Ultracold quantum gases – Problems

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Problems 1, 2 are neither long nor difficult and highly recommended. Problems 3, 5 are long but (in the opinion of the author) very instructive. Problem 4 is shorter but rather calculatory, and should be considered as optional.

1. Time-of-flight experiments

We consider the time evolution of a non-interacting gas (classical or quantum) initially at equilibrium in a trap potential $U(\boldsymbol{r})$. At $t = 0$, the potential is instantaneously switched off and the gas released to expand. The goal is to obtain an expression for the spatial density after an expansion time t (corresponding to the quantity measured experimentally using absorption imaging).

1.1. Classical version

A classical gas is described by its phase-space density $f(\mathbf{r}, \boldsymbol{p})$. From f one can obtain all physically interesting quantities, for instance

$$\mathcal{P}(\boldsymbol{p}) = \int d^3\boldsymbol{r}\, f(\mathbf{r}, \boldsymbol{p}) \ : \text{momentum distribution}$$
$$n_{\rm at}(\boldsymbol{r}) = \int d^3\boldsymbol{p}\, f(\mathbf{r}, \boldsymbol{p}) \ : \text{spatial distribution.}$$

Using Liouville's theorem, show that the spatial distribution $n(\boldsymbol{r}, r)$ for long times is proportional to the initial *momentum distribution* evaluated at $\mathbf{p} = \frac{M\mathbf{r}}{t}$. What condition must be imposed on the expansion time to reach this asymptotic regime ?

1.2. Quantum version

What is the momentum distribution of a quantum-mechanical particle prepared in the state $\psi_0(\boldsymbol{r})$? Using the stationary phase approximation (see Appendix A), show that the same conclusion as in the classical case is true for a time of flight experiment with $\psi(\boldsymbol{r}, t = 0) = \psi_0(\boldsymbol{r})$.

Solution:

2. BEC in a harmonic trap

The Gross-Pitaevskii energy functional describing a BEC of N atoms in a sherical harmonic trap is

$$E_N(\psi, \psi^*) = \int d^3\boldsymbol{r} \left(-\frac{\hbar^2}{2M}\psi^* \Delta\psi + \frac{1}{2}M\omega^2 r^2 |\psi|^2 + \frac{g}{2}|\psi|^4 \right),$$

with $g = 4\pi\hbar^2 a/M$ and with a the $s-$wave scattering length. Functional minimization with respect to ψ^* yields the Gross-Pitaevskii equation :

$$\mu\psi = -\frac{\hbar^2}{2M}\Delta\psi + \frac{1}{2}M\omega^2 r^2 \psi + g|\psi|^2\psi$$

2.1.

Assume a spherical cloud of radius R. Without detailed calculation, give order of magnitude estimates for the kinetic energy, potential energy and interaction contributions to the total energy. It is advised to use the oscillator energy $\hbar\omega$ and oscillator length $a_{\rm ho} = \sqrt{\hbar/(M\omega)}$ to obtain dimensionless quantities.

2.2.

Discuss in what limits the kinetic energy or the interaction can be neglected. Can the potential energy be neglected ?

2.3.

We now assume to be in the limit of large interactions. Compute the chemical potential, mean energy and cloud radius.

3. BEC hydrodynamics

The stationary Gross-Pitaevskii equation can be generalized to time-dependent problems as follows :

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2M}\Delta\psi + U(\boldsymbol{r})\psi + g|\psi|^2\psi$$

3.1.

Write the BEC wavefunction as $\psi = \sqrt{n}e^{i\theta}$, and obtain equations of motion for n and θ. How to interpret these equations ?

3.2.

We now consider an infinite uniform system with mean density n_0 (potential $U = 0$). Consider small deviations from the equilibrium solution, $n = n_0 + \delta n$, $\theta = \theta_0 + \delta\theta$, obtain the equations of motion for δn and $\delta\theta$. Obtain the dispersion relation of the normal modes of these equation of motions, and discuss their behavior at low and high energies.

4. Bose-Hubbard model for $U \to 0$

For a non-interacting gas, we know that the atoms will condense in the lowest Bloch state at $\mathbf{q} = 0$. If there are exactly N atoms in the system, the many-body state at zero temperature will be given by

$$|\Psi_N\rangle = \frac{1}{\sqrt{N!}}\left(\hat{b}^\dagger_{\mathbf{q}=0}\right)^N|\varnothing\rangle = \frac{1}{\sqrt{N!}}\left(\frac{1}{\sqrt{N_s}}\sum_i \hat{a}^\dagger_i\right)^N|\varnothing\rangle. \tag{1}$$

Here $\hat{b}_{\mathbf{q}=0}$ is an annihilation operator for a particle in the Bloch state $\mathbf{q} = 0$, N_s is the total number of sites, and $\overline{n} = N/N_s$ is the filling fraction. We note $\{n_i\}$ a configuration of occupation numbers for which the site i contains n_i particles, and $|\{n_i\}\rangle = \prod_i |n_i\rangle_i$ the corresponding Fock state.

Show that the probability $p(n_i)$ to find n_i atoms at one particular site i approximately follow a Poisson distribution when N, N_s are both large with $\overline{n}$ finite.

You will need the multinomial formula

$$\left(\sum_{i=1}^N a_i\right)^M = \sum_{\{n_i\}_{i=1,\cdots,N},\sum_i n_i = M}\prod_{i=1}^N \frac{M! a_i^{n_i}}{n_i!}$$

and Stirling's formula,

$$N! \approx_{N\to\infty} \sqrt{2\pi N}N^N e^{-N}.$$

5. Approximate ground state of the Bose-Hubbard model

We consider here a simplified version of the Gutzwiller trial wave function, where one truncates the on-site Fock basis to just three states,

$$|\phi_i\rangle = c(n_0-1)|n_i = n_0-1\rangle_i + c(n_0)|n_i = n_0\rangle_i + c(n_0+1)|n_i = n_0+1\rangle_i. \tag{2}$$

Here n_0 is the integer closest to the average filling fraction $\overline{n}$ and the nearest integers. Taking the normalization of $|\phi_i\rangle$ into account, the coefficients can be parametrized as

$$c(n_0-1) = \cos(\chi)\sin(\theta)\, e^{i\phi_-}, \tag{3}$$
$$c(n_0) = \cos(\theta), \tag{4}$$
$$c(n_0+1) = \sin(\chi)\sin(\theta)\, e^{i\phi_+}, \tag{5}$$

where $\theta, \chi \in [0, \pi/2]$ and $\phi_\pm \in [0, 2\pi]$.

5.1.

Compute the average filling factor (number of atoms per lattice site) for the trial wavefunction above. What parameters correspond to a commensurate filling of the lattice ($n_0 = \overline{n}$) ?

5.2. Commensurate filling $\overline{n} = n_0$

We focus now on the commensurate case $\overline{n} = n_0$.

5.2.1.

Compute the free energy of the trial state. Hint : separate the kinetic energy part from the local parts. Be careful with the tunneling terms in the former.

5.2.2.

Minimize the free energy with respect to the trial parameters $\chi, \theta, \phi_\pm$. Discuss the result for the ground state wavefunction when U increases from 0.

5.2.3.

Calculate the superfluid order parameter as defined in the Lectures.

A. The method of stationary phase

Given an integral of the form

$$I = \int_a^b dx f(x) e^{i\phi(x)}, \tag{6}$$

where ϕ varies rapidly in the interval $[a, b]$ and f varies slowly, one expands the phase around the stationary phase points x_ν where $d\phi/dx = 0$,

$$\phi(x) \approx \sum_\nu \phi(x_\nu) + \frac{1}{2}\phi''(x_\nu)(x - x_\nu)^2 + \cdots, \tag{7}$$

and set $f(x) \approx f(x_\nu)$ in the integrand. Then one breaks up the integral into several pieces around each of the x_ν, and extend the integration bounds to $\pm\infty$ for each piece (this gives a good approximation since the fast oscillations average out the contributions far from the stationary points). This gives

$$I \approx \sum_\nu f(x_\nu) e^{i\sum_\nu \phi(x_\nu)} \int_{-\infty}^{+\infty} dx e^{i\frac{1}{2}\phi''(x_\nu)(x-x_\nu)^2} \tag{8}$$

$$= \sum_\nu f(x_\nu) e^{i\sum_\nu \phi(x_\nu)} \sqrt{\frac{2\pi}{|\phi''(x_\nu)|}} e^{i\arg[\phi''(x_\nu)] - i\frac{\pi}{4}}. \tag{9}$$

The Gaussian integral is calculated using contour integration. This method can be generalized to more than 1 dimension ("saddle-point integration").