The two-dimensional Fermi gas

M2 of quantum physics 2012-2013

Quantum mechanics exam

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Consider a gas of non relativistic fermionic particles of mass m having spin 1/2, living in a two dimensional space. Particles with opposite spin state $\uparrow$ and $\downarrow$ undergo s-wave binary interactions of range b, and at the end of the calculation we will take the zero-range limit ($b \to 0$) for a fixed value of the two-dimensional scattering length a. There is no external potential acting on the gas, simply, the gas is confined in a square box of size L, $\mathbf{r} \in [0, L[^2$, such that periodic boundary conditions of period L along the orthogonal axis x and y can be imposed on the wave function. We work in the grand canonical ensemble where we fix the chemical potential μ rather than the total number of particles N. In addition, we assume zero temperature, $T = 0$, such that the gas is in its ground state. We shall eventually take the thermodynamic limit where L tends to infinity with μ fixed.

Since we do not restrict here to the weakly interacting regime we are led to use the BCS variational approach, which approximates the ground state of the gas with a condensate of pair of particles; a reasonable approximation in two dimensions because the existence of a condensate in the thermodynamic limit is not forbidden at $T = 0$. We shall obtain approximate expressions for the total density of the gas ρ and for the gap Δ, the latter parameter appearing in the spectrum of elementary excitation. We shall then test the theory by comparing it with current cold atoms experiments.

We recommend to consider each question in its order of appearance. Lecture notes taken during the course of Y. Castin and during the tutorials of C. Trefzger are allowed as well as the handout of the course of Y. Castin. The use of a calculator is authorized for the required numerical applications.

1 Description of the model and diagonalization of the BCS Hamiltonian

As we saw in section 3.3.9 of the course a Dirac delta interaction does not make any sense in two dimensions, the simplest substitute that we will use here, is a Kronecker delta interaction in a lattice model. Thus, we suppose that particle's position $\mathbf{r}$ is forced to be on a square lattice of eigenaxis x and y and lattice spacing b, with the ratio L/b being constant. This allows us to restrict particle's wave vectors $\mathbf{k}$ to belong to the first Brillouin zone of the lattice,

$$\mathbf{k} \in \mathrm{FBZ} = [-\pi/b, \pi/b[^2 \tag{1}$$

Unlike what has been done during the course we will work in the grand canonical ensemble, so that we introduce the grand canonical Hamiltonian $H = H_{\rm can} - \mu \hat{N}$, where $H_{\rm can}$ is the Hamiltonian in the canonical ensemble and $\hat{N}$ the total number of particles operator. The chemical potential μ can have here any sign.

We work in second quantization. We introduce the discretized version of the field operator $\hat{\psi}_\sigma(\mathbf{r})$, that annihilates a particle of spin state $\sigma \in \{\uparrow, \downarrow\}$ at the site of the lattice pointed by $\mathbf{r}$, with a normalization convention such that the anticommutation rules

$$\{\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}(\mathbf{r}')\} = 0 \quad \text{and} \quad \{\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\} = \frac{\delta_{\mathbf{r},\mathbf{r}'}\delta_{\sigma,\sigma'}}{b^2} \tag{2}$$

reproduce those of the Dirac delta continuous space in the limit $b \to 0$. The grand canonical Hamiltonian of the lattice model is then

$$H = \sum_{\mathbf{r},\sigma} b^2 \hat{\psi}^\dagger_\sigma \left[h_0 - \mu\right] \hat{\psi}_\sigma + g_0 \sum_{\mathbf{r}} b^2 \hat{\psi}^\dagger_\uparrow \hat{\psi}^\dagger_\downarrow \hat{\psi}_\downarrow \hat{\psi}_\uparrow \tag{3}$$

In the one-body term we have introduced the shorthand notation

$$h_0 = -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}, \tag{4}$$

where the discrete Laplacian operator $\Delta_{\mathbf{r}}$ is defined by the fact that it admits, on the lattice, the function $\mathbf{r} \mapsto \exp(i\mathbf{k}\cdot\mathbf{r})$ as an eigenfunction with eigenvalue $-k^2$, where $\mathbf{k}$ belongs to the first Brillouin zone. We thus have

$$h_0 e^{i\mathbf{k}\cdot\mathbf{r}} = E_k e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \forall \mathbf{k} \in \text{FBZ}, \quad \text{with} \quad E_k = \frac{\hbar^2 k^2}{2m}, \tag{5}$$

although $\mathbf{r}$ is here a discrete variable. Moreover, the bare coupling constant g_0 appearing in the on-site interaction is adjusted so as to reproduce the desired value of the two-dimensional scattering length a, which leads to

$$g_0 = \frac{2\pi\hbar^2}{m}\frac{1}{\ln(\mathcal{C}b/a)} \tag{6}$$

where the value of the numerical constant $\mathcal{C} > 0$ is known but irrelevant for what follows. We work here in the regime of weak interaction range, in particular

$$b \ll a, \tag{7}$$

so that interactions are attractive, $g_0 < 0$, and lead to the BCS pairing between fermions of opposite spin. In order to approximate the ground state of H we thus introduce the unnormalized BCS variational states

$$|\Phi\rangle = \exp\left[\sum_{\mathbf{r}_1,\mathbf{r}_2} b^4 \Phi(\mathbf{r}_1,\mathbf{r}_2)\hat{\psi}^\dagger_\uparrow(\mathbf{r}_1)\hat{\psi}^\dagger_\downarrow(\mathbf{r}_2)\right]|0\rangle \tag{8}$$

where $|0\rangle$ is the vacuum of particles. The value of the "pair field" $\Phi(\mathbf{r}_1,\mathbf{r}_2)$ has to be obtained by minimizing the energy functional

$$E[\Phi] = \langle H \rangle = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} \tag{9}$$

1.1 Stationarity condition of the energy

a) Using a simple argument show that for all Φ :

$$\langle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\uparrow \rangle = \langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow \rangle = 0 \tag{10}$$

b) We call Φ_0 the minimizer of $E[\Phi]$ and $\langle \ldots \rangle_0$ the expectation value taken in the corresponding BCS state $|\Phi_0\rangle$. Why can we suppose that $\Phi_0(\mathbf{r}_1, \mathbf{r}_2)$ is (i) a real-valued function, (ii) a function of $\mathbf{r}_1 - \mathbf{r}_2$ only, (iii) an even function of $\mathbf{r}_1 - \mathbf{r}_2$? These three properties of Φ_0 are supposed to be satisfied in what follows.

c) Deduce that for all $\mathbf{r}$,

$$\langle \hat{\psi}_\uparrow^\dagger(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \rangle_0 = \langle \hat{\psi}_\downarrow^\dagger(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) \rangle_0 = \frac{\rho}{2} \tag{11}$$

where ρ is thus the total density of particles in the BCS state of minimal energy. To this end you may introduce the unitary transformation $\hat{U}$ that, for each particle, changes the state $|\uparrow\rangle$ to $|\downarrow\rangle$ and the state $|\downarrow\rangle$ to $-|\uparrow\rangle$.

d) Also, show that the gap of the BCS state of minimal energy,

$$\Delta = g_0 \langle \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \rangle_0, \tag{12}$$

is real, is independent of the position $\mathbf{r}$ and can be taken to be non-negative. To this end you may introduce the unitary transformation $\hat{U}'$ that, for each particle, changes the state $|\uparrow\rangle$ to $|\downarrow\rangle$ and the state $|\downarrow\rangle$ to $|\uparrow\rangle$.

e) We perform an infinitesimal variation $\delta\Phi$ of the pair field Φ around the minimizer Φ_0. Give the corresponding variation $\delta|\Phi\rangle$ of the BCS state to first order in $\delta\Phi$, in the form $W|\Phi_0\rangle$, where W is an operator quadratic in the field operators that you will write explicitly.

f) Calculate the variation of $E[\Phi]$ around Φ_0 to first order in $\delta\Phi$. Conclude that

$$\langle W^\dagger (H - E[\Phi_0]) \rangle_0 = 0 \tag{13}$$

To obtain this result you may consider the variations $\delta\Phi$ and $i\delta\Phi$ of the field of the pairs.

1.2 The BCS Hamiltonian

A central role in the BCS theory is played by the quadratic Hamiltonian

$$\mathcal{H} = E_{\rm aj} + \sum_{\mathbf{r},\sigma} b^2 \hat{\psi}_\sigma^\dagger [h_0 - \tilde{\mu}] \hat{\psi}_\sigma + \sum_{\mathbf{r}} b^2 \left[\hat{\psi}_\uparrow^\dagger \hat{\psi}_\downarrow^\dagger \Delta + \text{h.c.} \right], \tag{14}$$

where the value of $E_{\rm aj}$ will be specified in the upcoming question 1.2, and we have set

$$\tilde{\mu} = \mu - \frac{1}{2} g_0 \rho \tag{15}$$

We will show here that in the framework of the variational BCS theory the Hamiltonian $\mathcal{H}$ stands as a substitute for the complete Hamiltonian H to calculate the energy and the spectrum of elementary excitations. We will need the energy functional corresponding to the expectation value of $\mathcal{H}$ in a BCS state :

$$\mathcal{E}[\Phi] = \frac{\langle\Phi|\mathcal{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle} \tag{16}$$

Notice that in this equation ρ and Δ appearing in $\mathcal{H}$ are quantities relative to the minimizer Φ_0 and thus are independent of Φ.

a) Give, in terms of g_0, L, ρ and Δ, the value of $E_{\rm aj}$ such that

$$\langle H\rangle_0 = \langle\mathcal{H}\rangle_0, \quad \text{that is} \quad E[\Phi_0] = \mathcal{E}[\Phi_0], \tag{17}$$

and we will use this choice in what follows. We recall that Wick's theorem is applicable to the evaluation of expectation values in the BCS state.

b) It is admitted here that as a consequence of Wick's theorem, one has

$$\langle W^\dagger H\rangle_0 = \langle W^\dagger\mathcal{H}\rangle_0 \tag{18}$$

for any variation $\delta\Phi$ of the pair field, the operator W being introduced in question 1.1e. Conclude that Φ_0 is a stationary point, not only of the functional $E[\Phi]$, but also of the functional $\mathcal{E}[\Phi]$. Note that this remarkable property is robust, meaning that it subsists, *mutatis mutandis*, also if the properties (i), (ii) and (iii) of Φ_0 discussed in the question 1.1b are not satisfied, as for example in the presence of an external potential.

c) It is admitted here that all the eigenstates of $\mathcal{H}$ are BCS states. Conclude that the wanted BCS state $|\Phi_0\rangle$, which is the best variational approximation of the ground state of H, must be the ground state of $\mathcal{H}$.

d) Close to the thermodynamic limit, consider a weakly excited eigenstate of H whose BCS variational approximation corresponds to the pair field Φ_e. We recall that Φ_e is always a stationary point of $E[\Phi]$, even if it is not the minimizer. Generalize the previous reasoning to show that $|\Phi_e\rangle$ is almost an eigenstate of $\mathcal{H}$. Use the fact that the expectation values of $\hat\psi_\uparrow\hat\psi_\downarrow$ and of $\hat\psi^\dagger_\sigma\hat\psi_\sigma$ in the BCS state $|\Phi_e\rangle$ differ in a negligible way from their corresponding expectation values in the state $|\Phi_0\rangle$. Conclude that the weakly excited eigenstates of $\mathcal{H}$ constitute the BCS variational approximation for the weakly excited eigenstates of the complete Hamiltonian H.

1.3 Implicit equations

The procedure allowing us to put the quadratic Hamiltonian $\mathcal{H}$ in its canonical form, and thus to diagonalize it, was explained in section 3.2 of the course and was explicitly implemented for the case of the BCS theory in the tutorial number 6. It is then sufficient

here to recall some results. The following modal decomposition of the field operators is available :

$$\hat{\psi}_\uparrow(\mathbf{r}) = \sum_{\mathbf{k}} b_{\mathbf{k}\uparrow} \frac{U_k}{L} e^{i\mathbf{k}\cdot\mathbf{r}} - b^\dagger_{\mathbf{k}\downarrow} \frac{V_k}{L} e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{19}$$

$$\hat{\psi}_\downarrow(\mathbf{r}) = \sum_{\mathbf{k}} b_{\mathbf{k}\downarrow} \frac{U_k}{L} e^{i\mathbf{k}\cdot\mathbf{r}} + b^\dagger_{\mathbf{k}\uparrow} \frac{V_k}{L} e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{20}$$

where the operators $b_{\mathbf{k}\sigma}$, obeying usual anticommutation relations, annihilate a quasi-particle (or elementary excitation) of wave vector $\mathbf{k}$ and of energy

$$\epsilon_k = \left[(E_k - \tilde{\mu})^2 + \Delta^2\right]^{1/2}, \tag{21}$$

where E_k is defined in equation (5), and $\tilde{\mu}$ is defined in equation (15). We also give the following relation, satisfied by the real-valued amplitudes U_k and V_k of the eigenmodes :

$$(U_k + iV_k)^2 = \frac{E_k - \tilde{\mu} + i\Delta}{\epsilon_k} \tag{22}$$

a) Give the value of $U_k V_k$ as a function of Δ and ϵ_k.

b) Calculate the expectation value of $\hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r})$ in the ground state of $\mathcal{H}$. Deduce a first implicit equation, called the gap equation, that you will simplify under the assumption $\Delta \neq 0$. Verify that in the thermodynamic limit it leads to

$$\frac{-1}{g_0} = \int_{\mathrm{FBZ}} \frac{d^2k}{(2\pi)^2} \frac{1}{2\epsilon_k} \tag{23}$$

c) Recall the normalization condition satisfied by U_k and V_k. Deduce the value of V_k^2 as a function of $E_k - \tilde{\mu}$ and ϵ_k.

d) Calculate the expectation value of $\hat{\psi}^\dagger_\uparrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})$ in the ground state of $\mathcal{H}$. Deduce a second implicit equation, called the density equation. Verify that it takes the following form in the thermodynamic limit :

$$\rho = \int_{\mathrm{FBZ}} \frac{d^2k}{(2\pi)^2} \left(1 - \frac{E_k - \tilde{\mu}}{\epsilon_k}\right) \tag{24}$$

2 Results in the zero range limit

In this part it will be shown that, as remarkable as it is, it is possible to solve analytically the implicit gap equation (23) and the density equation (24), in the limit where the lattice spacing b tends to zero. This will yield explicit values of Δ and ρ as functions of the chemical potential μ.

As stated in the general introduction, the limit $b \to 0$ has to be taken for a fixed value of the two-dimensional scattering length a. In practice, we will use the known fact that in this limit, a system of only two particles of opposite spin admits in free space ($L \to \infty$)

one and only one bound state, called a dimer, of energy at rest given in the *canonical* ensemble by

$$e_0 = -\frac{4\hbar^2 e^{-2\gamma}}{ma^2} \tag{25}$$

where $\gamma = 0.577\,215\ldots$ is the Euler-Mascheroni constant. This property is true for all values (non infinite and non zero) of the scattering length a. The amplitude of the interactions will be then conveniently represented in the final result by $|e_0|$ rather than by a.

2.1 Explicit solutions

a) Using equation (6), check that in the limit $b \to 0$, $\tilde{\mu}$ defined in (15) can be identified to μ, which will be done in what follows.

b) Show that the right hand side of the density equation (24) admits a finite (non-infinite) limit when $b \to 0$.

c) Calculate explicitly the integral over $\mathbb{R}^2$ that appears in the previous question. In polar coordinates, after having done the angular integration, you will perform the change of variable $x = E_k$ in the radial integral. You should obtain ρ as a simple function of $m/\hbar^2$, μ et Δ.

d) Does the right hand side of the gap equation (23) converge when $b \to 0$? Answer the same question for the left hand side of this equation.

e) We give the two-dimensional generalization of a result of section 3.3.9 of the course : in a system of only two particles of opposite spin and zero total momentum, the $T(z)$ matrix associated to the Hamiltonian H_{can} (in the canonical ensemble) of the lattice model admits the following matrix elements

$$\langle \mathbf{k}|T(z)|\mathbf{k}'\rangle = \frac{1}{\frac{1}{g_0} - \int_{\text{FBZ}} \frac{d^2q}{(2\pi)^2} \frac{1}{z-2E_q}} \tag{26}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are relative wave vectors of the two particles and $z \in \mathbb{C} \setminus \mathbb{R}$. From analytic properties of the resolvent of the Hamiltonian H_{can} for two particles of zero total momentum, obtain an expression of $1/g_0$ in terms of an integral involving E_k and the energy $e_0 < 0$ of the bound state.

f) With the help of the previous question, eliminate g_0 in the left hand side of equation (23). By collecting all contributions, obtain only one integral over $\mathbf{k}$, which you will show to be convergent in the limit $b \to 0$ with e_0 fixed.

g) Calculate the corresponding integral over $\mathbb{R}^2$, by using recommendations of question 2.1c, as well as the change of variable $x - \mu = \Delta \sinh\theta$. We also recall the explicit form of the inverse function

$$\operatorname{arcsinh} X = \ln(X + \sqrt{1+X^2}) \tag{27}$$

which is useful to determine the limit of a primitive in $x = +\infty$. Finally, you should obtain a simple expression for $\operatorname{arcsinh}(\mu/\Delta)$ as a function of $\Delta/|e_0|$.

h) By applying the hyperbolic sine function to the previously obtained equation, derive an explicit simple expression of μ as a function of Δ and $|e_0|$.

i) Conclude that $\mu^2 + \Delta^2$ is a perfect square.

j) Given the answers to the questions 2.1c, 2.1h and 2.1i, recover the result which was obtained in 1989 by Mohit Randeria and his collaborators :

$$\Delta = [|e_0|(|e_0| + 2\mu)]^{1/2} \quad (28)$$

$$\rho = \frac{m}{2\pi\hbar^2}(|e_0| + 2\mu) \quad (29)$$

2.2 Physics discussion

a) For a fixed value of the amplitude of the interactions, what is the domain of variation of the chemical potential μ compatible with the hypothesis $\Delta \neq 0$?

b) Show that the elementary excitation spectrum ϵ_k has a forbidden band of which you will give the width as a function of μ and Δ. You will treat the cases $\mu < 0$ and $\mu > 0$ separately.

c) We now change the amplitude of the interactions. Towards which state does the gas tend to when $a \to +\infty$? Note that the total density of the ideal gas of spin 1/2, at zero temperature and of Fermi energy E_F, is simply given by $mE_F/(\pi\hbar^2)$ in two dimensions.

d) Finally we consider the limit $a \to 0^+$ at fixed density ρ. How does e_0 behave in this limit ? And ρa^2 ? And μ ? And the width of the forbidden band in the excitation spectrum ? What is then the state of the gas ? Carefully justify your answer.

3 Comparison with experiments

In the last decade experimentalists have been able to realize in the laboratories strongly degenerate fermionic gases of atoms, that is with a temperature T such that $k_B T \ll E_F$. We assume that this corresponds in practice to zero temperature. In addition, by strongly confining the atoms along z using a harmonic potential, we freeze their motion along z in the vibrational ground state, which allows experimentalists to realize an effective two-dimensional gas in the xy plane. As two atoms in the opposite spin states $\uparrow$ and $\downarrow$ interact in the real three-dimensional space with the s-wave scattering length a_{3D}, an effective interaction takes place in the two-dimensional gas, with a known two-dimensional scattering length a, leading to

$$e_0 = -A\hbar\omega_z \, e^{(2\pi)^{1/2}\ell_z/a_{3D}} \quad (30)$$

where $A \simeq 0.288$, ω_z is the angular frequency of an atom along z and $\ell_z = [\hbar/(m\omega_z)]^{1/2}$ is the size of the harmonic oscillator ground state along z.

Moreover, we can access the excitation spectrum of the two-dimensional gas by trying to induce an atomic transition from the spin state $|\uparrow\rangle$ to another, initially empty, internal

state $|d\rangle$, which is $\hbar\omega_0$ higher in energy, by absorption of a radiofrequency photon of angular frequency ω and negligible momentum. We then detect the presence or absence of an atom in the internal state $|d\rangle$ according to the value of the detuning $\delta = \omega - \omega_0$. More precisely, it is found experimentally that the transition of an atom from $|\uparrow\rangle$ to $|d\rangle$ is possible only if the detuning is *larger* than a threshold value δ_S, $\delta > \delta_S$.

As the amplitude of the atomic interactions between $\uparrow$ and $\downarrow$ is adjustable by using a magnetic Feshbach resonance, we can measure the threshold detuning δ_S for several values of e_0, at a fixed surface density of the two-dimensional fermionic gas. On the other hand, the final state d must have a negligible atomic interaction with $\uparrow$ and $\downarrow$. Here are some values obtained in 2012 in the group of Martin Zwierlein at the MIT for a gas of ^{6}Li, corrected by the anharmonicity effect of the confinement along z :

ℓ_z/a_{3D}	δ_S/ω_z
-0.409	0.085 ± 0.015
-0.177	0.147 ± 0.015
0.007	0.253 ± 0.015

a) Initially, the two-dimensional gas is in its ground state, the internal state $|d\rangle$ is empty and the electromagnetic field contains a photon of energy $\hbar\omega$. Give the energy E_i of this initial state, as a function of $E[\Phi_0]$ and of $\hbar\omega$.

b) Suppose that an atom has undergone a transition to the internal state $|d\rangle$, after having absorbed a radiofrequency photon, and that the latter has left an elementary excitation of wave vector $\mathbf{k}$ in the two-dimensional gas. In which wave vector is the atom having undergone the transition ? Give the energy E_f of the final state of the complete system, as a function of $E[\Phi_0]$, $\hbar\omega_0$, ϵ_k, E_k and μ. As we are here in the grand canonical ensemble you will remember to include the contribution $-\mu$ to the energy in $|d\rangle$.

c) Using energy conservation $E_f = E_i$, show that

$$\hbar\delta_S = \inf_{\mathbf{k}\in\mathbb{R}^2} (\epsilon_k + E_k - \mu) \tag{31}$$

d) Show that the function $x \mapsto x + (x^2+1)^{1/2}$ is positive and increasing on $\mathbb{R}$. Deduce the value of $\hbar\delta_S$ as a function of μ and Δ then, using the answers to the questions 2.1h and 2.1i, as a function of e_0 only.

e) Compare with the experimental results given in the table. For which point(s) is there good agreement ?

f) To determine the first correction to e_0 due to a non-zero range (of order ℓ_z) of the effective two-dimensional interaction in the experiments we introduce the expansion of the two-dimensional scattering amplitude f_k for weak relative wave number k :

$$\frac{-1}{f_k} = 1 + \frac{2i}{\pi}\left[\ln(e^\gamma ka/2) - \frac{\ln 2}{2}k^2\ell_z^2 + \ldots\right] \tag{32}$$

Deduce the corrected value $|e_0^{\rm corr}| = |e_0|[1 - (\ln 2)\frac{|e_0|}{\hbar\omega_z} + \ldots]$, and show that this correction, although heuristic, substantially improves the agreement with the experiment.