 \left[\frac{(x + q)^2}{1 + x^2} \right].$$

I don't get the factor of 2π claimed in the problem, but I suspect this is different convention for spectral function. Plot of lineshape is

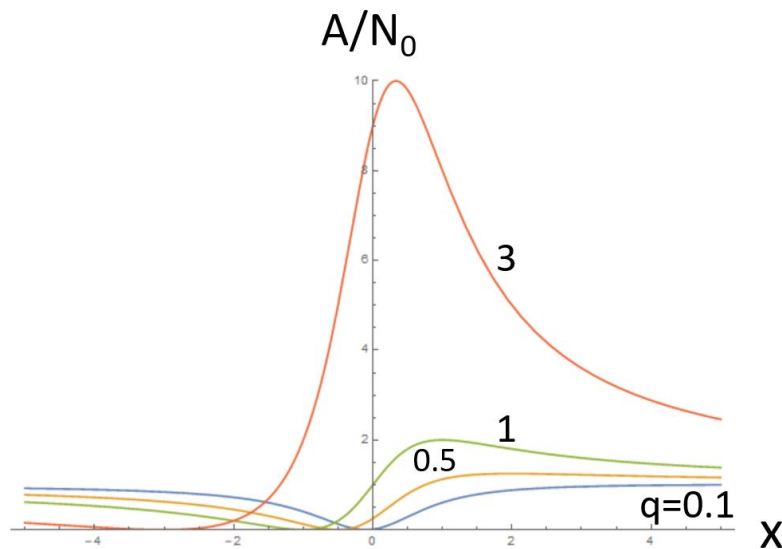


FIG. 4: Types of lineshapes possible within Fano description. Spectral function on impurity or nearby site vs. x for $q = 0.1, 0.5, 1, 3$.

The interpretation of the Fano factor q is not trivial, but it can be shown to represent the interference between the tunneling of a localized d electron and a conduction band electron. For more information, see the beautiful paper by Lu Yu and co-workers, H. G. Luo, T. Xiang, X. Q. Wang, Z. B. Su, and L. Yu Phys. Rev. Lett. 92, 256602. Note this paper is written for the Anderson model including a large Hubbard U term, and most of the interest is in the interference between the conduction electrons and the Kondo resonance, which we do not have here ($U = 0$). The resonance seen for large q in the STM differential conductance at $\propto A(\mathbf{r}, \mathbf{r}, \omega - eV)$, where V is the applied bias, is called the Fano resonance. Even for smaller q the large asymmetry of the conductance is a signal of the interference between two tunneling processes involving a localized level at finite energy.

The *Fano profile* formula (29) 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. 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.

