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Superconductivity, superfluidity and magnetism
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TD6: Interacting Bose fluids

1 Bogolyubov theory for the soft-disk gas

In this exercise we shall generalize Bogolyubov theory seen in the lectures to the case of a generic pair potential $V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}')$. We shall introduce the following definitions for the potential and its Fourier transform $\tilde{V}_{\rm int}(\boldsymbol{q})$:

$$\tilde{V}_{\rm int}(\boldsymbol{q}) = \int d^3r \; e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \; V_{\rm int}(\boldsymbol{r}) \qquad V_{\rm int}(\boldsymbol{r}) = \frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \; \tilde{V}_{\rm int}(\boldsymbol{q}) \tag{1}$$

where $\mathcal{V}$ is the volume of the system.

1.1

Write Gross-Pitaevskii equation for the condensate wavefunction $\Psi_0(\boldsymbol{r})$ in the presence of the interaction potential $V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}')$; show that the uniform condensate wavefunction

$$\Psi_0(\boldsymbol{r}) = \sqrt{n_0} = \sqrt{N_0/\mathcal{V}} \tag{2}$$

containing N_0 particles is a solution of the equation, with chemical potential

$$\mu = n_0 \tilde{V}_{\rm int}(\boldsymbol{q}=0) \; . \tag{3}$$

1.2

We shall now build Bogolyubov theory starting from this condensate wavefunction. We recall the Bogolyubov quadratic Hamiltonian

$$\begin{aligned}\hat{\mathcal{H}}_2 &= \sum_{\boldsymbol{q}\neq 0} (\epsilon_{\boldsymbol{q}} - \mu) \; \hat{a}^\dagger_{\boldsymbol{q}} \hat{a}_{\boldsymbol{q}} \\ &+ \frac{n_0}{2} \int d^3r \int d^3r' V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}') \left(\delta\hat{\psi}(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}') + \text{h.c.} + 2\delta\hat{\psi}^\dagger(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}') + 2\delta\hat{\psi}^\dagger(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}) \right)\end{aligned} \tag{4}$$

where

$$\delta\hat{\psi}(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\boldsymbol{q}\neq 0} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \; \hat{a}_{\boldsymbol{q}} \qquad \hat{a}_{\boldsymbol{q}} = \frac{1}{\sqrt{\mathcal{V}}} \int d^3r \; e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \; \delta\hat{\psi}(\boldsymbol{r}) \tag{5}$$

and $\epsilon_{\boldsymbol{q}} = \hbar^2 q^2/(2m)$.
Put the Hamiltonian in the form

$$\hat{\mathcal{H}}_2 = \frac{1}{2} \sum_{\boldsymbol{q}\neq 0} \begin{pmatrix} \hat{a}^\dagger_{\boldsymbol{q}} \\ \hat{a}_{-\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} A_{\boldsymbol{q}} & B_{\boldsymbol{q}} \\ B_{\boldsymbol{q}} & A_{\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} \hat{a}_{\boldsymbol{q}} \\ \hat{a}^\dagger_{-\boldsymbol{q}} \end{pmatrix} \tag{6}$$

and determine the $A_{\boldsymbol{q}}$, $B_{\boldsymbol{q}}$ coefficients.

1.3

The Bogolyubov quasi-particle spectrum is given by $E_{\boldsymbol{q}} = \sqrt{A_{\boldsymbol{q}}^2 - B_{\boldsymbol{q}}^2}$. Show that

$$E_{\boldsymbol{q}} = \sqrt{\epsilon_{\boldsymbol{q}} \left(\epsilon_{\boldsymbol{q}} + 2n_0 \tilde{V}_{\text{int}}(\boldsymbol{q}) \right)} \ . \tag{7}$$

What happens in the case of a contact potential $V_{\text{int}}(\boldsymbol{r} - \boldsymbol{r}') = g\ \delta(\boldsymbol{r} - \boldsymbol{r}')$?

1.4

We shall now consider the soft-disk potential

$$V_{\text{int}}(\boldsymbol{r} - \boldsymbol{r}') = \begin{cases} V_0 & |\boldsymbol{r} - \boldsymbol{r}'| < R \\ 0 & \text{otherwise} \ . \end{cases} \tag{8}$$

We start by calculating its Fourier transform. Using polar coordinates, show that

$$\tilde{V}_{\text{int}}(\boldsymbol{q}) = 4\pi V_0 \int_0^R dr\ r^2\ \frac{\sin(qr)}{qr} \tag{9}$$

and conclude that

$$\tilde{V}_{\text{int}}(\boldsymbol{q}) = \frac{4\pi V_0 R^3}{(qR)^3} \left[\sin(qR) - qR\cos(qR)\right] \ . \tag{10}$$

1.5

The dispersion relation can be written in the dimensionless form

$$e_x = \frac{2mR^2}{\hbar^2} E_{\boldsymbol{q}} = x\sqrt{x^2 + \frac{D}{x^3}\left(\sin x - x\cos x\right)} \ . \tag{11}$$

What is x? Motivate why the parameter D can be interpreted as the ratio between the potential energy change when modifying the condensate wavefunction on the length scale of R, and the kinetic energy cost of introducing an inhomogeneity on the same length scale.

1.6

Plot the dispersion relation e_x for various values of D, and estimate numerically (i.e. approximately) the critical value D_{c1} at which a so-called *roton minumum* appears in the dispersion relation; for which value of $x = x_{\text{rot}}$ does that occur?

1.7

Increasing the value of D even further, estimate approximately the value D_{c2} at which the dispersion relation becomes *gapless* at the roton wavevector. What happens for $D > D_{c2}$? Is the uniform condensate wavefunction stable to small perturbations? What would be in your opinion a stable solution?

2 Condensate fraction for a hard-disk wavefunction

Following Penrose and Onsager (1956) we calculate the condensate fraction associated with a model wavefuction for ^{4}He (proposed originally by R. P. Feynman). Such wavefunction is the same as the "Boltzmann weight" for a system of hard spheres of diameter a and centers in the positions $\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N$:

$$\Psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N) = \frac{1}{\sqrt{Z_N^{(c)}}}\; F_N(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N) \tag{12}$$

where

$$F_N(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N) = \begin{cases} 1 & |\boldsymbol{r}_i - \boldsymbol{r}_j| > a, \; \forall i \neq j \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

2.1

Show that $Z_N^{(c)}$ is the configurational partition function (namely the partition function for the position space only) of the hard sphere gas in the distinguishable-particle case (or $N!\; Z_N^{(c)}$ for the indistinguishable-particle case).

2.2

Justify that, for $|\boldsymbol{r} - \boldsymbol{r}'| > a$:

$$F_N(\boldsymbol{r}, \boldsymbol{r}_2, ..., \boldsymbol{r}_N)\; F_N(\boldsymbol{r}', \boldsymbol{r}_2, ..., \boldsymbol{r}_N) = F_{N+1}(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}_2, ..., \boldsymbol{r}_N) \tag{14}$$

2.3

The one-body density matrix at $T = 0$ takes the form

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = N \int d^3r_2 ... d^3r_N \Psi_0(\boldsymbol{r}, \boldsymbol{r}_2, ..., \boldsymbol{r}_N)\Psi_0(\boldsymbol{r}', \boldsymbol{r}_2, ..., \boldsymbol{r}_N). \tag{15}$$

Justify that, for $|\boldsymbol{r} - \boldsymbol{r}'| > a$

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \frac{Z_{N+1}^{(c)}}{Z_N^{(c)}} \frac{1}{N+1}\; \rho_2(\boldsymbol{r}, \boldsymbol{r}') \tag{16}$$

where $\rho_2(\boldsymbol{r}, \boldsymbol{r}')$ is the so-called pair correlation function, namely $\rho_2(\boldsymbol{r}, \boldsymbol{r}')\; d^3r\; d^3r'$ gives the probability of finding any two spheres (out of $N + 1$) with centers in the infinitesimal volumes d^3r and d^3r' centered around $\boldsymbol{r}$ and $\boldsymbol{r}'$ respectively.

2.4

Justify that, in the limit $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$, $\rho_2(\boldsymbol{r}, \boldsymbol{r}') \to (N/V)^2$ (where $N \gg 1$). Reminding yourself of the relationship between the condensate density n_0 and the one-body density matrix, show that

$$n_0 = z\left(\frac{N}{V}\right)^2 \tag{17}$$

where $z = (Z_{N+1}^{(c)}/Z_N^{(c)})\; N!/(N+1)!$.

2.5

We introduce the function

$$f(v_N) = \frac{1}{N} \log \frac{Z_N^{(c)}}{N!\; v_0^N} \qquad (N \to \infty) \tag{18}$$

where $v_N = V/N$ and v_0 is a reference volume. What is its physical meaning? Show that

$$\frac{1}{N+1} \log \frac{Z_{N+1}^{(c)}}{(N+1)!\; v_0^{N+1}} \approx f(v_N) - \frac{v_N}{N} \frac{\partial f}{\partial v}(v_N) \tag{19}$$

and consequently in the thermodynamic limit ($v_N \to v$ independent of N)

$$\log(z/v_0) \approx f(v) - v\frac{\partial f}{\partial v}(v) \ . \tag{20}$$

2.6

We now consider the hard-sphere gas with both kinetic and configurational terms of the partition function. The equation of state of a classical interacting gas is given by

$$P = k_B T \left(\frac{N}{V} + \frac{\partial}{\partial V} \log \frac{Z_N^{(c)}}{V^N} \right) \tag{21}$$

How do we obtain the ideal gas limit?
The second term on the right-hand side, stemming from interactions, can be calculated via the so-called virial expansion when the range of the interaction potential is small compared to the interparticle distance (in our case $na^3 \ll 1$, where $n = N/V$)

$$P = k_B T \left[\frac{N}{V} + B_2 \left(\frac{N}{V}\right)^2 + B_3 \left(\frac{N}{V}\right)^3 + ... \right] \tag{22}$$

For the hard-sphere gas, this expansion gives

$$B_2 = \frac{2\pi}{3} a^3 \tag{23}$$

From Eqs. (21) and (22) find a differential equation for $Z_N^{(c)}$ and hence for $f(v)$. Show that it is solved by

$$f(v) = \log v - \frac{2\pi}{3}\frac{a^3}{v} + 1 \tag{24}$$

2.7

Calculate z as a function of v and a. Using the data for ^{4}He, $a = 2.56$ Å and $v = 46.2$ Å^3, calculate the condensate fraction $N_0/N = n_0 V/N$. How does it compare with the value measured in ^{4}He by neutron scattering ($N_0/N = 6 - 8$ %) ?