M1- Sciences de la Matière, A. A. 2023-2024
Superconductivity, superfluidity and magnetism
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Midterm take-home exam – March 4-8th, 2024

Cet examen est un devoir-maison: afin de mieux tester vos connaissances, vous êtes encouragé.e.s à le travailler seul.e.s, mais aussi à vous servir de tout le matériel que vous le souhaitez, et notamment du matériel du cours et des TDs. Le sujet d'examen ne nécessite pas de données que vous ne puissiez pas trouver dans le cours et les TDs. Le temps que vous allez passer dans la préparation de votre copie est laissé à votre discretion, mais idéalement il ne devrait pas dépasser les 3 heures.

1 Short questions

These questions only require a short answer/ a short calculation!

Q1. Can you give a qualitative argument to explain why ^{4}He does not solidify at ambient pressure?

Solution: He is an atom which is both light and chemically inert. The He-He interaction potential has a shallow minimum at 0.265 nm with a depth of approximately 11 K; at this temperature the thermal de Broglie wavelength of an He atom is approximately 0.4 nm, namely larger than the interparticle spacing. This means that at the temperature at which the solid should form, the quantum uncertainty on the position of the atom is larger than the lattice spacing, and therefore quantum fluctuations essentially prevent the atoms from solidifying in a static pattern.

Q2. Consider a 1d Bose gas in a harmonic potential, $V(x) = m\omega^2 x^2/2$, and be $\Psi_0(x)$ the macroscopic wavefunction describing a Bose-Einstein condensate. What is the difference between the macroscopic wavefunction in the case of the ground-state of the ideal Bose gas, and that in the presence of interactions, i.e. the solution to the Gross-Pitaevskii equation? *Hint:* use the Thomas-Fermi approximation to solve the Gross-Pitaevskii equation.

Solution: In the case of the ideal Bose gas the macroscopic wavefunction for the ground state is a Gaussian, $\Psi_0(x) \sim \sqrt{N} e^{-x^2/2\sigma^2}$ where $\sigma = \sqrt{\hbar/m\omega}$. Instead in the case of the Thomas-Fermi solution to the Gross-Pitaevskii equation $\Psi_0(x) = (\mu - V(x))/g$, namely $\Psi_0(x)$ is an inverted parabola, much broader than the Gaussian, because of the presence of interactions.

Q3. Spin-spin interactions in magnetic solids come from the magnetic dipole moment associated with the spin: true or false? Provide some argument to justify your answer.

Solution: False, the magnetic dipole associated with the spins cannot account for the spin-spin interactions. Two magnetic dipoles of 1 Bohr magneton each, placed at 1 Åof distance, have an interaction energy of about 1K, much too weak to justify the appearance of magnetism at temperatures of hundreds or even thousands of K.

Q4. Be $\psi_1(x)$, $\psi_2(x)$ and $\psi_3(x)$ three orthonormal single-particle wavefunctions. Write the wavefunction associated to each of these three-particle states

$$|\Psi_B\rangle = b_1^\dagger b_2^\dagger b_3^\dagger |0\rangle \qquad |\Psi_F\rangle = f_1^\dagger f_2^\dagger f_3^\dagger |0\rangle \tag{1}$$

in terms of the ψ_1, ψ_2, ψ_3 wavefunctions. Here $b_i^\dagger$ $(i = 1, 2, 3)$ creates a boson in ψ_i, while $f_i^\dagger$ creates a fermion.

Solution: One should build the 3×3 matrix $\{\psi_i(x_j)\}$, and then obtain the many-body wavefunction as the matrix permanent for bosons, and the matrix determinant for fermions.

Q5. Consider the two electronic states in first quantization

$$\Psi_\pm = \frac{1}{2}\left[\psi_1(x_1)\psi_2(x_2) \pm \psi_2(x_1)\psi_1(x_2)\right]\left(|\uparrow_1\downarrow_2\rangle \mp |\downarrow_1\uparrow_2\rangle\right) \ . \tag{2}$$

Write these states in terms of the states in second quantization

$$f_{1,\uparrow}^\dagger f_{2,\downarrow}^\dagger|0\rangle \qquad f_{1,\downarrow}^\dagger f_{2,\uparrow}^\dagger|0\rangle \tag{3}$$

where $f_{i,\sigma}^\dagger$ creates an electron in state $\psi_i(x)|\sigma\rangle$.

Solution: We have that

$$f_{1,\uparrow}^\dagger f_{2,\downarrow}^\dagger|0\rangle \to \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)|\uparrow_1\downarrow_2\rangle - \psi_2(x_1)\psi_1(x_2)|\downarrow_1\uparrow_2\rangle\right)$$

and

$$f_{1,\downarrow}^\dagger f_{2,\uparrow}^\dagger|0\rangle \to \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)|\downarrow_1\uparrow_2\rangle - \psi_2(x_1)\psi_1(x_2)|\uparrow_1\downarrow_2\rangle\right)$$

. Hence

$$\Psi_\pm = \frac{1}{\sqrt{2}}\left(f_{1,\uparrow}^\dagger f_{2,\downarrow}^\dagger|0\rangle \mp f_{1,\downarrow}^\dagger f_{2,\uparrow}^\dagger|0\rangle\right) \ .$$

Q6. Two fermions with $S = 1/2$ can bind to form a composite boson with $S = 0$ or 1. Consider the field operator

$$\hat{\phi}_y(x) = \hat{\psi}_\uparrow(x + y/2)\ \hat{\psi}_\downarrow(x - y/2) \tag{4}$$

destroying a pair of fermions of opposite spins at distance y and with center of mass in x. Provide a simple condition on x, x' and y under which the operators $\hat{\phi}_y(x)$ and $\hat{\phi}_y(x')$ satisfy bosonic commutation relations at different positions, i.e. $[\hat{\phi}_y(x), \hat{\phi}_y^\dagger(x')] = 0$ and $[\hat{\phi}_y(x), \hat{\phi}_y(x')] = 0$.

Solution: If we require that $|x - x'| > y$, namely that the composite bosons are further apart than their size, than we are guaranteed that the pairs of fermionic operators creating and destroying them commute with each other.

2 Hong-Ou-Mandel effect

In this exercise, we consider a very important effet of interference between two identical particles, the so-called Hong-Ou-Mandel effect. The setup to observe this effect implies a so-called beam-splitter transformation, namely the linear transformation of two input states ϕ_1, ϕ_2 into two output states ψ_1, ψ_2:

$$|\psi_1\rangle = \cos\theta|\phi_1\rangle + e^{i\phi}\sin\theta|\phi_2\rangle \tag{5}$$

$$|\psi_2\rangle = \sin\theta|\phi_1\rangle - e^{i\phi}\cos\theta|\phi_2\rangle \tag{6}$$

See Fig. 1(a) for an illustration. Throughout the exercise we will assume that the particles of interest can be bosons *or* fermions.

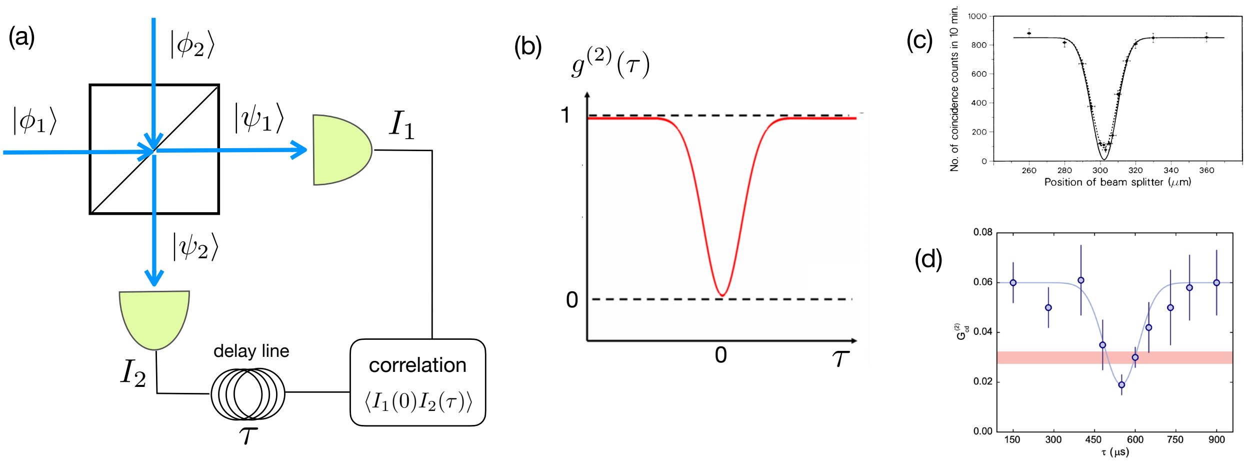

Figure 1: Hong-Ou-Mandel (HOM) effect: (a) scheme of a beam-splitter experiment, with input modes a_1, a_2 and output modes b_1, b_2. The number of particles detected at the two output ports translates into two signals of intensity I_1 and I_2 which are recombined and correlated; (b) dependence of the $g^{(2)}$ function on the delay time τ between the two signals I_1 and I_2, in the case of bosons; (c) and (d): HOM experiment done with (c) photons (C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. 1987) and (d) with atoms (R. Lopes et al., Nature 2015).

2.1

Be $a_1, a_1^\dagger$ and $a_2, a_2^\dagger$ the operators that destroy and create particles in states ϕ_1 and ϕ_2 respectively; and $b_1, b_1^\dagger$ and $b_2, b_2^\dagger$ the operators that destroy and create particles in states ψ_1 and ψ_2 respectively. Write down the linear relationship between a_1, a_2 and b_1, b_2.

Solution:

$$b_1 = \cos\theta\ a_1 + e^{-i\phi}\sin\theta\ a_2 \qquad b_2 = \sin\theta\ a_1 - e^{-i\phi}\cos\theta\ a_2$$

2.2

Calculate the number operators of output particles $b_1^\dagger b_1$, $b_2^\dagger b_2$ as a function of the input operators $a_{1(2)}, a_{1(2)}^\dagger$. What is the relationship between the number of incoming particles, $a_1^\dagger a_1 + a_2^\dagger a_2$, and the number of outgoing ones, $b_1^\dagger b_1 + b_2^\dagger b_2$?

Solution:

$$b_1^\dagger b_1 = \cos^2\theta\ a_1^\dagger a_1 + \sin^2\theta\ a_2^\dagger a_2 + \sin\theta\cos\theta(e^{-i\phi} a_1^\dagger a_2 + e^{i\phi} a_2^\dagger a_1)$$

$$b_2^\dagger b_2 = \sin^2\theta\ a_1^\dagger a_1 + \cos^2\theta\ a_2^\dagger a_2 - \sin\theta\cos\theta(e^{-i\phi} a_1^\dagger a_2 + e^{i\phi} a_2^\dagger a_1)$$

The number of incoming particles is equal to that of outgoing ones.

2.3

We denote with $|n_1, n_2\rangle$ an incoming Fock state for the a_1, a_2 particles, such that $a_1^\dagger a_1 |n_1, n_2\rangle = n_1 |n_1, n_2\rangle$ and $a_2^\dagger a_2 |n_1, n_2\rangle = n_2 |n_1, n_2\rangle$. What is the outgoing number of particles at the two ports, $\langle b_1^\dagger b_1\rangle$ and $\langle b_2^\dagger b_2\rangle$? And under which condition does one get $\langle b_1^\dagger b_1\rangle = \langle b_2^\dagger b_2\rangle$?

Solution:

$$\langle b_1^\dagger b_1\rangle = \cos^2\theta\ n_1 + \sin^2\theta\ n_2 \qquad \langle b_2^\dagger b_2\rangle = \sin^2\theta\ n_1 + \cos^2\theta\ n_2$$

Clearly for $n_1 = n_2 = n$ one has $\langle b_1^\dagger b_1\rangle = \langle b_2^\dagger b_2\rangle = n$ for any mixing angle θ. Otherwise for $\theta = \pi/4$ one has $\langle b_1^\dagger b_1\rangle = \langle b_2^\dagger b_2\rangle = (n_1 + n_2)/2$.

2.4

After the answer to the previous question, you may think that the beam splitter redistributes the incoming particles uniformly at the output ports. Let us examine the situation more closely by looking at the correlation between the output ports, namely the product $b_1^\dagger b_1 b_2^\dagger b_2$. Calculate this operator as a function of the incoming-state operators $a_{1(2)}, a_{1(2)}^\dagger$, and by retaining only the terms which conserve the particle numbers in the two incoming states (namely which commute with $a_1^\dagger a_1$ and $a_2^\dagger a_2$). Use the bosonic commutation and fermionic anti-commutation relations to express the result in terms of the incoming particle numbers n_1 and n_2.

Solution:

$$\begin{aligned} b_1^\dagger b_1 b_2^\dagger b_2 &= \cos^2\theta \sin^2\theta\ (n_1^2 + n_2^2) + (\cos^4\theta + \sin^4\theta)\ n_1 n_2 - \sin^2\theta\cos^2\theta\,(n_1 + n_2 + 2\eta\ n_1 n_2) \\ &+ \ \text{(terms not conserving the incoming populations)} \end{aligned}$$

with $\eta = 1$ for bosons and $\eta = -1$ for fermions.

2.5

Considering the case $n_1 = n_2 = 1$, show that

$$\langle b_1^\dagger b_1 b_2^\dagger b_2\rangle = \begin{cases} 1 & \text{for fermions} \\ \cos^2(2\theta) & \text{for bosons} \end{cases} . \tag{7}$$

What is special about bosons?

Solution: The result follows directly from that of the previous question as a special case. As one can see, for bosons this number can vanish, precisely when one has a 50-50 beam splitter with $\theta = \pi/4$.

2.6

In a Hong-Ou-Mandel experiment particles are continuously sent into the beam splitter; particles at the output ports are detected, and the detection generates two signals I_1 and I_2 proportional to the number $b_1^\dagger b_1$ and $b_2^\dagger b_2$ of detected particles. These signals are then correlated, so as to reconstruct the second-order correlation function

$$g^{(2)}(\tau) = \frac{\langle I_1(0) I_2(\tau)\rangle}{\langle I_1\rangle\langle I_2\rangle} = \frac{\langle (b_1^\dagger b_1)(0)(b_2^\dagger b_2)(\tau)\rangle}{\langle b_1^\dagger b_1\rangle\langle b_2^\dagger b_2\rangle} \tag{8}$$

where τ is a delay time imposed between the acquisition of the two signals. The typical outcome of a Hong-Ou-Mandel experiment done with bosons is shown in Fig. 1(b) (with concrete examples with photons in Fig. 1(c) and with atoms in Fig. 1(d)). Based on the result of the previous question, can you explain what you see in the figure?

Solution: The $g^{(2)}(\tau)$ function is 1 for large $|\tau|$, as the signals at large time difference become uncorrelated. On the other hand, for $\tau = 0$ the function goes to zero in a 50-50 beam splitter (or, more generally, to $\cos^2(2\theta) \leq 1$) because of the two-particle interference effect outlined above.

3 Stoner instability and ferromagnetism in a Fermi gas

In this exercise we consider a Fermi gas of *interacting* electrons, possessing a spin 1/2. We shall be interested in single-particle states which are then joint states of position ($\boldsymbol{r}$) and spin (σ), of the form $|\boldsymbol{r}, \sigma\rangle$; and of momentum ($\hbar\boldsymbol{k}$) and spin, of the form $|\boldsymbol{k}, \sigma\rangle$ with $\sigma = \uparrow, \downarrow$. The corresponding operators destroying and creating particles in these states are indicated as $\psi_\sigma(\boldsymbol{r}), \psi^\dagger_\sigma(\boldsymbol{r})$, and $c_{\boldsymbol{k},\sigma}, c^\dagger_{\boldsymbol{k},\sigma}$, respectively.

3.1

We start from the non-interacting Fermi gas at $T = 0$ in three-dimensional space. The Hamiltonian of the system in second quantization reads

$$H_{\text{kin}} = \sum_{\sigma=\uparrow,\downarrow} \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} \, c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} \tag{9}$$

where $\epsilon_{\boldsymbol{k}} = \hbar^2 k^2/2m$. Since electrons obey the Pauli exclusion principle, in the ground state at $T = 0$ they occupy all the single particle states with energy smaller than the Fermi energy $\epsilon_{\boldsymbol{k}} \leq \epsilon_F$, namely all the states with momentum smaller than the Fermi momentum $|\boldsymbol{k}| \leq k_F$, such that the density reads

$$n = \frac{N}{V} = \sum_\sigma \frac{1}{V} \sum_{\boldsymbol{k}:|\boldsymbol{k}|\leq k_F} \tag{10}$$

where N is the total particle number, and V the volume of the system. In the limit of $N, V \to \infty$ you can transform the sum $V^{-1} \sum_{\boldsymbol{k}}(...)$ into an integral. Show then that, for a Fermi gas with two spin states and density n

$$k_F = (3\pi^2 n)^{1/3} \tag{11}$$

and therefore, defining the densities of spin $\uparrow$ and spin $\downarrow$ particles $n_\uparrow = N_\uparrow/V$ and $n_\downarrow = N_\downarrow/V$

$$k_{F,\uparrow} = (6\pi^2 n_\uparrow)^{1/3} \qquad k_{F,\downarrow} = (6\pi^2 n_\downarrow)^{1/3} \; . \tag{12}$$

Solution:

$$n = \frac{N}{V} = \frac{(2)}{(2\pi)^3} \frac{4\pi}{3} k_F^3$$

hence the result, in which the factor of 2 is omitted in the case of a single spin species.

3.2

Write the density of kinetic energy of the gas as a sum over k-space, then as an integral, and show that it can be written as

$$e_{\text{kin}} = \frac{\langle H_{\text{kin}} \rangle}{V} = \frac{3}{5} \left(\, n_\uparrow \epsilon_{F,\uparrow} + n_\downarrow \epsilon_{F,\downarrow} \, \right) \tag{13}$$

where $\epsilon_{F,\sigma} = \frac{\hbar^2 k_{F,\sigma}^2}{2m}$.

Solution: The average energy reads:

$$\frac{\langle H_{\text{kin}}\rangle}{V} = \sum_\sigma \frac{\hbar^2}{2m}\frac{4\pi}{(2\pi)^3}\int_0^{k_{F,\sigma}} dk\ k^4 = \sum_\sigma \frac{3}{5} n_\sigma \epsilon_{F,\sigma}\ .$$

3.3

Introducing the polarization variable

$$p = \frac{N_\uparrow - N_\downarrow}{N} \tag{14}$$

rewrite $N_\uparrow$ and $N_\downarrow$ in terms of N and p, and show that

$$e_{\text{kin}}(p) = \frac{e_{\text{kin}}(0)}{2}\left[(1+p)^{5/3} + (1-p)^{5/3}\right] \tag{15}$$

where $e_{\text{kin}}(0)$ is the kinetic energy density at zero polarization. Prove that the energy minimum is obtained for $p = 0$.

Solution: Given that $N_\uparrow = \frac{1+p}{2}N$, $N_\downarrow = \frac{1-p}{2}N$, the result follows directly from the fact that $n_\sigma \epsilon_{F,\sigma} \sim n_\sigma^{5/3} \sim (1+\sigma p)^{5/3}$. Since $de_{\text{kin}}(p)/dp \sim [(1+p)^{2/3} - (1-p)^{2/3}]$, the only solution to $de_{\text{kin}}(p)/dp = 0$ is for $p = 0$.

3.4

We now add interactions to the picture, namely the potential energy (in second quantization)

$$H_{\text{pot}} = \frac{1}{2}\sum_{\sigma\sigma'}\int_V d^3r \int_V d^3r' \psi^\dagger_\sigma(\boldsymbol{r})\psi^\dagger_{\sigma'}(\boldsymbol{r}')V(\boldsymbol{r}-\boldsymbol{r}')\psi_{\sigma'}(\boldsymbol{r}')\psi_\sigma(\boldsymbol{r})\ . \tag{16}$$

In the following we will assume a contact interaction between the fermions, $V(\boldsymbol{r}-\boldsymbol{r}') = g\ \delta(\boldsymbol{r}-\boldsymbol{r}')$, and $g > 0$. Using the transformation from the $\psi^\dagger_\sigma(\boldsymbol{r})$ operators to the $c_{\boldsymbol{k},\sigma}$ operators, show that

$$H_{\text{pot}} = \frac{g}{2V}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}}\sum_{\sigma\sigma'} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma}\ . \tag{17}$$

Solution: Since $\psi_\sigma(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{V}} c_{\boldsymbol{k},\sigma}$ and

$$\int_V d^3r\ e^{i(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4)\cdot\boldsymbol{r}} = V\ \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,-\boldsymbol{k}_3-\boldsymbol{k}_4}$$

one obtains the result above.

3.5

We would then like to calculate the expectation value of the potential energy on the state of the electron gas with lowest kinetic energy (as considered above), but possessing a finite polarization p. Such a state is generically a Fock state on the single-particle basis $|\boldsymbol{k},\sigma\rangle$. Justify why $\langle c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma}\rangle$ is finite for this state only in two cases

1. $\boldsymbol{q} = 0$;
2. $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$ and $\sigma = \sigma'$.

Evaluate the expectation value in the two cases, accounting correctly for the fermionic anticommutation relations.

Solution: The two cases above are the only ones in which the operator $c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma}$ conserves the populations $N_{\boldsymbol{k},\sigma}$ of the states $|\boldsymbol{k},\sigma\rangle$. The first case leads to the expectation value

$$\langle c^\dagger_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma} \rangle = N_{\boldsymbol{k}\sigma} N_{\boldsymbol{k}'\sigma'} - N_{\boldsymbol{k}\sigma} \delta_{\boldsymbol{k},\boldsymbol{k}'} \delta_{\sigma,\sigma'}$$

while the second case gives

$$\langle c^\dagger_{\boldsymbol{k}',\sigma} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k}',\sigma} c_{\boldsymbol{k},\sigma} \rangle = -N_{\boldsymbol{k}\sigma} N_{\boldsymbol{k}'\sigma} + N_{\boldsymbol{k}\sigma} \delta_{\boldsymbol{k},\boldsymbol{k}'} \ .$$

3.6

Show that

$$\langle H_{\text{pot}} \rangle = \frac{g}{4V} \ N^2 (1 - p^2) \ . \tag{18}$$

Solution: We have that

$$\langle H_{\text{pot}} \rangle = \frac{g}{2V} \sum_{\boldsymbol{k}\boldsymbol{k}'} \sum_{\sigma\sigma'} N_{\boldsymbol{k},\sigma} N_{\boldsymbol{k}',\sigma'} (1 - \delta_{\sigma\sigma'}) = \frac{g}{2V} \left(N^2 - N_\uparrow^2 - N_\downarrow^2 \right)$$

which leads to the above result.

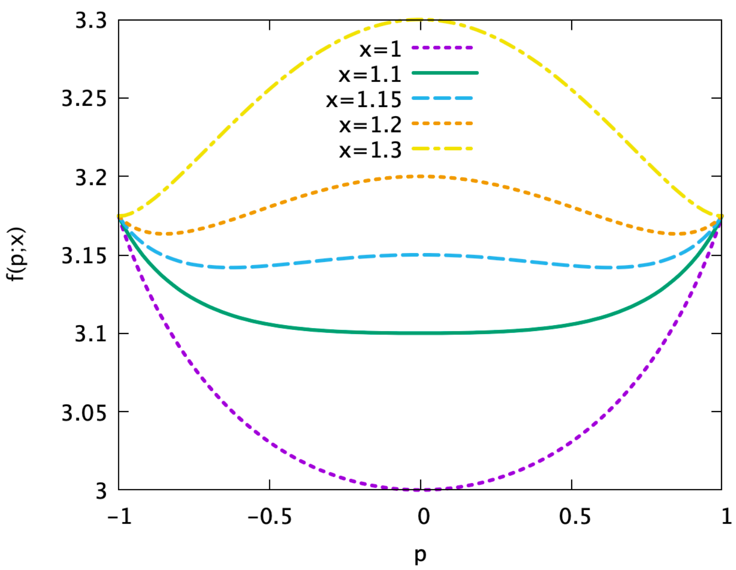

Figure 2: $f(p;x)$ function.

3.7

The expectation value of the total energy is then of the form

$$\langle H_{\text{kin}} + H_{\text{pot}} \rangle = E_0 \; f(p; x) \tag{19}$$

where

$$f(p; x) = (1 + p)^{5/3} + (1 - p)^{5/3} + x(1 - p^2) \tag{20}$$

and the parameters E_0 and x are to be determined. The function $f(p; x)$ is shown in Fig. 2. Can you deduce that interactions may lead to *ferromagnetism* in a Fermi gas, and how?

Solution: $E_0 = \frac{3}{10} N \epsilon_F$ and $x = \frac{5gn}{6\epsilon_F}$. When x is sufficiently large, i.e. interactions are sufficiently strong, the minima of the energy is no longer at zero polarization p but at a finite one, and for even stronger interactions one obtains $p = 1$, i.e. full polarization. This means that the Fermi gas is unstable to spontaneous polarization at strong repulsive interactions, and it is expected to develop ferromagnetism.