PHY635, II-Semester 2022/23, Assignment 3 solution

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(1) Bose-Einstein condensation in different numbers of dimensions Revisit the calculation of section 3.2.

(a) Then adapt it to a 2D and a 1D harmonic trap. Find the condensation temperature in either case. [5 pts]

Solution: *As before we find the lowest temperature T_c where $N_0 \approx 0$ is still possible at $\tilde{\mu} = 0$. Using $\beta_c = \frac{1}{k_B T_c}$ we start as in the lecture notes, but now have a summation only over 2 indices n_x and n_y*

$$N = \sum_{\mathbf{n} \neq (00)} \frac{1}{\exp[\beta_c(\hbar\omega(n_x + n_y)) - \underset{=0}{\underset{\downarrow}{\tilde{\mu}}}] - 1} \tag{1}$$

$$\approx \int dn_x dn_y \frac{1}{\exp[\beta_c(\hbar\omega(n_x + n_y))] - 1}, \qquad \textit{Let } n'_{x/y} = \hbar\omega\, n_{x/y} \tag{2}$$

$$\approx \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \int_0^\infty dn'_x dn'_y \frac{1}{e^{n'_x + n'_y} - 1}$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \sum_{p=1}^\infty \int d^2\mathbf{n} e^{-p(n'_x + n'_y)}, \qquad \textit{where we used } \underbrace{\left[\sum_{p=1}^\infty e^{-p\alpha} = \frac{1}{e^\alpha - 1}\right]}_{\textit{geometric series}} \tag{3}$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \sum_{p=1}^\infty \underbrace{\left(\int_0^\infty dn'_x e^{-pn'_x}\right)}_{=1/p} \left(\int_0^\infty dn'_y e^{-pn'_y}\right) \tag{4}$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \sum_{p=1}^\infty \frac{1}{p^2} = \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \frac{\pi^2}{6} \tag{5}$$

where the series can be e.g. done with mathematica. Thus in a 2D trap, the condensation temperature is $k_B T_c = \sqrt{6}\hbar\omega N^{1/2}/\pi$.

It should now be clear that in 1D we just remove yet one more integration/summation index and power of $\left(\frac{k_B T_c}{\hbar\omega}\right)$, and thus end up with

$$N = \left(\frac{k_B T_c}{\hbar\omega}\right) \sum_{p=1}^\infty \underbrace{\left(\int_0^\infty dn'_x e^{-pn'_x}\right)}_{=1/p}$$

instead of the second to last line. However now we notice that the series does not converge. Thus formally we need $T_c = 0$, there is no Bose-Einstein condensation in a strictly 1D system.

(b) Next adapt it to a 3D equal side length infinite square well potential. [5 pts]

Solution: *Again we attempt to stick as closely as possible to the earlier calculation, this time we keep the three dimensions, but swap the energy for that of a particle in the infinite square well potential. Assuming a cubic box of side length a, the energy in 3D is given by*

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2(n_x^2+n_y^2+n_z^2)}{2ma^2}. \tag{6}$$

We thus start from

$$N \approx \int dn_x dn_y dn_z \frac{1}{\exp[\frac{\beta_c\hbar^2\pi^2(n_x^2+n_y^2+n_z^2)}{2ma^2}]-1}, \tag{7}$$

and use a slightly different substitution $n'_{x/y/z} = \frac{\sqrt{\beta_c}\hbar\pi}{\sqrt{2m}a} n_{x/y/z}$, thanks to which

$$N \approx \left(\frac{\sqrt{2m}a}{\sqrt{\beta_c}\hbar\pi}\right)^3 \int dn'_x dn'_y dn'_z \frac{1}{\exp[n_x'^2+n_y'^2+n_z'^2]-1}, \tag{8}$$

The integral appears amenable to spherical 3D polar coordinates in the space $[n'_x n'_y n'_z]$, hence we define a radial coordinate $n = \sqrt{n_x'^2+n_y'^2+n_z'^2}$. The corresponding angular integrations trivially give (4π). Then

$$N \approx (4\pi)\left(\frac{\sqrt{2m}a}{\sqrt{\beta_c}\hbar\pi}\right)^3 \underbrace{\int_0^\infty dn \frac{n^2}{\exp[n^2]-1}}_{=\frac{1}{4}\sqrt{\pi}\zeta(3/2)}, \tag{9}$$

which we can reshuffle to yield: $k_B T_c = \frac{\pi\hbar^2}{2ma^2}\left(\frac{N}{\zeta(3/2)}\right)^{2/3}$.

(c) Compare all dimensions and systems you have inspected and discuss the dependence of critical temperature on the number of dimensions and system details. [2 pts]

Solution: *We found that the power law with which the critical temperature depends on parameters and atom numbers change with both, number of dimensions and details of potential.*

(2) Grand canonical ensemble Consider a collection of non-interacting ~~particles~~ Bosons[1] in the ~~infinite square well potential $V(x)$ (zero between $x = 0$ and $x = a$, infinite outside).~~ 2D harmonic trap $V(x) = m\omega^2(x^2+y^2)/2$. For whatever reasons[2], assume these to be in contact with an environment at temperature $T > T_{\text{crit}}$ and also exchanging particles with it. Find the chemical potential required to have a given mean number N

[1] We meant Bosons, you can do it for Fermions as well

[2] theoretical ones

of particles in the box. [8 pts]

Solution: *The starting point is again Eq. (1) as before, however now we have nonzero $\tilde{\mu} = \mu - \hbar\omega$.*

$$N = \sum_{\mathbf{n}\neq(00)} \frac{1}{\exp[\beta[\hbar\omega(n_x + n_y) - \tilde{\mu}]] - 1} \tag{10}$$

and $\beta = 1/(k_B T)$ (not T_{crit}). Nonetheless we can do all the subsequent steps as before:

$$N \approx \int dn_x dn_y \frac{1}{\exp[\beta[\hbar\omega(n_x + n_y) - \tilde{\mu}]] - 1}, \qquad \textit{Let } n'_{x/y} = \hbar\omega\, n_{x/y} \tag{11}$$

$$\approx \left(\frac{k_B T}{\hbar\omega}\right)^2 \int_0^\infty dn'_x dn'_y \frac{1}{e^{n'_x + n'_y - \tilde{\mu}'} - 1}. \tag{12}$$

where we defined $\tilde{\mu}' = \beta\tilde{\mu}$. Then as before

$$N = \left(\frac{k_B T}{\hbar\omega}\right)^2 \sum_{p=1}^{\infty} \int d^2\mathbf{n} e^{-p(n'_x + n'_y - \tilde{\mu}')}, \qquad \textit{where we used } \underbrace{\left[\sum_{p=1}^{\infty} e^{-p\alpha} = \frac{1}{e^\alpha - 1}\right]}_{\textit{geometric series}} \tag{13}$$

$$= \left(\frac{k_B T}{\hbar\omega}\right)^2 \sum_{p=1}^{\infty} e^{-p\tilde{\mu}'} \underbrace{\left(\int_0^\infty dn'_x e^{-pn'_x}\right)}_{=1/p} \left(\int_0^\infty dn'_y e^{-pn'_y}\right) \tag{14}$$

$$= \left(\frac{k_B T}{\hbar\omega}\right)^2 \sum_{p=1}^{\infty} \frac{e^{-p\tilde{\mu}'}}{p^2} = \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \frac{\pi^2}{6} Li_2(e^{-\tilde{\mu}'}) \tag{15}$$

where Li denotes the polylogarithm. Eq. (15) contains μ' and N so in principle (at least numerically) we can find μ' and hence μ in terms of the target mean atom number N and other system parameters. However since the relation involves special functions, it is not straightforward to do this explicitly.

(3) Bose gas thermometry: Consider a partially condensed Bose gas of a mean number of $\bar{N} = 10^5$ ^{87}Rb atoms in an isotropic harmonic trap with trapping frequency $\omega = (2\pi)100$ Hz. Assume the atoms do not interact, because interactions are switched off using a Feshbach resonance, which we will discuss later.

(a) Find the specific heat $C = \partial E/\partial T$ of the Bose-gas above and below $T = T_{\text{crit}}$, where E is the total energy of a Bose gas using the canonical ensemble. [2pts]

Solution: *See Pethik and Smith, section 2.4.*

(b) Using a mathematica script or analytical calculations, find the atom numberdensity $\rho(r)$ as a function of radial distance from the centre of the trap r. Show plots of this for $T = 0$, $T = T_{\text{crit}}/2$ and $T > T_{\text{crit}}$. [5 pts]

Solution: *Let us calculate the density in a partially Bose condensed and otherwise thermal state from scratch, assuming a density matrix* $\hat{\rho} = \sum_{\mathbf{N}} p_{\mathbf{N}} |\, \mathbf{N} \,\rangle\langle\, \mathbf{N} \,|$ *and field operator* $\hat{\Psi}(\mathbf{r}) = \sum_k \varphi_k(\mathbf{r})\hat{a}_k$*, expressed in terms of Fock states and destruction operators for eigenstates* $\varphi_k(\mathbf{r})$ *of the isotropic 3D oscillator.*

In the above density matrix, we obtain a total density

$$\begin{aligned} \rho(\mathbf{r}) &= Tr[\hat{\rho}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})] = \sum_{\mathbf{N}} p_{\mathbf{N}} \langle\, \mathbf{N} \,|\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})|\, \mathbf{N} \,\rangle \\ &= \sum_{\mathbf{N}} p_{\mathbf{N}} \sum_{kk'} \varphi_k^*(\mathbf{r})\varphi_{k'}(\mathbf{r}) \underbrace{\langle\, \mathbf{N} \,|\hat{a}_k^\dagger \hat{a}_{k'}|\, \mathbf{N} \,\rangle}_{=N_k\delta_{kk'}} \\ &\overset{Eq.\ (3.10)}{=} \sum_k \bar{m}_k |\varphi_k(\mathbf{r})|^2 = N_{cond}|\varphi_0(\mathbf{r})|^2 + \sum_{k>0} \bar{m}_k |\varphi_k(\mathbf{r})|^2 \end{aligned} \tag{16}$$

with $\bar{m}_k$ *given by the Bose-Einstein distribution in Eq. (3.12). We thus just weigh the spatial probability density in each single particle state with the mean number of particles within it and sum up, which makes sense. In the last step we separated off the ground-state, which contains a BEC and thus cannot be described by the B.E. distribution.*

Now we review or read up on the isotropic 3D harmonic oscillator in spherical polar coordinates (we can use cartesian coordinates, but then the sum becomes near intractable). Resources I found for this are: Brandsden and Joachain, Quantum mechanics, chapter 7.6., this video [3] *and a document from the web which I shall co-upload with this solution. The eigenstates and energies are described by three quantum numbers* $n\ell m$ *governing energy and angular momentum as in the Hydrogen atom:*

$$\begin{aligned} \psi_{n\ell m}(\mathbf{r}) &= R_{n\ell}(r) Y_\ell^m(\theta, \varphi), \\ R_{n\ell}(r) &= \sqrt{\frac{2^{n+2}(n-\ell)!}{\pi^{1/2}(2n+1)!!} \frac{1}{\sigma^3}} \left(\frac{r}{\sigma}\right)^\ell e^{-\frac{r^2}{2\sigma^2}} L_{(n-\ell)}^{\ell+\frac{1}{2}}(r^2/\sigma^2), \\ E_n &= \hbar\omega(n + \frac{3}{2}), \qquad \sigma = \sqrt{\frac{\hbar}{m\omega}}. \end{aligned} \tag{17}$$

Like in the hydrogen atom the energy quantum number constrains the angular momentum, in the isotropic oscillator the rule is $\ell = 0, 2, 4, \cdots n$ *for even* n *and* $\ell = 1, 3, 5, \cdots n$ *for odd* n*.*

Expanding the sum in (16) in terms of these three quantum numbers we have:

$$\rho(\mathbf{r}) = N_{cond}|\varphi_0(\mathbf{r})|^2 + \sum_{n>0,\ell} \bar{m}_n |R_{n\ell}(r)|^2 \underbrace{\sum_m |Y_\ell^m(\theta, \varphi)|^2}_{=\frac{(2\ell+1)}{4\pi}}, \tag{18}$$

[3] In my copy below, I renamed the $n+\ell$ in the video into n and fixed typos in the normalisation factor.

where the identity used for spherical harmonics is the reason why the spherical polar wavefunctions are more practical here than the cartesian ones. For the remaining sum over Gaussians and Laguerre polynomials there might be analytical formulae, but we go the brute force approach to just sum these up numerically, as done in `Assignment3_Q3_solution_v4.nb`. *Sadly, even after doing the sum over m analytically, this runs for a very long time.*

Eventually though, it gives us plots as shown in Fig. 1, for $T = T_{crit}/2$. The outer part of the thermal cloud should be fit by

$$\rho_{therm}(r) = \frac{N_{exc}}{\pi^{3/2}R^3} e^{-\frac{r^2}{R^2}}, \tag{19}$$

with $R = \sqrt{2k_BT/(m\omega^2)}$ (See Pethik and Smith, red line in Fig. 1)[4] *For $T = 0$ we*

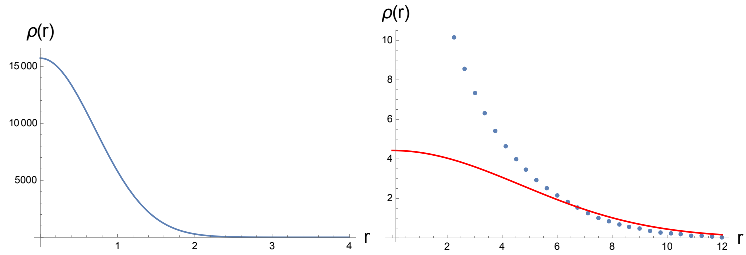

Figure 1: (left) Condensate density $\rho_{\text{cond}} = N_{\text{cond}}|\varphi_0(\mathbf{r})|^2$ and (right) thermal cloud $\rho(\mathbf{r}) - \rho_{\text{cond}}$ from Eq. (18) (dots) compared with semi-classical theory $\rho_{\text{therm}}(r)$ from Eq. (19), see Pethik and Smith. We use dimensionless units with $\hbar = m = \omega = 1$.

get only the part ρ_{cond}, for $T > T_{crit}$ we get only the part ρ_{therm}. See lecture Example 20 and Pethik and Smith, section 2.3. for some more discussion.

(c) How do you propose to use this to measure the temperature of the Bose gas? [3 pts]

Solution: *The width R of the thermal cloud depends on the temperature and since it takes a quite different shape from the condensate (bi-modal distribution, see example 20), we can separately fit both with a Gaussian and thus extract the temperature.*

[4]It should fit better I think, looks as if there is still some mistake in that script.