5.10: Appendix II- Ideal Bose Gas Condensation

We begin with the grand canonical Hamiltonian $K = H - \mu N$ for the ideal Bose gas,

$$K = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu)\, b^\dagger_{\mathbf{k}} b_{\mathbf{k}} - \sqrt{N} \sum_{\mathbf{k}} \left(\nu_{\mathbf{k}}\, b^\dagger_{\mathbf{k}} + \bar{\nu}_{\mathbf{k}}\, b_{\mathbf{k}}\right) \quad . \tag{5.10.1}$$

Here $b^\dagger_{\mathbf{k}}$ is the creation operator for a boson in a state of wavevector $\mathbf{k}$, hence $\left[b_{\mathbf{k}}\,,\,b^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k}\mathbf{k}'}$. The dispersion relation is given by the function $\varepsilon_{\mathbf{k}}$, which is the energy of a particle with wavevector $\mathbf{k}$. We must have $\varepsilon_{\mathbf{k}} - \mu \geq 0$ for all $\mathbf{k}$, lest the spectrum of K be unbounded from below. The fields $\{\nu_{\mathbf{k}}, \bar{\nu}_{\mathbf{k}}\}$ break a global $\mathsf{O}(2)$ symmetry.

Students who have not taken a course in solid state physics can skip the following paragraph, and be aware that $N = V/v_0$ is the total volume of the system in units of a fundamental "unit cell" volume. The thermodynamic limit is then $N \to \infty$. Note that N is not the boson particle number, which we'll call N_b.

Solid state physics boilerplate : We presume a setting in which the real space Hamiltonian is defined by some boson hopping model on a Bravais lattice. The wavevectors $\mathbf{k}$ are then restricted to the first Brillouin zone, $\hat{\Omega}$, and assuming periodic boundary conditions are quantized according to the condition $\exp\!\left(iN_l\, \mathbf{k} \cdot \mathbf{a}_l\right) = 1$ for all $l \in \{1, \ldots, d\}$, where $\mathbf{a}_l$ is the l^{th} fundamental direct lattice vector and N_l is the size of the system in the $\mathbf{a}_l$ direction; d is the dimension of space. The total number of unit cells is $N \equiv \prod_l N_l$. Thus, quantization entails $\mathbf{k} = \sum_l (2\pi n_l/N_l)\, \mathbf{b}_l$, where $\mathbf{b}_l$ is the l^{th} elementary reciprocal lattice vector ($\mathbf{a}_l \cdot \mathbf{b}_{l'} = 2\pi\delta_{ll'}$) and n_l ranges over N_l distinct integers such that the allowed $\mathbf{k}$ points form a discrete approximation to $\hat{\Omega}$.

To solve, we first shift the boson creation and annihilation operators, writing

$$K = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu)\, \beta^\dagger_{\mathbf{k}} \beta_{\mathbf{k}} - N \sum_{\mathbf{k}} \frac{|\nu_{\mathbf{k}}|^2}{\varepsilon_{\mathbf{k}} - \mu} \quad , \tag{5.10.2}$$

where

$$\beta_{\mathbf{k}} = b_{\mathbf{k}} - \frac{\sqrt{N}\, \nu_{\mathbf{k}}}{\varepsilon_{\mathbf{k}} - \mu} \qquad , \qquad \beta^\dagger_{\mathbf{k}} = b^\dagger_{\mathbf{k}} - \frac{\sqrt{N}\, \bar{\nu}_{\mathbf{k}}}{\varepsilon_{\mathbf{k}} - \mu} \quad . \tag{5.10.3}$$

Note that $\left[\beta_{\mathbf{k}}\,,\,\beta^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k}\mathbf{k}'}$ so the above transformation is canonical. The Landau free energy $\Omega = -k_B T \ln \Xi$, where $\Xi = \mathsf{Tr}\ e^{-K/k_B T}$, is given by

$$\Omega = N k_B T \int\limits_{-\infty}^{\infty} d\varepsilon\; g(\varepsilon)\, \ln\left(1 - e^{(\mu-\varepsilon)/k_b T}\right) - N \sum_{\mathbf{k}} \frac{|\nu_{\mathbf{k}}|^2}{\varepsilon_{\mathbf{k}} - \mu} \quad , \tag{5.10.4}$$

where $g(\varepsilon)$ is the density of energy states per unit cell,

$$g(\varepsilon) = \frac{1}{N} \sum_{\mathbf{k}} \delta\left(\varepsilon - \varepsilon_{\mathbf{k}}\right) to35pt\backslash\mathrm{rightarrowfill}_{N\to\infty} \int\limits_{\hat{\Omega}} \frac{d^d k}{(2\pi)^d}\, \delta\left(\varepsilon - \varepsilon_{\mathbf{k}}\right) \quad . \tag{5.10.5}$$

Note that

$$\psi_{\mathbf{k}} \equiv \frac{1}{\sqrt{N}} \left\langle b_{\mathbf{k}} \right\rangle = -\frac{1}{N} \frac{\partial\Omega}{\partial\bar{\nu}_{\mathbf{k}}} = \frac{\nu_{\mathbf{k}}}{\varepsilon_{\mathbf{k}} - \mu} \quad . \tag{5.10.6}$$

In the condensed phase, $\psi_{\mathbf{k}}$ is nonzero.

The Landau free energy (grand potential) is a function $\Omega(T, N, \mu, \nu, \bar{\nu})$. We now make a Legendre transformation,

$$Y(T, N, \mu, \psi, \bar{\psi}) = \Omega(T, N, \mu, \nu, \bar{\nu}) + N \sum_{\mathbf{k}} \left(\nu_{\mathbf{k}} \bar{\psi}_{\mathbf{k}} + \bar{\nu}_{\mathbf{k}} \psi_{\mathbf{k}}\right) \quad . \tag{5.10.7}$$

Note that

$$\frac{\partial Y}{\partial \bar{\nu}_{\mathbf{k}}} = \frac{\partial \Omega}{\partial \bar{\nu}_{\mathbf{k}}} + N\psi_{\mathbf{k}} = 0 \quad , \tag{5.10.8}$$

by the definition of $\psi_{\mathbf{k}}$. Similarly, $\partial Y/\partial\nu_{\mathbf{k}} = 0$. We now have

$$Y(T,N,\mu,\psi,\bar{\psi}) = Nk_BT\int\limits_{-\infty}^{\infty} d\varepsilon\; g(\varepsilon)\,\ln\left(1-e^{(\mu-\varepsilon)/k_bT}\right) + N\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}}-\mu)\,|\psi_{\mathbf{k}}|^2 \quad . \tag{5.10.9}$$

Therefore, the boson particle number per unit cell is given by the *dimensionless density*,

$$n = \frac{N_b}{N} = -\frac{1}{N}\frac{\partial Y}{\partial\mu} = \sum_{\mathbf{k}}|\psi_{\mathbf{k}}|^2 + \int\limits_{-\infty}^{\infty} d\varepsilon\,\frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_BT}-1} \quad , \tag{5.10.10}$$

and the condensate amplitude at wavevector $\mathbf{k}$ is

$$\nu_{\mathbf{k}} = \frac{1}{N}\frac{\partial Y}{\partial\bar{\psi}_{\mathbf{k}}} = (\varepsilon_{\mathbf{k}}-\mu)\,\psi_{\mathbf{k}} \quad . \tag{5.10.11}$$

Recall that $\nu_{\mathbf{k}}$ acts as an external field. Let the dispersion $\varepsilon_{\mathbf{k}}$ be minimized at $\mathbf{k}=\mathbf{K}$. Without loss of generality, we may assume this minimum value is $\varepsilon_{\mathbf{K}}=0$. We see that if $\nu_{\mathbf{k}}=0$ then one of two must be true:

- $\psi_{\mathbf{k}}=0$ for all $\mathbf{k}$
- $\mu=\varepsilon_{\mathbf{K}}$, in which case $\psi_{\mathbf{K}}$ can be nonzero.

Thus, for $\nu=\bar{\nu}=0$ and $\mu>0$, we have the usual equation of state,

$$n(T,\mu) = \int\limits_{-\infty}^{\infty} d\varepsilon\,\frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_BT}-1} \quad , \tag{5.10.12}$$

which relates the intensive variables n, T, and μ. When $\mu=0$, the equation of state becomes

$$n(T,\mu=0) = \overbrace{\sum_{\mathbf{K}}|\psi_{\mathbf{K}}|^2}^{n_0} + \overbrace{\int\limits_{-\infty}^{\infty} d\varepsilon\,\frac{g(\varepsilon)}{e^{\varepsilon/k_BT}-1}}^{n_>(T)} \quad , \tag{5.10.13}$$

where now the sum is over only those $\mathbf{K}$ for which $\varepsilon_{\mathbf{K}}=0$. Typically this set has only one member, $\mathbf{K}=0$, but it is quite possible, due to symmetry reasons, that there are more such $\mathbf{K}$ values. This last equation of state is one which relates the intensive variables n, T, and n_0, where

$$n_0 = \sum_{\mathbf{K}}|\psi_{\mathbf{K}}|^2 \tag{5.10.14}$$

is the dimensionless condensate density. If the integral $n_>(T)$ in Equation [condeqn] is finite, then for $n>n_0(T)$ we must have $n_0>0$. Note that, for any T, $n_>(T)$ diverges logarithmically whenever $g(0)$ is finite. This means that Equation [GDE] can always be inverted to yield a finite $\mu(n,T)$, no matter how large the value of n, in which case there is no condensation and $n_0=0$. If $g(\varepsilon)\propto\varepsilon^\alpha$ with $\alpha>0$, the integral converges and $n_>(T)$ is finite and monotonically increasing for all T. Thus, for fixed dimensionless number n, there will be a *critical temperature* T_c for which $n=n_>(T_c)$. For $T<T_c$, Equation [GDE] has no solution for any μ and we must appeal to Equation [condeqn]. The condensate density, given by $n_0(n,T)=n-n_>(T)$, is then finite for $T<T_c$, and vanishes for $T\geq T_c$.

In the condensed phase, the phase of the order parameter ψ inherits its phase from the external field ν, which is taken to zero, in the same way the magnetization in the symmetry-broken phase of an Ising ferromagnet inherits its direction from an applied field h which is taken to zero. The important feature is that in both cases the applied field is taken to zero *after* the approach to the thermodynamic limit.