

1 (10 points)

1.1

Using Dyson's equation and the self-energy $\Pi_q(\omega_n)$ to second order in Λ , we get the following expression for the full phonon propagator:

$$D_q(\omega_n) = \frac{1}{(D_q^0(\omega_n))^{-1} - \Pi_q(\omega_n)} = \frac{1}{M\beta} \left[\omega_n^2 + \Omega_q^2 + 2\Lambda^2\Omega_q \sum_k \frac{f_k - f_{k+q}}{-i\omega_n + \varepsilon_k - \varepsilon_{k+q}} \right]^{-1}$$

We perform the analytic continuation

$$-i\omega_n \rightarrow \omega + i\eta$$

to obtain the retarded correlation function

$$D_q^R(\omega) = -\frac{1}{M} \frac{1}{-(\omega + i\eta)^2 + \Omega_q^2 + 2\Lambda^2\Omega_q \sum_k \frac{f_k - f_{k+q}}{\omega_n + \varepsilon_k - \varepsilon_{k+q} + i\eta}} = -\frac{1}{M} \frac{1}{-(\omega + i\eta)^2 - \Omega_q^2 + \Pi_q^R}$$

with Π_q^R defined as

$$\Pi_q^R(\omega) = -2M\Lambda^2\Omega_q \sum_k \frac{f_k - f_{k+q}}{\omega + \varepsilon_k - \varepsilon_{k+q} + i\eta}$$

1.2

Splitting the self-energy into its real and imaginary part, we can see that the real part modifies the phonon dispersion Ω_q :

$$D_q^R(\omega) = -\frac{1}{M} \frac{1}{-(\omega + i\eta)^2 + \underbrace{\Omega_q^2 + \text{Re}[\Pi_q^R]}_{\tilde{\Omega}_q^2} - i \text{Im}[\Pi_q^R]}$$

Let us now inspect the structure of the self-energy. For simplicity, we will consider the case of zero temperature in one dimension only. Here, the Fermi-factors are $f_k - f_{k+q} = \theta(k - k_F) - \theta(k + k_F - k)$, i.e. they give 1 within a shell of width q below the Fermi-surface and are zero otherwise. The self-energy correction is therefore a correction to the phonon dispersion as a result of coupling to the Fermi sea.

1.3

We evaluate the self-energy correction for one dimensional case assuming $\varepsilon_k = k^2/2m$. For this, we have to perform the sum

$$\begin{aligned} \sum_k \frac{f_k - f_{k+q}}{\omega + \varepsilon_k - \varepsilon_{k+q} + i\eta} &= \frac{L}{2\pi} \int_{k_F - q}^{k_F} dk \frac{1}{\omega - kq/m - q^2/2m + i\eta} + \frac{L}{2\pi} \int_{-k_F}^{-(k_F - q)} dk \frac{1}{\omega - kq/m - q^2/2m + i\eta} \\ &= \frac{mL}{2\pi q} \left[\ln \left(\frac{\omega + i\eta - (2k_F q + q^2)/2m}{\omega + i\eta - (2k_F q - q^2)/2m} \right) + \ln \left(\frac{\omega + i\eta + (2k_F q + q^2)/2m}{\omega + i\eta + (2k_F q - q^2)/2m} \right) \right] \\ &= \frac{mL}{2\pi q} \left[\ln \left(\frac{[\omega + i\eta]^2 - [(2k_F q + q^2)/2m]^2}{[\omega + i\eta]^2 - [(2k_F q - q^2)/2m]^2} \right) \right] \end{aligned}$$

The sum diverges for small ω and $k = \pm 2k_F$. This divergence signals an *instability* of the system towards a formation of the *dimerized phase*, also known as Peierls instability. Physically electron-phonon systems in 1D are known to dimerize (i.e. in a lattice model every other bond becomes slightly shorter), polyacetylene being a prominent example of this phenomenon.

In dimensions higher than 1 the effect is also present but is weaker: the self energy itself remains finite but its derivative has a divergence. The phonon dispersion thus develops a kink at $\pm 2k_F$ which is known as the *Kohn anomaly*. This is also a measurable effect.

2 (10 points)

2.1

Assuming that a positive ionic background cancels out the Hartree contribution the total ground state energy in the Hartree-Fock approximation is given by

$$E_{tot}^{HF} = E_{\text{non-int}} + E^{ex}$$

where

$$E^{ex} = -\frac{3e^2 p_f}{4\pi} = -\frac{3}{2} \left(\frac{3}{2\pi} \right)^{2/3} \frac{1}{r_s} E_0 N$$

was derived in D&S (6.2.13). We are left to compute the free-electron piece $E_{\text{non-int}}$:

$$E_{\text{non-int}} = \frac{1}{2m} \sum_{\sigma=\uparrow\downarrow} \sum_{|\mathbf{p}| < p_F} \mathbf{p}^2 = 2 \cdot \frac{1}{2m} V \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \mathbf{p}^2 = 2 \cdot \frac{1}{2m} \frac{4\pi V}{(2\pi)^3} \frac{p_F^5}{5} = 2 \cdot \frac{3}{10} \left(\frac{9\pi}{4} \right)^{2/3} \frac{1}{r_s^2} N E_0$$

In total, we get

$$E_{tot}^{HF} = \left(\frac{3}{5} \left(\frac{9\pi}{4} \right)^{2/3} \frac{1}{r_s^2} - \frac{3}{2} \left(\frac{3}{2\pi} \right)^{2/3} \frac{1}{r_s} \right) N E_0 = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right) N E_0$$

as a final expression.

2.2

If the electron gas is polarized, we need to add up the contributions of the two spin species to the ground state energy. We introduce N_σ , the number of electron with spin $\sigma = \pm$ and define the corresponding $r_{s\sigma}$

$$\frac{4}{3} \pi (r_{s\sigma} a_0)^3 = \frac{V}{N_\sigma}.$$

The ground state energy is now

$$E_{tot}^{HF} = \sum_{\sigma} \left(\frac{2.21}{r_{s\sigma}^2} - \frac{0.916}{r_{s\sigma}} \right) N_\sigma E_0$$

where

$$\begin{aligned} N_\sigma &= \frac{N + \sigma N M}{2} = N \frac{1 + \sigma M}{2} \\ r_{s\sigma} &= r_s (1 + \sigma M)^{-\frac{1}{3}} \end{aligned}$$

The last relation between r_s and $r_{s\sigma}$ was obtained by recalling the definition

$$\frac{4}{3}\pi(r_s a_0)^3 = \frac{V}{N/2}.$$

Inserting this yields

$$\begin{aligned} E_{tot}^{HF} &= \frac{1}{2} \sum_{\sigma} \left(\frac{2.21}{r_s^2} (1 + \sigma M)^{\frac{5}{3}} - \frac{0.916}{r_s} (1 + \sigma M)^{\frac{4}{3}} \right) N E_0 \\ &= \left(\frac{2.21}{r_s^2} \left[\sum_{\sigma} \frac{1}{2} (1 + \sigma M)^{\frac{5}{3}} \right] - \frac{0.916}{r_s} \left[\sum_{\sigma} \frac{1}{2} (1 + \sigma M)^{\frac{4}{3}} \right] \right) N E_0 \end{aligned}$$

2.3

We compute the difference in the ground dstate energy between the fully polarized and unpolarized state

$$\begin{aligned} E_{tot}^{HF}(M=1) - E_{tot}^{HF}(M=0) &= \left(\frac{2.21}{r_s^2} \left[\frac{1}{2} 2^{\frac{5}{3}} - 1 \right] - \frac{0.916}{r_s} \left[\frac{1}{2} 2^{\frac{4}{3}} - 1 \right] \right) N E_0 \\ &= \left(\frac{2.21}{r_s^2} 0.587 - \frac{0.916}{r_s} 0.260 \right) N E_0 \end{aligned}$$

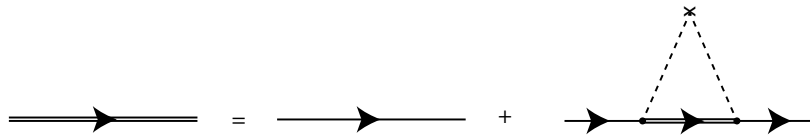
Above a critical value of $r_s^c = 5.45$, the energy difference becomes negative and the fully magnetized state ($M=1$) has lower energy.

One may think about this in the following way: for larger r_s the average spacing between electrons increases while the electron density and p_F decrease correspondingly. This lowers the non-interacting ground state energy $E_{\text{non-int}}$. We have derived that $E_{\text{non-int}}$ falls as $1/r_s^2$. The exchange energy, which is a negative correction, also decreases, but only as $1/r_s$. Thus, for large enough r_s , the exchange correction dominates. This leads to the well known but rather counter-intuitive result that interactions in the electron gas become more important in the *dilute limit*, a purely quantum effect rooted in the Pauli exclusion principle.

The exchange correction is larger for the fully magnetized state ($-0.916 \cdot 2^{1/3} N E_0 / r_s$ compared to $-0.916 N E_0 / r_s$). Intuitively, this is because the Pauli principle has the largest effect when all particles are indistinguishable (i.e. have the same spin).

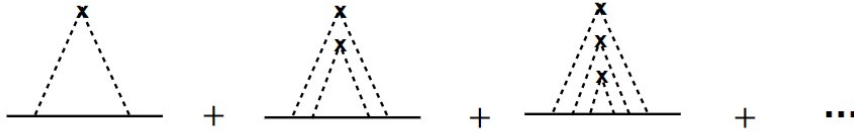
3 (5 bonus points)

The series can be summed up as shown in the figure below. This approach is sometimes called *self consistent Born approximation*. The resulting Dyson equation then implicitly determines G but typically cannot be solved analytically.



In the case of short-range impurity potential, however, we can work out an analytic expression for the series. The key observation is that the Fourier transform of the impurity potential is momentum independent

for short-range impurities modeled by randomly distributed δ -function potentials, $U_q = U$. Using this, the expression corresponding to the diagrams



becomes

$$\begin{aligned}
 & U^2 \sum_{p_1} G^0(p) G^0(p_1) G^0(p) + U^4 \sum_{p_1 p_2} G^0(p) G^0(p_1) G^0(p_2) G^0(p_1) G^0(p) + \dots \\
 = & U^2 [G^0(p)]^2 \left(\sum_{p_1} G^0(p_1) + U^2 \sum_{p_1} [G^0(p_1)]^2 \sum_{p_2} G^0(p_2) + U^4 \sum_{p_1} [G^0(p_1)]^2 \sum_{p_2} [G^0(p_2)]^2 \sum_{p_3} G^0(p_3) + \dots \right)
 \end{aligned}$$

Defining

$$\begin{aligned}
 x &= \sum_p G^0(p) \\
 y &= \sum_p [G^0(p)]^2
 \end{aligned}$$

we can write this as

$$U^2 [G^0(p)]^2 (x + U^2 xy + U^4 xy^2 + U^6 xy^3 + \dots) = U^2 [G^0(p)]^2 x (1 + U^2 y + U^4 y^2 + U^6 y^3 + \dots)$$

We recognize the geometric series which we sum up to get the final expression

$$U^2 [G^0(p)]^2 \frac{x}{1 - U^2 y} .$$