Long-range order in (quasi-) 2D systems

Suppose we have a many-body system that is described by some order parameter Ψ. The OP could be a real scalar quantity (e.g., in the Ising model, the z-component of average magnetization, which we called M in lecture 8) a complex scalar (as in the case of a superconductor or liquid ^4He), a vector (as in the 3D Heisenberg model, where it is the spin magnetization density $\mathbf{S}$) or something more complicated (as e.g. in the case of some liquid crystals or superfluid ^3He). Rather generically, the Hamiltonian (or free energy) of the *isolated* system (no external fields) may possess some invariance with respect to one or more symmetry operations on Ψ. E.g. the Hamilton of an isolated Ising system has the form

$$H = -J \sum_{ij=n.n.} \sigma_i \sigma_j \tag{1}$$

and is clearly invariant under the symmetry operation of simultaneous inversion of all spins ($\sigma_i \to -\sigma_i$), which is equivalent to $M \to -M$. Formally, this is reflected in the fact that the free energy (or equivalently the partition function) is a function only of M^2. Similarly, the free energy of the GL model of BCS superconductivity contains only terms of the form $f(|\Psi|^2)$ and $|\nabla\Psi|^2$, and thus is invariant[1] under (global) phase rotations (gauge transformations) $\Psi \to \Psi \exp i\alpha$, where $\alpha \neq f(r)$. The Heisenberg Hamiltonian

$$H = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2}$$

is invariant under the operations of the group O(3) (simultaneous rotation of all the spins around the same axis by the same angle). And so on.

In practice, the symmetry is likely to be broken by various external fields, which may or may not be "weak." For example, the symmetry of the Ising Hamiltonian is broken by an external magnetic field in the z-direction, and that of the Heisenberg Hamiltonian, by one in an arbitrary direction; in the latter case the added term is explicitly of the form

$$-\boldsymbol{\mathcal{H}} \cdot \sum_i \mathbf{S}_i \tag{3}$$

which shows that the Hamiltonian is still invariant under a subgroup of O(3), namely those corresponding to rotations around the field axis. In the case of BCS superconductivity it is strictly speaking impossible to break the gauge symmetry of the closed system by any physical mechanism, since it is equivalent to a different choice of overall phase for the single-particle wave functions, which has no physical significance. The best one can do is to insert terms in the Hamiltonian which couple the BCS phase of the system in question (defined,

[1] As is of course the original Hamiltonian, since an overall change of phase simply corresponds to multiplying the single-electron wave function by $e^{i\alpha/2}$, which has no physical significance.

say, as "the electrons within layer n" of a layered material) to that of its neighbors; the Josephson-type coupling discussed in lecture 8, namely

$$\epsilon = -J \sum_m (\Psi_n^* \Psi_{n+1} + c.c.) \tag{4}$$

is just such a term. (The free energy is, of course, still invariant under simultaneous phase rotation of all the Ψ_n through the same angle).[2]

In the following it may be easiest to visualize what is going on in terms of a model of spins subject to an exchange interaction and, possibly, an external magnetic field; to mimic a complex scalar order parameter we can specialize to the so-called XY model, where the spins lie entirely within a plane (say the xy-plane) and are coupled by an interaction that is isotropic within this plane, e.g.

$$H = -J \sum_{\substack{ij \\ \text{ln}}} (S_{xi} S_{xj} + S_{yi} S_{yj}) - S_x \mathcal{H} \qquad (J > 0, \text{ferromagnetic}) \tag{5}$$

The complex order parameter Ψ is then $S_x + iS_y$. The Ising model involves only one axis and the Heisenberg model term three equivalent axes, so the XY model is in some range intermediate between them. From the point of view of symmetry it is completely equivalent to the case of a superfluid/superconductor.

We now want to pose a question concerning the condition for ferromagnetism, or more generally for so-called "long-range order." There are at least two obvious ways of doing this:

(1) Does the system possess a finite expectation value of Ψ (i.e. of $\mathbf{S}$) in the thermodynamic limit when $\mathcal{H} \to 0$?

(2) Are the correlations of $\Psi(\mathbf{r})$ and $\Psi(\mathbf{r}')$ of infinite range with respect to $|\mathbf{r} - \mathbf{r}'|$?

There is actually a close connection between these two criteria, as can be seen as follows: For any quantity A that can be treated as classical (as can the total spin of the system in the thermodynamic limit) the fluctuations $\langle A^2 \rangle$ are related to the susceptibility χ_{AA} by the standard relation (a special case of the fluctuation dissipation theorem)

$$\langle A^2 \rangle = kT \chi_{AA} \tag{6}$$

Consider the quantity $\Psi \equiv \int \Psi(\mathbf{r}) d\mathbf{r}$ ($\equiv$ (something related to) total spin $\mathbf{S}$ for a magnetic model). If the correlation $\langle \Psi(\mathbf{r}) \Psi^*(\mathbf{r}') \rangle$ is of finite range (i.e. if the quantity in $\langle\ \rangle$ tends to zero "sufficiently fast" (see below) as $|\mathbf{r} - \mathbf{r}'| \to \infty$) then $\langle \Psi^2 \rangle$ is of order N in the thermodynamic limit and thus so is χ_{AA}; this then means that we should expect the total spin S to be proportional to $N\mathcal{H}$ and to vanish in the limit $\mathcal{H} \to 0$. If, on the other hand,

[2] The question of whether the "absolute" phase of the order parameter of a superconductor or superfluid can be given a meaning, e.g. by comparison with a "phase standard," is a still highly debated one; see e.g. AJL in *Bose Einstein Condensation*, ed. D. W. Snoke et al., Dunningham and Burnett, PRL, **82** 3729 (1999).

the correlation is of infinite range, i.e. $\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle$ tends to a finite (nonzero) value as $|\mathbf{r}-\mathbf{r}'|\to\infty$, then by the same argument χ_{AA} is of order N^2 and we expect, formally, the value of S induced by a field $\mathcal{H}$ to be proportional to $N^2\mathcal{H}$ and thus still of order N if $N\to\infty$ and $\mathcal{H}\to 0$ in such a way that $N\mathcal{H}\geq$ const. An interesting intermediate case is that the correlation falls off according to a power law, see below.

Although this argument is not at all rigorous, it focuses attention on the necessity of taking the thermodynamic limit $N\to\infty$ and the limit $\mathcal{H}\to 0$ in the correct way. Consider as an example Ising's original argument concerning the 3D version of his model, in which spins within a plane are infinitely tightly coupled and spins on neighboring planes have coupling J. For this model he correctly obtained the result, valid for any value of the field $\mathcal{H}$.

$$S=\frac{N\sinh N_s\mu\mathcal{H}/kT}{\sqrt{\sinh^2 N_s\mu\mathcal{H}/kT+e^{-2N_sJ/T}}} \tag{7}$$

where N_s is the number of spins in a plane and for a large rectangular volume of constant shape is $\propto N^{2/3}$. If we take the limits (as Ising did) in the order $\mathcal{H}\to 0$ then $N\to\infty$, clearly it is zero. On the other hand, if we take it in the opposite order, it is clear that $S=N$! (This particular example is a bit pathological because of the unphysically strong form of the in-plane coupling). In a system with "reasonable" (generally, short-range) interactions we need to take the limit in such a way that the limit of the product $(N\mathcal{H})$ is large compared to kT/μ; if we do not, then the fluctuations corresponding to a uniform rotation of all spins simultaneously will mean that the total magnetization is much less than N. In other words, we need a field that, though weak, is still sufficiently strong to stabilize the system against (uninteresting) rotations as a whole. This consideration is common to cases with discrete symmetry (like the Ising model), where the relevant "rotations" are only through π, and those with continuous symmetry (like the isotropic Heisenberg model) where they can be arbitrarily small. However, the next part of the argument requires us to distinguish these two cases. For a model with discrete symmetry and short-range forces the minimum energy to form a "domain wall" is proportional to N^{d-1} (e.g. for the Ising model in 1D it is 2J), and it turns out that while in 1D long-range order is destroyed at any nonzero temperature[3], it is stable in 2D up to a critical temperature, which is independent of N in the thermodynamic limit (in particular, this follows for the Ising model from Onsager's explicit solution). For the case of a continuous symmetry, which is more interesting in the present context, the situation is a bit different; as shown in lecture 1, in 3D the condition $(N\mu\mathcal{H}/k_BT\gg 1)$ is compatible with a value of the single-spin orientation energy $\mu\mathcal{H}$ which is still small compared to the lowest spin-wave energy ($\sim k^2_{\rm min}\sim N^{-2/d}$); however, in 1D this is no longer true in the thermodynamic limit, and in 2D the situation is "marginal,"

[3]This may be seen from the fact that the "kinks" are independent, and while the probability to form a kink between two neighboring sites is $\exp -J/k_BT\ll 1$, the number of independent pairs of sites $\propto N$.

since the quantities kT/N and $k^2_{\min}$ scale in the same way with N. Thus the question of the existence or not of LRO in 1D and, even more, in 2D is nontrivial.

So let's consider the 2D case rather more quantitatively. We will take as a convenient example a GL model such as the XY model for which the OP is a complex scalar, so that the symmetry in question is a phase rotation. We will examine explicitly criterion (6): does the correlation $\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle$ have finite or infinite range? The *exact* expression for this correlation is given within GL theory by the formula ($\int \mathcal{D}\Psi \equiv$ functional integral)

$$\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle_T = \frac{\int \mathcal{D}\Psi(\mathbf{r}'')(\exp -F\{\Psi(\mathbf{r}'')\}/kT)\Psi(\mathbf{r})\Psi(\mathbf{r}')}{\int \mathcal{D}\Psi(\mathbf{r}'')\exp -F\{\Psi(\mathbf{r}'')\}/kT} \tag{8}$$

In general it is not possible to evaluate this expression in closed form because of the occurrence of terms higher than quadratic in $\Psi(\mathbf{r})$ in the free energy. However, we can proceed as follows: Consider first the "mean-field" solution, that is the form of the function in $\Psi(\mathbf{r})$ which corresponds to the absolute minimum of the free energy $F\{\Psi(\mathbf{r})\}$. As we saw in lecture 8, for $T < T_c$ (the MF transition temperature, defined by $\alpha(T) = 0$)

$$\Psi(\mathbf{r}) = \text{const.} = \big(-\alpha(T)/\beta\big)^{1/2} \equiv \Psi_0 \tag{9}$$

Now expand the free energy around this value, and keep terms only up to second order in $\delta\Psi(\mathbf{r}) \equiv \Psi(\mathbf{r}) - \Psi_0$. It is convenient to split $\delta\Psi(\mathbf{r})$ into an "amplitude" term $\delta\Psi_\parallel$ which changes $|\Psi|^2$ and a "phase" term $\delta\Psi_\perp$ which preserves $|\Psi|^2$; from symmetry, the free energy cannot contain cross-terms between these. The fluctuational free energy associated with amplitude fluctuations has a finite contribution from the terms $\alpha(T)\,|\Psi|^2 + \frac{1}{2}\beta(T)\,|\Psi|^4$, as well as from the gradient term:

$$F^{fl}_\parallel(T) = \int \big\{2\,|\alpha(T)|\;\;|\delta\Psi_\parallel(r)|^2\;\; + \gamma(T)\;|\underline{\nabla}(\delta\Psi_\parallel)|^2\big\}dr \tag{10}$$

Because even the long-wavelength fluctuations have a "gap" $\alpha(T)$, it follows that except right at the mean-field T_c where $\alpha(T) \to 0$ the amplitude fluctuations cannot drive the LRO to zero (Problem). By contrast, let us write the phase fluctuations in the form

$$\Psi(\mathbf{r}) \to \Psi_0\;\exp\;i\varphi(\mathbf{r}) \qquad\qquad [\text{so, formally, } \delta\Psi_\perp(\mathrm{r}) = \Psi_0(\mathrm{i}\varphi(\mathrm{r}) - \frac{1}{2}\varphi^2(\mathrm{r}) + ...).] \tag{11}$$

It is clear that this kind of fluctuation, which preserves $|\Psi|^2$, has *no* restoring force from the "bulk" terms in F, and the only contribution is from the gradient term

$$F^{fl}_\perp(T) = \gamma(T)\;|\Psi_0|^2\;\int d\mathbf{r}\;(\underline{\nabla}\varphi)^2(r) \tag{12}$$

If we expand $\varphi(\mathbf{r})$ in a (d-dimensional) Fourier series

$$\varphi(r) = (2\pi)^{-d/2}\Omega^{-1/2}\sum_{\mathbf{k}}\varphi_k\;\exp\;i\mathbf{k}\cdot\mathbf{r} \tag{13}$$

then $F_\perp^{fl}(T)$ is a sum of contributions from the different k's:

$$F_\perp^{fl}(T) = (2\pi)^{-d}\gamma(T)|\Psi_0|^2 \sum_{\mathbf{k}} k^2 \varphi_{\mathbf{k}}^* \, \varphi_{-\mathbf{k}} \tag{14}$$

So far, the dimensionality d of the system has not entered explicitly.

Now, let us use the above results to evaluate the correlation $\langle \Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle$. In the approximation of neglecting amplitude fluctuations, this is simply $|\Psi_0|^2 \ \langle \exp \ i\big(\varphi(\mathbf{r}) - \varphi(\mathbf{r}')\big)\rangle$. Moreover, in view of the uncorrelated Gaussian nature of the fluctuations φ_k (see below), we can write

$$\langle \exp i\big(\varphi(\mathbf{r}) - \varphi(\mathbf{r}')\big)\rangle = \exp -\frac{1}{2}\langle[\varphi(\mathbf{r}) - \varphi(\mathbf{r}')]^2\rangle \equiv \exp -Q(|\mathbf{r}-\mathbf{r}'|) \tag{15}$$

We therefore have to calculate the quantity

$$Q(|\mathbf{r}-\mathbf{r}'|) \equiv \frac{1}{2}\langle[\varphi(\mathbf{r}) - \varphi(\mathbf{r}')]^2\rangle = \sum_{\mathbf{k}} \langle \varphi_{\mathbf{k}}\varphi_{-\mathbf{k}}\rangle (1 - \exp i\mathbf{k}\cdot\mathbf{r} - \mathbf{r}') \times 1/(2\pi)^d\Omega \tag{16}$$

Now, within our approximation for the fluctuational free energy (above) the latter is just a sum of contributions from the different $\mathbf{k}$, and the probability of a given set of values $\varphi_{\mathbf{k}}\varphi_{-\mathbf{k}}$ is just the product over the probabilities for each $\mathbf{k}$ separately. Thus we find[4]

$$\langle \varphi_{\mathbf{k}} \ \varphi_{-\mathbf{k}}\rangle = \int \frac{d(\varphi_{\mathbf{k}} \ \varphi_{-\mathbf{k}})\{\exp -\big(\beta\gamma(T)k^2 \ |\Psi_0|^2 \ \varphi_{\mathbf{k}} \ \varphi_{-\mathbf{k}}\big)\}}{\int d(\varphi_{\mathbf{k}} \ \varphi_{-\mathbf{k}}) \exp -\big(\beta\gamma(T)|\Psi_0|^2 \ k^2\varphi_{\mathbf{k}}\varphi_{-\mathbf{k}}\big)} = \frac{1}{2}Ak^{-2} \tag{17}$$

where the constant $A(T)$ is given by

$$A(T) \equiv \frac{k_B T(2\pi)^d}{\gamma(T) \ |\Psi_0|^2} \tag{18}$$

This formula is still valid independently of dimensionality.

Where the dimensionality comes in is at the final stage of inverting the Fourier transform to obtain $Q(|\mathbf{r}-\mathbf{r}'|) \equiv Q(r)$:

$$\begin{aligned} Q(r) &= \frac{1}{2} \ \frac{A(T)}{(2\pi)^d\Omega} \sum_{\mathbf{k}} \frac{(1-\cos\mathbf{k}\cdot\mathbf{r})}{k^2} = \frac{A(T)}{2} \ \cdot \frac{1}{(2\pi)^d} \int d^d\mathbf{k} \frac{1-\cos\mathbf{k}\cdot\mathbf{r})}{k^2} \\ &= \frac{1}{2}\cdot\frac{2A(T)}{(2\pi)^d}\int_0^{k_c} d^d\mathbf{k}\frac{\sin^2\frac{1}{2}\mathbf{k}\cdot\mathbf{r}}{k^2} = \frac{2k_BT}{(2\pi)^d \ \gamma \ |\Psi_0|^2}\int_0^{k_c} d^d\mathbf{k}\frac{\sin^2\frac{1}{2}\mathbf{k}\cdot\mathbf{r}}{k^2} \end{aligned} \tag{19}$$

[4]There is a slightly delicate point involved in the "counting" of the fluctuations: since $\varphi_{\mathbf{k}} \equiv \varphi_{-\mathbf{k}}^*$, we need to take $\varphi_{\mathbf{k}}$ and $\varphi_{-\mathbf{k}}$ together, and this gives rise to the factor of 1/2.

where, if necessary, the integral must be cut off at an upper limit k_c of the order of the value of the k for which the GL expression breaks down; this is typically of order $\xi^{-1}(T)$ where $\xi(T) \equiv \big(\gamma(T)/\alpha(T)\big)^{-1/2}$ is the GL correlation length introduced in lecture 8. In the following, we assume we are interested in values of $r \gg \xi(T)$. It is clear that in the 3D case the integral over $d^3\mathbf{k}$ gives an expression which is *independent* of r for $r \gg \xi(T)$, and proportional to $\xi^{-1}(T)$. So in this case the effect of fluctuations is to depress the magnitude of the quantity $\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle$ for such large values of $|\mathbf{r}-\mathbf{r}'|$, but it still tends to a nonzero asymptotic value.

In 1 and 2D the situation is qualitatively different because of the infrared-divergent behavior of the integral $\int d^dk/k^2$. In fact, in the 1D case, we have

$$Q(r) = \tilde{A}r, \qquad \tilde{A} \equiv \big(2A(T)/\pi\big) \cdot \int_0^\infty \frac{\sin^2 x}{x^2} dx \tag{20}$$

Hence, in this case, the quantity $\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle$ falls off *exponentially* with r. It is convenient to write the result in the form

$$\langle\Psi(x)\Psi^*(x')\rangle = |\Psi_0|^2 \exp -|x-x'|/\xi'(T) \tag{21}$$
$$\xi'(T) \equiv R\xi(T)$$

where $\xi(T) \equiv (\gamma/\alpha(T))^{1/2}$ (see lecture 8) and $R(T) \sim (\alpha^2/\beta)\xi/k_BT$ is of the order of the free energy per unit correlation length in units of k_BT. For T not too close to T_c, if the 3D transition is well described by MF theory, R is typically $\gg 1$; in particular this is true for the superconducting case. We see therefore that there is no LRO at any finite T in a 1D system described by a GL free energy with a continuous symmetry; moreover, it is clear that the susceptibility (obtained as above by integrating over the volume) should be proportional to N not N^2, i.e. the system behaves "normally" on the application of a weak external "magnetic field."[5] Nevertheless, when examined on length scales short compared to $\xi'(T)$ (which can still be very long compared to microscopic lengths such as the interparticle distance) the system may look very much "as if" it possessed LRO.

In the 2D case, the expression for $Q(\mathbf{r})$ is messy because of the effect of the angular averaging, but it is clear that for $r \gg k_c^{-1} \sim \xi(T)$ this gives simply a factor of $\pi/2$ and thus $Q(r) = k_BT/4\pi\gamma|\Psi_0|^2 ln(r/\xi)+$ const. Hence, the quantity $\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle$ falls off according to a *power law*:

$$\langle\Psi(\mathbf{r})\Psi^*(\mathbf{r}')\rangle \sim \big(\xi(T)/|\mathbf{r}-\mathbf{r}'|\big)^{\eta(T)} \tag{22}$$

where $\eta(T) = k_BT/\big(4\pi\gamma(T)\ |\Psi_0|^2\big)$. For the special case of a neutral bosonic superfluid such as ^4He for which $\gamma(T)$ can be shown (see lecture 10) to be equal to $\hbar^2/2m^2$ times the superfluid density $\rho_s(T)$, this can be written

$$\eta(T) \sim\ k_BT/\big(2\pi\rho_s(T)\hbar^2/m^2\big) \tag{23}$$

[5] A much more detailed study of the 1D GL system, largely by computational methods, has been carried out by Scalapino et al., Phys. Rev. **86**, 3409 (1972).

where $\rho_s(T)$ is the 2D superfluid density (superfluid mass/unit area). Note that in this case the susceptibility is "normal" if $\eta(T) > 2$, otherwise it increases faster than N in the thermodynamic limit. Hence we might expect a qualitative change in the behavior of the system at the point $\eta(T) = 2$, i.e. when the superfluid density satisfies

$$\rho_s(T) = \frac{1}{4\pi}[\frac{m}{\hbar}]^2 k_B T \tag{24}$$

This (or an equivalent extension for other types of order) indeed turns out to be the case, although the analysis requires us to go beyond the consideration of small fluctuations around homogenous equilibrium (see next lecture).

The above arguments are physically appealing but not rigorous, since they depend on (a) an appeal to an effective GL form of free energy and (b) approximation of the free energy of fluctuations around the MF solution by a quadratic expression. A rigorous proof of the absence of LRO at any nonzero temperature in 1 or 2D was found by Hohenberg[6] for the specific case of a superfluid or superconductor, and applied by Mermin and Wagner[7] to other types of ordering (magnetic and crystalline); it is usually known as the Hohenberg-Mermin-Wagner theorem. I will give the proof explicitly for the case of a neutral Bose superfluid under the normal assumption that we can pretend that the quantity $\langle a_0 \rangle \equiv \int \langle \psi(\mathbf{r}) \rangle d\mathbf{r}$ exists.

Suppose $\hat{H}$ is the Hamiltonian of the system, all expectation values $\langle \quad \rangle$ are taken in thermal equilibrium and A and C are any two *arbitrary* operators. Then there exists a famous inequality[8] due to Bogoliubov:

$$\frac{1}{2}\langle \{A, A^\dagger\} \rangle \cdot \langle \big[[C, H], C^\dagger\big] \rangle \geq k_B T \langle [C, A] \rangle^2 \tag{25}$$

($[\ ,\ ] \equiv$ commutator, $\{\ ,\ \} \equiv$ anticommutator)

In the case of a Bose superfluid, take A to be the $k-th$ Fourier component of the particle destruction operator $\hat{\psi}(r)$, i.e. $A \equiv a_{\mathbf{k}}$, and C to be the $-k$'th component of the density fluctuation operator, $\rho_{-\mathbf{k}}$. Then since $[\rho_{-k}, a_k] = a_0$, the Bogoliubov inequality takes the form

$$\frac{1}{2}\big(2\langle n_k \rangle + 1\big) \cdot \langle \big[[\rho_{\mathbf{k}}, H], \rho_{-}\mathbf{k}\big] \rangle \geq k_B T \langle a_0 \rangle^2 = k_B T n_0 \tag{26}$$

where at the last step I have made the usual assumption that $\langle a_0 \rangle^2$ can be equated with the condensate occupation number n_0. Now for a Hamiltonian without velocity-dependent

[6] P. C. Hohenberg, Phys. Rev. **158**, 383 (1967).

[7] N. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[8] For the proof, which is straightforward and based on a Schwartz inequality, see Mermin and Wagner, loc. cit.

forces, the double commentator of $\rho_{\mathbf{k}}$ with $\hat{H}$ is simply given by the well known f-sum rule result, namely $n\hbar^2k^2/m$. Thus we obtain Hohenberg's lemma:

$$\boxed{n_k \geq \frac{mk_BT}{\hbar^2k^2} \cdot \frac{n_0}{n} - \frac{1}{2}} \tag{27}$$

which is true independently of dimension d.

A crude physical interpretation of Hohenberg's lemma runs as follows: Suppose there are n_0 particles per unit volume in the condensate. The operator $\rho_{\mathbf{k}}$ effects (among other things) the removal of a particle from the state 0 (the condensate) and its placing in the state $\mathbf{k} \neq 0$. Because $\rho_{\mathbf{k}}$ commutes with the potential energy, the only energy cost of this operation is the change in KE, namely $\hbar^2k^2/2m$. At least if this energy is $\ll k_BT$, we should therefore expect the population of the state $\mathbf{k}$ to be at least of the order $k_BT/(\hbar^2k^2/2m)$ times the original fractional probability n_0/n of the groundstate being populated. This gives the lemma (to within a constant ~ 1, of course).

It is clear that in 1 or 2D, if $n_0/n \neq 0$, the density of "uncondensed" particles

$$n_n \equiv \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \to \frac{1}{2\pi}^d \int d^2\mathbf{k} n_{\mathbf{k}} \geqslant \frac{1}{(2\pi)^d} \cdot \frac{1}{2} \int_0^{k_0} \left(\frac{k_0^2}{k^2} - 1\right) d^2\mathbf{k} \tag{28}$$

$$\left(k_0^2 \equiv \left(\frac{2mk_BT}{\hbar^2} \quad \frac{n_0}{n}\right)\right)$$

must diverge, so that we cannot fulfill the obvious constraint $n_n + n_0 = n$. Thus the assumption of nonzero n_0/n is inconsistent, i.e. we recover the result that there can be no LRO in 1 or 2D (at any nonzero T). In 3D the assumption is not internally inconsistent, but application of the lemma then yields an upper limit on the condensate fraction $n_0(T)/n$ at any finite T (a not universally known, and quite useful result, see Problem).

A number of comments regarding the HMW theorem are in order. First, one may wonder how would it be modified by the application of a small "symmetry-breaking" field, which in the Bose case would give rise to an extra term in the Hamiltonian of the form

$$\Delta H = -(\lambda_0 \hat{a}_0 + H.c.) \qquad \lambda_0 \to 0. \tag{29}$$

Of course, in the real (particle-conserving) situation such a term is unphysical, but its analogs in cases of other types of broken symmetry are perfectly realistic (e.g. in the XY model, λ_0 would correspond to a weak magnetic field along some axis in the xy-plane). It is clear that the only change in the derivation is that the double commutator $\langle [\rho_{\mathbf{k}}, H], \rho_{\mathbf{k}} \rangle$ now acquires an extra term of the form $\lambda_0(\langle a_0^+ \rangle + \langle a_0 \rangle)$ ($= 2\lambda_0 \langle a_0 \rangle$ if we assume λ_0 and hence $\langle a_0 \rangle$ is real). Thus, Hohenberg's lemma is generalized to

$$n_k \geq \frac{mk_BT}{\hbar^2k^2 + 2m\lambda_0\langle a_0 \rangle} \left(\frac{n_0}{n}\right) - \frac{1}{2} \tag{30}$$

We now no longer get a divergence in the sum over k, but since we must maintain the constraint $\sum_k n_k + n_0 = n$, the lemma puts an upper limit on n_0 as a function of λ_0 (Problem).

A second obvious question is: How seriously should we take the theorem for real-life physical systems, which needless to say have finite dimension L? After all, the infrared logarithmic divergence of the quantity n_n in eqn. (28) only arose because we implicitly took the limit $L \to \infty$ and therefore replaced the sum in its definition by an integral. So let's go back to eqn. (27) and perform the sum over $\mathbf{k} \equiv (2\pi n_x/L,\ 2\pi n_y/L)$ where n_x and n_y are both integers such that $n_x n_y \neq 0$ (i.e. both cannot simultaneously be zero, as this would correspond to the condensate). Without evaluating the sum in detail, it is intuitively clear that its order of magnitude is given by an integral cut off at $k \sim 2\pi/L$. Hence we find that the lower limit on n_n (eqn. (28)) is given in order of magnitude by

$$n_n^{min} \sim \frac{1}{8\pi} k_0^2 \ \ln k_0 L \qquad\qquad \left(k_0 \equiv \left(\frac{2\pi m k_B T}{\hbar^2} \ \frac{n_0}{n} \right)^{1/2} \right) \tag{31}$$

Defining a characteristic "degeneracy" temperature T_0 by the condition that the thermal de Broglie wavelength $\lambda_L(T)$ be of order of the interparticle separation, or more formally by $T_0 \equiv n\hbar^2/2\pi m k_B$, we can rewrite (31) as

$$n_n^{min} \sim \frac{1}{8\pi^2} \left(\frac{T}{T_0} \right) n_0 \ln \left\{ (L/\lambda_L(T) \cdot (n_0/n)^{1/2} \right\} \tag{32}$$

and thus, since $n_n + n_0 \equiv n$, the limit on n_0/n is given by the implicit equation

$$\frac{n_0}{n} \leq \left(1 + \frac{1}{8\pi^2} \ \frac{T}{T_0} \ln \left\{ (L/\lambda_L(T)(n_0/n)^{1/2} \right\} \right)^{-1} \tag{33}$$

Let's ask for the smallest value $L_{\min}$ of k for which the HMW requires n_0 to be less than, say, 10% of n (the approximate value it has in real (3D) liquid ^4He). The answer is approximately

$$L_{min} \sim \frac{\lambda_T}{3} \exp \alpha \frac{T_0}{T} \qquad\qquad \alpha \sim \frac{9}{8\pi} \tag{34}$$

(where the value of α should be taken only as an order of magnitude). Thus, e.g. for a 1cm^2 monolayer film of $^4He(T_0 \sim 3K)$ the HMW becomes essentially irrelevant for $T \ll 50\ mK$, a temperature regime not difficult to reach experimentally. For other kinds of 2D phase transition the situation is even worse (or better!)): e.g. in the case of crystalline order T_0 is replaced by a temperature that is at least of the order of the Debye temperature, so to see HMW-type effects in (say) a graphene crystal at a few degrees would require the crystal to extend from here to the moon! The moral is that before taking the theorem too seriously in a real-life situation, one should carefully put in the numbers.

Incidentally, we note that the theorem is not in contradiction with the estimates given earlier for the fall-off of the correlation $C(\mathbf{r},\mathbf{r}') \equiv \langle\Psi(\mathbf{r})\Psi(\mathbf{r}')\rangle$, namely $C(\mathbf{r},\mathbf{r}') \sim |\mathbf{r}-\mathbf{r}'|^{-\eta(T)}$ where $\eta(T) \equiv k_BT/2\pi\rho_s(T)(\hbar^2/m)$: the quantity n_0/n is proportional to N^{-2} times the double integral of $C(\mathbf{r}\mathbf{r}')$ over $\mathbf{r}$ and $\mathbf{r}'$, which is proportional to N for $\eta(T) > 2$ and to $N^{2-\eta/2}$ for $\eta(T) < 2$, so for $\eta(T) \neq 0$ the condensate fraction indeed vanishes in the thermodynamic limit.

Finally, we must ask how the results we have obtained, either by the phenomenological GL technique or by Hohenberg's theorem, apply to the realistic case of quasi-2D geometries, that is to a set of planes with weak but nonzero interplane coupling. Obviously, in the limit of a very anisotropic continuum the generalization in each case is straightforward: if $k\|$ denotes the component(s) of $\mathbf{k}$ parallel to the rods/planes and $k_\perp$ the "perpendicular" component(s), then in the GL formulation we must make the replacement

$$\gamma k^2 \to \gamma_\| k_\|^2 + \gamma_\perp k_\perp^2 \tag{35}$$

while in the Hohenberg theorem, if we define "parallel" and "perpendicular masses" $m_\|, m_\perp$, then we must make the replacement

$$k^2/m \to k_\|^2/m_\| + k_\perp^2/m_\perp \tag{36}$$

Since the original 3D expressions can be recovered (up to a multiplying constant) by a rescaling of the different components of $\mathbf{k}$, we see that the very anisotropic 3D case is equivalent in the present context (only) to a fully 3D case, and in particular that LRO is possible.

However, it is physically obvious that if we keep the in-plane (etc.) properties and also T constant, and gradually turn down the interplane coupling, there must come a point at some nonzero value of this coupling at which we recover the "truly" 2D behavior; so the above argument, which if taken seriously would suggest that an infinitesimal transverse coupling should stabilize LRO, cannot be the whole truth.

Formally, this comes about because when the magnitude k_0 of the maximum transverse wave vector that can be appreciably thermally excited, namely $k_0 \sim (k_BT/\gamma_\perp\ |\Psi_0|^2)^{1/2}$, becomes comparable to the inverse interplane spacing, we can no longer use the continuum model and must return to the discrete form of the coupling energy, namely

$$F_\perp = -J\sum_{mn}\int(\Psi_i^*\ \Psi_j + c.c.)dr_\| \tag{37}$$

(or an equivalent replacement in the Hamiltonian). It is clear that the maximum value of this free energy per plane is $2J|\Psi_0|^2$ per unit area.

Will this be enough to stabilize the LRO? To answer this question, we note that when viewed from any one plane the interplane coupling essentially looks like an external magnetic field. Moreover, the differential susceptibility per unit area of the isolated plane is given by the quantity (apart from a multiplying constant)

$$\chi_0 \equiv N^{-1}(k_B T)^{-1} \iint dr\ dr' \langle \Psi(\mathbf{r})\ \Psi(\mathbf{r}') \rangle \tag{38}$$

which as we have seen is proportional to a constant for $\eta(T) > 2$ but to a positive power of N for $\eta(T) < 2$. Thus we conclude that for $\eta(T) < 2$ an infinitesimal interplane coupling will stabilize LRO, while for $\eta(T) > 2$ a minimum value of J will be required. We postpone for now the question of what this minimum value is.

[Relation of ODLRO and superfluidity]