

Ultracold quantum gases – Solutions of Problems

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1 Time-of-flight experiments

1.1 Classical version

Liouville's theorem implies that a phase-space element of volume $d^3\mathbf{r}_0 d^3\mathbf{p}_0$ centered on $(\mathbf{r}_0, \mathbf{p}_0)$ is conserved along the classical trajectories. For the situation considered here, the particles undergo ballistic flight for $t > 0$: $f(\mathbf{r}, \mathbf{p}, t) = f_0(\mathbf{r}(t), \mathbf{p}_0, t)$ with $\mathbf{r}(t) = \mathbf{r}_0 + \frac{\mathbf{p}_0}{M}t$, $\mathbf{p}(t) = \mathbf{p}_0$ the classical trajectory evolving from $(\mathbf{r}_0, \mathbf{p}_0)$. The spatial density reads

$$n_{\text{at}}(\mathbf{r}, t) = \int d^3\mathbf{p}_0 f_0(\mathbf{r}(t), \mathbf{p}_0) = \int d^3\mathbf{r}_0 \int d^3\mathbf{p}_0 f_0(\mathbf{r}_0, \mathbf{p}_0) \delta\left(\mathbf{r}_0 + \frac{\mathbf{p}_0}{M}t - \mathbf{r}(t)\right)$$

For long times, the terms $\propto t$ in the δ function dominate. We can then approximate

$$\begin{aligned} n_{\text{at}}(\mathbf{r}, t) &\approx \int d^3\mathbf{r}_0 \int d^3\mathbf{p}_0 f_0(\mathbf{r}_0, \mathbf{p}_0) \delta\left(\frac{\mathbf{p}_0}{M}t - \mathbf{r}(t)\right) \\ &\approx \left(\frac{M}{t}\right)^3 \int d^3\mathbf{r}_0 f\left(\mathbf{r}_0, \frac{M\mathbf{r}}{\hbar t}\right) \\ &= \left(\frac{M}{t}\right)^3 \mathcal{P}_0\left(\frac{M\mathbf{r}}{t}\right). \end{aligned}$$

If Δr_0 and Δp_0 are the initial sizes of the position and momentum distributions, respectively, the asymptotic regime is reached when $\Delta p_0 t / M \gg \Delta r_0$.

1.2 Quantum version

The momentum distribution is given by

$$\mathcal{P}_0(\mathbf{p}) = \left| \int \frac{d^3\mathbf{r}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \psi_0(\mathbf{r}) \right|^2 = |\tilde{\psi}_0(\mathbf{k})|^2,$$

the modulus square of the Fourier transform $\tilde{\psi}_0(\mathbf{k})$ of ψ_0 .

To compute the time evolution, we express the initial wave function before release in the plane wave basis,

$$\psi_0(\mathbf{r}, t=0) = \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} \tilde{\psi}_0(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (1)$$

The evolution is due to the free particle Hamiltonian, leading to

$$\psi(\mathbf{r}, t) = \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} \tilde{\psi}_0(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \frac{\hbar\mathbf{k}^2 t}{2M})} \quad (2)$$

For long enough times, the phase factor determines the integral. It oscillates very rapidly, thus averaging the integral to zero, except near the points of stationary phase $k_i = Mx_i/\hbar t$ ($i = x, y, z$). The stationary phase approximation then yields

$$\psi(\mathbf{r}, t) \approx \tilde{\psi}_0\left(\mathbf{k} = \frac{M\mathbf{r}}{\hbar t}\right) e^{i\frac{M\mathbf{r}^2}{2\hbar t}} \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} e^{i(\delta\mathbf{k}\cdot\mathbf{r} - \frac{\hbar\delta\mathbf{k}^2 t}{2M})} = \left(\frac{M}{i\hbar t}\right)^{3/2} \tilde{\psi}_0\left(\mathbf{k} = \frac{M\mathbf{r}}{\hbar t}\right) e^{i\frac{M\mathbf{r}^2}{2\hbar t}}. \quad (3)$$

This result becomes exact as $t \rightarrow \infty$, where the integral over the oscillating exponential tends to a δ function. Taking the modulus squared gives the desired result.

2 BEC in a harmonic trap

2.1

Order-of-magnitude estimates for a cloud of N atoms, of typical size R , in a spherical trap of frequency ω :

$$E_{\text{kin}} \sim N \frac{\hbar^2}{MR^2} = N\hbar\omega \frac{a_{\text{ho}}^2}{R^2}, \quad E_{\text{pot}} \sim NM\omega^2 R^2 = N\hbar\omega \frac{R^2}{a_{\text{ho}}^2}, \quad E_{\text{int}} \sim N\hbar\omega \frac{Na a_{\text{ho}}^2}{R^3}$$

2.2

$$\frac{E_{\text{kin}}}{E_{\text{pot}}} \sim \frac{a_{\text{ho}}^4}{R^4}, \quad \frac{E_{\text{int}}}{E_{\text{pot}}} \sim \frac{Na a_{\text{ho}}^4}{R^5}, \quad \frac{E_{\text{int}}}{E_{\text{kin}}} \sim \frac{Na}{R}.$$

Kinetic energy negligible if $R \ll Na$ and interaction energy negligible if $R \gg Na$. The potential energy can never be neglected: Both kinetic and interaction contributions would favor $R \rightarrow \infty$, and the potential energy is necessary to balance them and keep the equilibrium size finite.

2.3

For strong repulsive interactions [$\chi = \frac{Na}{a_{\text{ho}}} \gg 1$, equivalent to saying that the cloud size \gg healing length (check!)], we can neglect the kinetic energy. The equilibrium density profile is determined by the balance between the potential and interaction energy terms,

$$n(\mathbf{r}) = |\psi(\mathbf{r})|^2 = \begin{cases} \frac{\mu - \frac{1}{2}M\omega^2 r^2}{g}, & \mu \geq \frac{1}{2}M\omega^2 r^2, \\ 0, & \mu \leq \frac{1}{2}M\omega^2 r^2, \end{cases} \text{ or } n(\mathbf{r}) = \begin{cases} n_{0m} \left[1 - \left(\frac{r}{R_{\text{TF}}} \right)^2 \right], & r \leq R_{\text{TF}}, \\ 0, & r \geq R_{\text{TF}}. \end{cases}$$

The Thomas-Fermi radius (edge of the cloud where $n = 0$) is $R_{\text{TF}} = \sqrt{\frac{2\mu_{\text{TF}}}{M\omega^2}}$, and the peak density is $n_{0m} = \frac{\mu}{g}$.

For the normalization condition, one finds the chemical potential :

$$\mu_{\text{TF}} = \frac{\hbar\omega}{2} (15\chi)^{2/5} \gg \hbar\omega.$$

Note the scaling with atom number, $\mu_{\text{TF}} \propto N^{2/5}$ and $R_{\text{TF}} \propto N^{1/5}$. The condition for strong repulsive interactions, $R \ll Na$, amounts to $\chi = \frac{Na}{a_{\text{ho}}} \gg 1$.

The various contribution to the energy are

$$E_{\text{pot}} = \frac{3}{7}\mu N \quad E_{\text{int}} = \frac{2}{7}\mu N.$$

3 BEC hydrodynamics

3.1

Separating real and imaginary part, we get

$$\frac{\partial n}{\partial t} + \nabla \cdot \left(n \frac{\hbar}{M} \nabla \theta \right) = 0 \quad -\hbar \frac{\partial \theta}{\partial t} = -\frac{\hbar^2}{2M} \frac{\Delta \sqrt{n}}{\sqrt{n}} + \frac{\hbar^2}{2M} \nabla^2 \theta + U + gn.$$

The first equation looks like a continuity equation, if we identify $\mathbf{v}_s = \frac{\hbar}{M} \nabla \theta$ with the fluid velocity field. Taking the gradient of the second equation, one finds

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{v}_s) = 0, \quad M \frac{\partial}{\partial t} \mathbf{v}_s = -\nabla \cdot \left(\mu_{\text{loc}} + \frac{1}{2} M \mathbf{v}_s^2 \right),$$

$$\mu_{\text{loc}} = -\frac{\hbar^2}{2M} \frac{\Delta \sqrt{n}}{\sqrt{n}} + gn + U(\mathbf{r}).$$

These equations look like the continuity and Euler equations describing a *perfect* fluid with density n and velocity field \mathbf{v}_s , with an “extra”, purely quantum term $-\frac{\hbar^2}{2M} \frac{\Delta \sqrt{n}}{\sqrt{n}}$ in the pressure. Note that the pressure for a uniform weakly-interacting Bose gas is $P = gn^2/2$, so that $\nabla P/n = g \nabla n$. The absence of viscosity indicates that the flow of a fluid in a BEC state will be dissipation-free, or equivalently *superfluid*.

3.2

We start from the hydrodynamic equations above, and linearize them around the equilibrium solution. This gives after some algebra

$$\frac{\partial \delta n}{\partial t} + \frac{\hbar n_0}{M} \nabla^2 \delta \theta = 0, \quad -\hbar \frac{\partial}{\partial t} \delta \theta = \left(g - \frac{\hbar^2}{4M} \frac{\nabla^2}{n_0} \right) \delta n.$$

We decompose δn , $\delta \theta$ in normal modes appropriate for a uniform medium, *i.e.* plane waves,

$$\delta n \propto \sum_{\mathbf{k}} \delta n_{\mathbf{k}} e^{i(\mathbf{k} \cdot \mathbf{r} - \frac{E_{\mathbf{k}} t}{\hbar})}, \quad \delta \theta \propto \sum_{\mathbf{k}} \delta \theta_{\mathbf{k}} e^{i(\mathbf{k} \cdot \mathbf{r} - \frac{E_{\mathbf{k}} t}{\hbar})},$$

where the dispersion relation $E_{\mathbf{k}}$ is common to both modes. This gives the two eigenmode equations

$$\begin{aligned} -i E_{\mathbf{k}} \delta n_{\mathbf{k}} &= \frac{\hbar^2 k^2 n_0}{M} \delta \theta_{\mathbf{k}} = 2n_0 \epsilon_{\mathbf{k}} \delta \theta_{\mathbf{k}}, \\ i E_{\mathbf{k}} \delta \theta_{\mathbf{k}} &= \left(g + \frac{\hbar^2 k^2}{4M n_0} \right) \delta n_{\mathbf{k}} = \left(g + \frac{1}{2n_0} \epsilon_{\mathbf{k}} \right) \delta n_{\mathbf{k}}, \end{aligned}$$

with $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / (2M)$ the free particle dispersion relation.

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} (\epsilon_{\mathbf{k}} + 2g n_0)}$$

For low-energy $E_{\mathbf{k}} \ll g n_0$, the excitations are sound waves with linear dispersion relation) $E_{\mathbf{k}} \approx \hbar c_s k$. The speed of sound is $c_s = \sqrt{\frac{g n_0}{M}}$. For “high energies” $E_{\mathbf{k}} \gg g n_0$, the excitations behave as free particles but for a k -independent energy shift, $E_{\mathbf{k}} \approx \epsilon_{\mathbf{k}} + g n_0$.

4 Bose-Hubbard model for $U \rightarrow 0$

Using the multinomial formula, we rewrite the N -particle wavefunction as

$$|\Psi_N\rangle = \sum_{\{n_i\}, \sum_i n_i = N} \sqrt{\frac{N!}{N_s^N \prod_i n_i!}} |\{n_i\}\rangle.$$

The probability $p(n_i)$ is found by taking the expectation value of the projector on the subspace spanned by Fock states with exactly n_i particles at site i . This is

$$p(n_i) = \frac{N!}{N_s^N n_i!} \underbrace{\sum_{\{n_j\}, \sum_j n_j = N - n_i} \frac{1}{\prod_{j \neq i} n_j!}}_{= \frac{1}{(N - n_i)!} (N_s - 1)^{N - n_i}} = \underbrace{\frac{N!}{(N - n_i)!}}_{\approx N^{n_i}} \underbrace{\frac{(N_s - 1)^{N - n_i}}{N_s^N}}_{\approx e^{-N/N_s} / N_s^{n_i}} \frac{1}{n_i!},$$

where we used the multinomial formula again and Stirling’s formula to simplify the factorials. The probability $p(n_i)$ can thus be rewritten as

$$p(n_i) \approx e^{-\bar{n}} \frac{\bar{n}^{n_i}}{n_i!},$$

up to small corrections $\sim 1/N, 1/N_s$ that vanish in the thermodynamic limit $N, N_s \rightarrow \infty$. This is a Poisson distribution, with mean value \bar{n} and standard deviation $\sqrt{\bar{n}}$.

5 Approximate ground state of the Bose-Hubbard model

5.1

The average filling is given by

$$\bar{n} = n_0 - \sin^2(\theta) \cos(2\chi). \quad (4)$$

For $\chi = \pi/4$, the atomic filling is thus commensurate with the lattice with n_0 atoms per site on average.

5.2 Commensurate filling $\bar{n} = n_0$

5.2.1

The free energy is

$$\frac{\langle \mathcal{G}_{\text{BH}} \rangle_{\text{Gutzwiller}}}{N_s} = \mathcal{G}_{J=0} + \frac{U}{2} \sin^2(\theta) - \frac{zJ}{4} \sin^2(2\theta) \left(2n_0 + 1 + 2\sqrt{n_0(n_0 + 1)} \cos(\phi_+ - \phi_-) \right), \quad (5)$$

where $z = 6$ is the number of nearest neighbors in 3D and where $\mathcal{G}_{J=0}$ is the purely local free energy for vanishing tunneling and n_0 atoms per site.

5.2.2

Minimizing with respect to the phases ϕ_{\pm} yields immediately $\cos(\phi_+ - \phi_-) = 1$. In order to minimize the kinetic energy, one wants to delocalize the wave function over the largest possible domain, with a phase as uniform as possible (this is true as well for arbitrary filling fractions). Taking this into account, the free energy simplifies to

$$\frac{\langle \mathcal{G}_{\text{BH}} \rangle_{\text{Gutzwiller}}}{N_s} = \mathcal{G}_{J=0} + \frac{U}{2} \sin^2(\theta) - \frac{zJ}{4} A(n_0) \sin^2(2\theta). \quad (6)$$

where the coefficient $A(n_0) = (\sqrt{n_0} + \sqrt{n_0 + 1})^2$. The variational free energy is minimized with respect to θ when

$$(1) \quad \cos(2\theta) = \frac{U}{zJA(n_0)} \quad \text{or} \quad (2) \quad \sin(2\theta) = 0.$$

The first solution exists if the ratio U/zJ is lower than a critical value,

$$U \leq U_c = zJA(n_0) = zJ \left(2n_0 + 1 + 2\sqrt{n_0(n_0 + 1)} \right). \quad (7)$$

and it has the lowest free energy.

5.2.3

The lowest energy solution for $U \leq U_c$ corresponds to an order parameter

$$\alpha = \langle \hat{a}_i \rangle = \begin{cases} \sqrt{\frac{A(n_0)}{2} \left[1 - \left(\frac{U}{U_c} \right)^2 \right]} & \text{if } U \leq U_c, \\ 0 & \text{if } U \geq U_c, \end{cases} \quad (8)$$

with a condensate fraction $f_c = |\alpha|^2/n_0$. When U becomes larger than the critical value U_c , only the second solution is possible, with free energy $\mathcal{G}_{J=0}$ and $\alpha = f_c = 0$.