A liquid-gas transition for bosons in 1d with attractive interaction

"Quantum fluids" exam M1 ICFP 2016-2017

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1 The model

We consider a one-dimensional homogeneous gas of N bosons of mass m. The bosons are non-relativistic, have no spin and interact through a two-body zero-range interaction potential $V_{ij} = g\delta(x_i - x_j)$, where x_i and x_j are the positions of the particles and g is a constant assumed to be negative $g < 0$. The system is in equilibrium at a temperature T and consists of a box of length L with periodic boundary conditions.

1.1 Solution via Bethe ansatz in free space

The model of N bosons in 1D which interact through an attractive Dirac potential is integrable via Bethe ansatz. The solution in free space (without box quantization) is particularly simple and will be the starting point of our study. One finds that in free space each eigenstate of the system is composed of a collection of i fragments, with i an arbitrary integer from 1 to N. Each fragment is formed by a certain number n_i of bound atoms (called n_i-mers), where n_i may vary from 1 to N, and has a well-defined center-of-mass momentum k_i. The energy of the eigenstates becomes

$$E = \sum_{i=1}^{\#\text{fragments}} \left[E_0(n_i) + \frac{\hbar^2 k_i^2}{2 n_i m} \right] \qquad \text{with} \qquad E_0(n) = -\frac{m g^2}{24\hbar^2} n(n^2-1) \tag{1}$$

Here $E_0(n)$ represents the internal energy of the n-mer and $\frac{\hbar^2 k_i^2}{2nm}$ its kinetic energy. We shall see that the interaction energy, though taking into account, does not affect the spectrum. On the one hand, the integrability imposes the scattering of n-mers to be purely elastic, while the interaction between n-mers, on the other hand, does not affect the spectrum (1) because the n-mers that scatter are asymptotically free.

In the following we will give the conditions under which we may use the same spectrum in presence of the quantization box. To this purpose we will need tools to describe two limiting cases more easily : the dimer on one hand and the N-mer with $N \gg 1$ on the other hand. We will also need a few results from scattering theory in 1D.

1.2 The dimer

We wish to find a two-body bound state (a dimer) for two atoms in 1D that interact through an attractive Dirac potential $V_{ij} = g\delta(x_i - x_j)$ with $g < 0$.

1. For cold atoms confined to one dimension, the constant g is related to the scattering length a (this is the 1D equivalent of the s-wave scattering length in 3D) through the relation
$$g = -\frac{\hbar^2}{ma} \tag{2}$$
Rederive the relation (2) between g and a up to a numerical prefactor by dimensional analysis. Find the equivalent relation in 3D.
2. Write the Schrödinger equation $H\phi(x) = E\phi(x)$ for the wave function $\phi(x)$ of the relative motion of two atoms. One should make a appear in the Hamiltonian and redefine the energy in a convenient way.
3. $\phi(x)$ has to be a continuous function. Explain why $\phi'(x)$ is discontinuous at $x = 0$ in our case.
4. Solve the Schrödinger equation and find the normalised wave function $\phi(x)$ of the bound state.
5. Calculate the spatial extension l of the dimer (half-width at $1/e$ of $\phi(x)$ relative to $\phi(0)$) and its energy E as a function of a. One should find $l = 2a$.

1.3 Scattering problem

We still consider the two-body problem, but this time with a positive energy in order to calculate the scattering amplitude of our attractive Dirac potential.

1. Write the Schrödinger equation $H\phi(x) = E\phi(x)$ for the wave function $\phi(x)$ of the relative motion of two atoms. One makes a appear in the Hamiltonian and one imposes $E = \frac{\hbar^2 k^2}{m}$.
2. We assume the ansatz of an incoming wave and a reflected wave for $x < 0$, and a transmitted wave for $x > 0$:
$$\phi(x<0) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx} \quad ; \quad \phi(x>0) = C\mathrm{e}^{ikx} \tag{3}$$
Write the matching conditions at zero for ϕ and ϕ'.
3. Express B and C as a function of A and deduce the expression of the transmission and reflection coefficients as a function of ka.
4. Derive that the scattering tends to total reflection at low energy $ka \ll 1$. As a consequence the Born regime in 1D is reached at high energy $\frac{1}{ka} \ll 1$, in contrast to 3D.
5. Comment on the fact that it is not necessary to regularise the Dirac potential in 1D.

1.4 The N-mer with $N \gg 1$ in mean-field approximation

We wish to find the ground state of the N-mer with $N \gg 1$ in the mean-field approximation. Starting from the Hamiltonian for N interacting atoms in 1D
$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} g\delta(x_i - x_j) \tag{4}$$
we consider the variational ansatz
$$|\psi\rangle = |\phi\rangle \otimes |\phi\rangle \otimes \ldots \otimes |\phi\rangle \tag{5}$$
and minimise the mean energy E
$$E = N\int_{\mathbb{R}} dx \left\{ \frac{\hbar^2}{2m}\left|\frac{d\phi}{dx}\right|^2 + \frac{g}{2}(N-1)|\phi|^4 \right\} \tag{6}$$

1. We will factorise a prefactor of E by dimensional analysis. Introducing the function ψ and the length ξ such that

$$\phi(x) = \frac{1}{\sqrt{\xi}}\psi\left(\frac{x}{\xi}\right) \tag{7}$$

   calculate ξ in a way that the kinetic energy and the mean-field energy in (6) have the same coefficient.

2. Reexpress the energy functional E in the following form

$$E[\phi, \phi^*] = \frac{mg^2}{\hbar^2}N(N-1)^2\epsilon[\psi, \psi^*] \tag{8}$$

   (we remind that $g < 0$) and give the expression of the functional $\epsilon[\psi, \psi^*]$ in which all the constants have disappeared.

3. To take into account the constraint on the norm of ψ we will minimise the functional

$$\mathcal{F}[\psi, \psi^*] = \epsilon[\psi, \psi^*] - \nu \int |\psi|^2 \tag{9}$$

   where ν is a Lagrange multiplier.

   Write the variation $\delta\mathcal{F}$ as function of the variations $\delta\psi$ and $\delta\psi^*$, and find the differential equation that is satisfied by the minimising function (or “minimiser”).

4. Show that one can rewrite the equation for the minimiser in the form

$$\psi'^2 + \psi^4 - 2|\nu|\psi^2 = 0 \tag{10}$$

   (one can limits oneself to $\psi \in \mathbb{R}$) what is the sign of ν ?

5. Solve equation (10) by quadrature. One has

$$\forall x \in]1, \infty[\qquad \frac{\mathrm{d}}{\mathrm{d}x}[\mathrm{arcosh}(x)] = \frac{1}{\sqrt{x^2-1}} \tag{11}$$

6. Starting from the result, reintroducing dimensionfull quantities and approximating $N-1$ by N for $N \gg 1$, one finds :
   (a) The wave function in mean-field approximation of the N-mer

$$\phi_0(x) = \frac{1}{2\xi^{1/2}}\frac{1}{\cosh\left[\frac{x-x_0}{2\xi}\right]} \tag{12}$$

   which is a bright soliton.

   (b) The chemical potential in mean-field approximation of the N-mer

$$\mu_0^{\mathrm{cm}} = -\frac{1}{8}\frac{mg^2}{\hbar^2}N^2 \tag{13}$$

   (c) The internal energy of the mean field of the N-mer

$$E_0^{\mathrm{cm}} = -\frac{1}{24}\frac{mg^2}{\hbar^2}N^3 \tag{14}$$

1.5 In a box with periodic boundary conditions

If one introduces a quantization box the problem becomes more involved, though still integrable by Bethe ansatz. Here we restrict ourselves to a simple limiting case in which the spectrum remains approximatively of the form (1) with the additional quantization condition.

$$k_i = \frac{2\pi q}{L} \qquad \text{with} \qquad q \in \mathbb{Z} \tag{15}$$

1. The first validity condition is that the internal structure and the energy of the bound states must be only slightly perturbed by the presence of the box. For this one requires that the extension of the n-mers should be smaller than L.

   Using the results of the previous sections, show that for $n \gg 1$ the extension of the n-mer is much smaller than that of the dimer, l. In what follows we can thus restrict ourselves to

   $$\frac{L}{l} \gg 1 \tag{16}$$

   We now wish to show that the liquid-gas transition takes place in the non-degenerate regime.

2. Starting from $E_0(N)$ calculate the chemical potential μ_0 of the N-mer. One neglects 1 compared to N^2.
3. Calculate the Fermi energy E_F of a fictitious gas of non-interacting fermions in 1D having the same density as our gas of bosons as a function of $\rho = N/L$.
4. Show that

   $$\frac{L}{l} = \pi \left(\frac{|\mu_0|}{E_F} \right)^{1/2} \tag{17}$$

5. Explain why one expects that the critical temperature of the liquid-gas transition is of the order of (or a fraction of) $|\mu_0|$.
6. Taking $k_B T_c \simeq |\mu_0|$, show that condition (16) implies that the liquid-gas transition takes place in the non-degenerate regime

   $$\rho\lambda \ll 1 \qquad \text{with} \qquad \lambda = \sqrt{\frac{2\pi\hbar^2}{m k_B T}} \tag{18}$$

   which will be the second validity condition of our study.
7. A third condition for using the spectrum (1) of the free space is that the energy shifts due to elastic collisions between n-mers, which are non-zero in the box, are negligible compared to the kinetic energy of the n-mers. We limit ourselves to clarifying this condition in the purely atomic phase. Show that the inequality

   $$\frac{\lambda}{l} \ll 1 \tag{19}$$

   guaranties that the scattering between thermal atoms is correctly described by the Born approximation.
8. Show that the inequality (19) is verified for temperatures of the order of $k_B T_c \sim |\mu_0|$ when $N \gg 1$.

9. Knowing that one is in the Born regime, explain why the interaction energy of an atom with the rest of the gas is ρg.
10. Show that

$$\frac{\rho|g|}{k_B T} = \frac{1}{\pi}(\rho\lambda)\left(\frac{\lambda}{l}\right) \tag{20}$$

which is $\ll 1$ under the conditions (18) and (19).

2 The liquid-gas transition

Under the conditions (16), (18) and (19) which we have identified, we can consider each configuration (eigen state) of the system as an ensemble $\{\mathcal{N}_n\}$ of $\mathcal{N}_n$ indistinguishable n-mers in equilibrium in the non-degenerate regime with $\sum_{n=1}^{N} n\mathcal{N}_n = N$.

2.1 Calculation of the critical temperature

1. Calculate the partition function of an atom in equilibrium in a 1D box with periodic boundary conditions as a function of λ and L. Consider the limit $L \gg \lambda$. Replace the obtained sum by an integral. Evaluate the integral.
2. Similarly, calculate the partition function of one n-mer (of mass nm) in equilibrium in a 1D box with periodic boundary conditions as a function of $E_0(n)$, $\beta = \frac{1}{k_B T}$, λ, n and L. Note that the internal and external partition functions factorise.
3. Write the partition function of an ideal gas of $\mathcal{N}_n$ indistinguishable n-mers in equilibrium in the non-degenerate regime.
4. The partition function of the system is a sum of partition functions Z_{conf} of the different configurations

$$Z = \sum_{\text{conf}} Z_{\text{conf}} \tag{21}$$

Write Z by replacing Z_{conf} by its expression.

If N is not too big, one can do a numerical study of the system by summing the configurations. For $N = 100$ and $L = 100l$ one then finds that the free energy $F = -k_B T \ln Z$ as a function of T/T_F (with $T_F = E_F/k_B$) suddenly changes its slope at $T_c \simeq 105 T_F$. One also finds that for $T > T_c$ the system is essentially composed out of atoms with few dimers, and for $T > T_c$ the system is essentially composed out of a big n-mer with few atoms. We will estimate T_c by considering two pure phases : one atomic phase for $T > T_c$ and a phase with one N-mer for $T < T_c$.

5. Show that one thus obtains the following equation for the critical temperature ($\beta_c = 1/k_B T_c$) :

$$\mathrm{e}^{-\beta_c E_0(N)} \frac{L\sqrt{N}}{\lambda_c} = \frac{1}{N!}\left(\frac{L}{\lambda}\right)^N \tag{22}$$

6. Take the logarithm and expand for big N, under the hypothesis that $\ln(L/\lambda_c) = O(\ln(N))$, to arrive at

$$\frac{1}{3}\beta_c|\mu_0| - \ln\left(\frac{\mathrm{e}}{\rho\lambda_c}\right) = O\left(\frac{\ln N}{N}\right) \tag{23}$$

7. Show the following implicit equation by neglecting the terms which vanish for large N

$$\frac{2}{3}\beta_c|\mu_0| + \ln\left(\frac{2}{3}\beta_c|\mu_0|\right) = \ln\left(\frac{\pi \mathrm{e}^2|\mu_0|}{6E_F}\right) \tag{24}$$

8. Show that one then has

$$\frac{2}{3}\beta_c|\mu_0| = W\left(\frac{\pi \mathrm{e}^2|\mu_0|}{6E_F}\right) \tag{25}$$

   where W is the Lambert function, which is the inverse function of $x \mapsto x\mathrm{e}^x$ for $x \geq -1$. For the parameters $N = 100$ and $L = 100l$ this gives an analytical estimate for the critical temperature $T_c^{\mathrm{analy}} \simeq 106T_F$ which is very close to the numerical value $T_c \simeq 105T_F$.

2.2 Can one neglect the fraction of atoms in the liquid phase ?

As in section 1.4, we will describe the liquid phase within the mean field approximation and we will determine its elementary excitations. The starting point is the time-dependent Gross-Pitaevskii equation for the mean field wave function $\phi(x,t)$ of the N-mer :

$$\mathrm{i}\hbar\partial_t\phi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\phi(x,t) - |g|N|\phi(x,t)|^2\phi(x,t) - \mu_0^{\mathrm{cm}}\phi(x,t) \tag{26}$$

1. As usual in the Bogoliubov method, derive the coupled linear system giving the time derivative of the fluctuations $\delta\phi(x,t)$ and $\delta\phi^*(x,t)$ (considered as independent variables), around the stationary solution $\phi_0(x) \in \mathbb{R}$ (that, as we saw, is a bright soliton localized around $x = x_0$).
2. We look for eigenmodes of the form $\delta\phi(x,t) = U(x)\mathrm{e}^{-\mathrm{i}\omega t}$ and $\delta\phi^*(x,t) = V(x)\mathrm{e}^{-\mathrm{i}\omega t}$, with $\omega > 0$. Give the differential system obeyed by $U(x)$ and $V(x)$.
3. Far from the soliton, one can replace ϕ_0 by 0 in the differential system. Show then that for $\hbar\omega > |\mu_0^{\mathrm{cm}}|$ (you will take for granted that there are no solutions for $\hbar\omega < |\mu_0\mathrm{cm}|$) $U(x)$ is a sum of plane waves of wavenumber k, and $V(x)$ is zero. Deduce that the Bogoliubov dispersion relation is

$$\epsilon_k = \frac{\hbar^2k^2}{2m} - \mu_0^{\mathrm{cm}} \tag{27}$$

4. Deduce from this result that the excitation spectrum is gapped. Give the gap and its physical interpretation.
5. Of which kind are the excitations predicted by the Bogoliubov approach ? Does this approach describe all the excitations in the system ?
6. Calculate the mean number of Bogoliubov excitations at a temperature T in the regime $\beta|\mu_0^{\mathrm{cm}}| \gg 1$ and $L \gg \lambda$.
7. Deduce that at the critical temperature T_c, that one will characterize using equation (23), the fraction of atoms in the liquid phase is given by

$$\left(\frac{N_{\mathrm{at}}}{N}\right)_{T=T_c} = \frac{(\rho\lambda_c)^2}{\mathrm{e}^3} \tag{28}$$