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 $d^3\boldsymbol{r}_0 d^3\boldsymbol{p}_0$ centered on $(\boldsymbol{r}_0, \boldsymbol{p}_0)$ is conserved along the classical trajectories. For the situation considered here, the particles undergo ballistic flight for $t > 0$: $f(\mathbf{r}, \boldsymbol{p}, t) = f_0(\mathbf{r}(t), \boldsymbol{p}_0, t)$ with $\boldsymbol{r}(t) = \boldsymbol{r}_0 + \frac{\boldsymbol{p}_0}{M}t$, $\boldsymbol{p}(t) = \boldsymbol{p}_0$ the classical trajectory evolving from $(\boldsymbol{r}_0, \boldsymbol{p}_0)$. The spatial density reads

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

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

$$\begin{aligned} n_{\rm at}(\boldsymbol{r}, t) &\approx \int d^3\boldsymbol{r}_0 \int d^3\boldsymbol{p}_0\, f_0(\mathbf{r}_0, \boldsymbol{p}_0)\delta\left(\frac{\boldsymbol{p}_0}{M}t - \boldsymbol{r}(t)\right) \\ &\approx \left(\frac{M}{t}\right)^3 \int d^3\boldsymbol{r}_{0\,0} f\left(\mathbf{r}_0, \frac{M\mathbf{r}}{\hbar t}\right) \\ &= \left(\frac{M}{t}\right)^3 \mathcal{P}_0\left(\frac{M\mathbf{r}}{t}\right). \end{aligned}$$

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

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

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,

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

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

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

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

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

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

2 Bose-Hubbard model for $U \to 0$

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

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

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

3 Approximate ground state of the Bose-Hubbard model

3.1

The average filling is given by

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

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

3.2 Commensurate filling $\overline{n} = n_0$

3.2.1

The free energy is

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

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.

3.2.2

Minimizing with respect to the phases $\phi_\pm$ 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

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

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,

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

and it has the lowest free energy.

3.2.3

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

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

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 $\alpha = f_c = 0$.