Decay of Order in Isotropic Systems of Restricted Dimensionality. I. Bose Superfluids

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The off-diagonal ordering of one- and two-dimensional Bose particle systems of finite thickness and cross-section is considered in the presence and absence of a symmetry-breaking field. It is shown rigorously, by applying Bogoliubov's inequality to a subdomain of the system, that no spontaneous ordering can occur; several definitions of long-range order are discussed. Explicit bounds on the order-order correlation function, integrated over a subdomain, are obtained which indicate how the short-range order decays with distance. Conditions under which information on the pointwise behavior of the correlation function can be inferred are also discussed. The inequalities are assessed numerically for real situations.

I. INTRODUCTION

Ordering or spontaneous symmetry breaking in systems admitting a continuous global symmetry operation (such as total spin rotation in an isotropic ferromagnet or gauge transformation in a Bose fluid) is of fundamental theoretical and experimental interest. Heuristic arguments, frequently based on thermodynamic considerations or simple concepts of elementary excitations, have long ago suggested that one- or two-dimensional systems cannot support long-range ordering or sustain a broken symmetry. Qualitatively it appears that the fluctuations in magnitude and "direction" of the local order parameter are so large in one or two dimensions as to break up any initially ordered state. (Conversely in a fully three-dimensional system a state of broken symmetry may be stable at low enough temperatures.) Recently Hohenberg[1] has demonstrated that an operator inequality, due originally to Bogoliubov,[2] can be used to substantiate these conclusions in superfluid and superconducting systems. Mermin and Wagner[3] considered isotropic Heisenberg ferromagnets and antiferromagnets and proved rigorously that spontaneous magnetization (or sublattice ordering) cannot occur at any nonzero temperature if the system is one or two dimensional. Similar rigorous arguments have been developed for other systems.[4] Chester, Fisher, and Mermin[5] have shown explicitly that these results remain valid even for a system extended in three dimensions provided the over-all cross section ($d=1$) or the over-all thickness ($d=2$) is finite.

The existing proofs[3,5] first introduce a *symmetry-breaking field* η (a magnetic field H in the case of a ferromagnet) into the Hamiltonian, *then* proceed to the thermodynamic limit (volume $V\to\infty$), and finally demonstrate that the induced order parameter $\Psi(\eta)$ [the magnetization $M(H)$, in a ferromagnet] vanishes as the η field is reduced to zero, $|\eta|\to 0$ ($H\to 0$). While the result Ψ_0 (or M_0) $\equiv 0$, obtained in this way is valuable, the arguments leave open certain basic questions:

(a) How does the static order-order correlation function $\sigma(\vec{r},\vec{r}')$ behave for large spatial separations of the arguments? In particular, one would like to show that $\sigma\to 0$ as $|\vec{r}-\vec{r}'|\to\infty$ to demonstrate the absence of any long-range order.

(b) Can the initial introduction of the symmetry-breaking field be avoided in proving the absence of spontaneous order? This question seems especially pertinent in the case of a Bose fluid,[6] where the appropriate "off-diagonal" or "anomalous" field η cannot be realized physically, and the relevance of the corresponding definition of Ψ_0 might be questioned.

We have found that if attention is concentrated on the correlation functions (with or *without* a symmetry-breaking field), Bogoliubov's inequality can again be manipulated to give rigorous answers to these questions.[7] We treat the case of a Bose system and a Heisenberg/Ising magnet in these articles. Section II introduces the notation and summarizes our specific results. Several types of long-range order are considered and discussed in detail in the later sections. A brief outline of the arguments is presented at the end of Sec. II. The remainder of this paper is devoted exclusively to the detailed proofs concerning anomalous or off-diagonal order in Bose particle systems.[7] The corresponding detailed arguments for spin systems are taken up in the following paper.

II. NOTATION AND SUMMARY OF RESULTS

To introduce the notation consider first an anisotropic Heisenberg ferromagnet of $\mathfrak{N}(\Omega)$ localized spins $\vec{S}(\vec{r})$ occupying the sites $\vec{r}$ of a regular lattice contained in a domain Ω. We take the Hamiltonian to be

$$\mathcal{H}_\Omega = -\tfrac{1}{2}\sum_{\vec{r}}\sum_{\vec{r}'}[J_x(\vec{r},\vec{r}')S^x(\vec{r})S^x(\vec{r}') + J_y(\vec{r},\vec{r}')S^y(\vec{r})S^y(\vec{r}') + J_z(\vec{r},\vec{r}')S^z(\vec{r})S^z(\vec{r}')]$$

$$-\sum_{\vec{r}} \vec{h}(\vec{r}) \cdot \vec{S}(\vec{r}) , \tag{2.1}$$

where $\vec{h}(\vec{r})$ is the external field in energy units ($\vec{h} = \frac{1}{2} g \mu_B \vec{H}$), while $J_\alpha(\vec{r}, \vec{r}\,')$ is the exchange coupling. Note that the terms with $\vec{r} = \vec{r}\,'$ represent single-spin anisotropy terms of magnitude $\frac{1}{2} J_\alpha(\vec{r}, \vec{r})\,(S^\alpha)^2$ ($\alpha = x, y, z$). We will allow $J_\alpha(\vec{r}, \vec{r}\,')$ to vary randomly (or regularly). The α component of the spontaneous magnetization per spin at temperature T is defined by the expression

$$M_0^\alpha(T) = \lim_{h_\alpha \to 0+} M^\alpha(\vec{h}, T)$$
$$\equiv \lim_{h_\alpha \to 0+} \lim_{\mathfrak{N}(\Omega) \to \infty} \mathfrak{N}(\Omega)^{-1} \sum_{\vec{r}} \langle S^\alpha(\vec{r}) \rangle_\Omega , \tag{2.2}$$

where the thermal average $\langle S^\alpha(\vec{r}) \rangle_\Omega$ is calculated in the presence of fixed (uniform) field $\vec{h}$ with $h_\alpha \neq 0$. This magnetic field is needed to break the underlying symmetry, which is (a) *spherical* if $J_x = J_y = J_z$, (b) *axial* or *cylindrical* (about the z axis) if $J_x = J_y \neq J_z$, or (c) merely *reflexive* if $J_x \neq J_y \neq J_z$. [Note in considering, say, the spontaneous magnetization in the x direction, $M_0^x(T)$, it is *not* essential that h_z or h_y vanish.]

The thermodynamic limit $\mathfrak{N}(\Omega) \to \infty$ is, of course, essential since the magnetization M_Ω^α in a finite system vanishes identically by symmetry if $h_\alpha = 0$. The system may be three dimensional in the sense that Ω contains many lattice layers, but if, in the thermodynamic limit, Ω may be contained between two parallel planes of a fixed, finite separation D_z, we say the dimensionality is *restricted* to $d = 2$.[5] Similarly, if Ω can be contained within a cylinder of fixed, finite rectangular cross section $D_y D_z$, the dimensionality is said to be restricted to $d = 1$.[5] We will refer to the infinite domain enclosing Ω as the "box" Λ.

In the case of a Bose system we take the Hamiltonian for a system of N particles in a bounded domain Ω to be

$$\mathcal{H}_{N,\Omega} = T_N + U_N + W_N , \tag{2.3}$$

where the kinetic-energy operator is

$$T_N = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 , \tag{2.4}$$

while $U_N = U_N(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ is the total interaction potential, which consists of the usual sum of two-body interaction terms, plus appropriate higher-order three-body, four-body, ..., terms.[8-10] Finally, $W_N(\vec{r}_1, \ldots, \vec{r}_N)$ is a sum of N single-body terms $W_1(\vec{r}_i)$, representing the wall potentials, which ensure that the many-body position wave functions $\Phi_N(\vec{r}_1, \ldots, \vec{r}_N)$ vanish continuously as any $\vec{r}_i$ approaches the boundary of the domain Ω. (The domain is assumed to be of sufficiently regular shape.[9,10])

For a Bose system the many-body wave functions must satisfy the condition of total symmetry:

$$\Phi_N(\ldots \vec{r}_i, \ldots \vec{r}_j, \ldots) = \Phi_N(\ldots \vec{r}_j, \ldots \vec{r}_i, \ldots) \quad (\text{all } i, j).$$

As is well known, the combinatorial difficulties associated with this restriction may be conveniently handled by the formalism of second quantization; we sketch this briefly here to bring out a few points relevant to our subsequent arguments. One starts with a set $\varphi_n(\vec{r})$ of continuous, differentiable single-particle wave functions which are complete in Ω, and vanishing on the boundary. (These might, but need not, be eigenfunctions of the Laplacian, i.e., of the kinetic energy.) If a_n and $a_n^\dagger$ are the corresponding annihilation and creation operators appropriate to Bose statistics,[11] we may construct the field operators

$$\psi(\vec{r}) = \sum_n \varphi_n(\vec{r}) a_n , \quad \psi^\dagger(\vec{r}) = \sum_n \varphi_n^*(\vec{r}) a_n^\dagger . \tag{2.5}$$

If, by convention, we suppose that each $\varphi_n(\vec{r})$ vanishes identically for $\vec{r}$ outside Ω, then the field operators are defined for all $\vec{r}$ and satisfy the formal commutation relations

$$[\psi(\vec{r}), \psi(\vec{r}\,')] = [\psi^\dagger(\vec{r}), \psi^\dagger(\vec{r}\,')] = 0 ,$$
$$[\psi(\vec{r}), \psi^\dagger(\vec{r}\,')] = \delta(\vec{r} - \vec{r}\,') \quad \text{for } \vec{r} \text{ and } \vec{r}\,' \text{ both in } \Omega$$
$$= 0 \qquad \text{otherwise.} \tag{2.6}$$

It is worth stressing, to avoid possible misunderstanding, that $\psi(\vec{r})$, $\psi^\dagger(\vec{r})$, and any of their linear or nonlinear combinations or derivatives, integrals, etc., are acceptable *operators* which do *not* have to satisfy any "boundary conditions." As usual the density operator is

$$\rho(\vec{r}) = \psi^\dagger(\vec{r})\, \psi(\vec{r}) , \tag{2.7}$$

while the number operator for the domain Ω is

$$\hat{N}_\Omega = \int_\Omega \rho(\vec{r})\, d\vec{r} . \tag{2.8}$$

The second-quantized Hamiltonian is then

$$\hat{\mathcal{H}}_\Omega = \hat{T}_\Omega + \hat{U}_\Omega + \hat{W}_\Omega , \tag{2.9}$$

with

$$\hat{T}_\Omega = -(\hbar^2/2m) \int_\Omega \psi^\dagger(\vec{r})\, \nabla^2 \psi(\vec{r})\, d\vec{r}$$
$$= (\hbar^2/2m) \int_\Omega \nabla \psi^\dagger(\vec{r}) \cdot \nabla \psi(\vec{r})\, d\vec{r} , \tag{2.10}$$

$$\hat{W}_\Omega = \int_\Omega W_1(\vec{r})\, \rho(\vec{r})\, d\vec{r} , \tag{2.11}$$

while $\hat{U}_\Omega$ is similarly a quadratic or higher-order functional of the density operator $\rho(\vec{r})$ alone.

For a particle system it is natural to use a *canonical* (i.e., particle-conserving) ensemble for the statistical mechanics. This means that in the calculation of the partition function $Z_{N,\Omega}$, and thermal averages $\langle \cdot \rangle_{N,\Omega}$, all traces are restricted to the subspace for which $\hat{N}_\Omega$ is just N times the identity operator. In taking the thermodynamic limit the number of particles N and the volume $V(\Omega)$ of the domain Ω are related as usual[9,10] by

$$N/V(\Omega)=\rho_\Omega \to \rho \quad \text{as } V(\Omega)\to\infty . \qquad (2.12)$$

We will make use of this canonical formulation below, but since it does not allow the analog of the magnetic symmetry-breaking terms, we will also consider the *grand-canonical* ensemble in which the traces are *unrestricted* and in which the Hamiltonian is taken in the form

$$\hat{\mathcal{H}}_{\mu,\Omega}=\hat{\mathcal{H}}_\Omega - \mu\hat{N}_\Omega - \hat{h}_\Omega . \qquad (2.13)$$

Here μ is the chemical potential (which is the analog of the longitudinal field h_z in the magnetic case[12]), while the symmetry-breaking part of the Hamiltonian is

$$\hat{h}_\Omega = \int_\Omega [\eta(\vec{r})\psi^\dagger(\vec{r})+\eta^*(\vec{r})\psi(\vec{r})]\,d\vec{r} , \qquad (2.14)$$

where the "off-diagonal" or "anomalous" fields $\eta(\vec{r})=\eta'(\vec{r})+i\eta''(\vec{r})$ are the analogs of the transverse magnetic fields $h^+(\vec{r})=h_x(\vec{r})+ih_y(\vec{r})$. Then the analog of expression (2.2) for the spontaneous magnetization is

$$\Psi_0(T)=\lim_{\eta\to 0+}\Psi(T,\eta)$$
$$\equiv \lim_{\eta\to 0+}\ \lim_{V(\Omega)\to\infty} V(\Omega)^{-1}\int_\Omega d\vec{r}\,\langle\psi(\vec{r})\rangle_\Omega , \qquad (2.15)$$

where $\langle\cdot\rangle_\Omega$ denotes the grand-canonical thermal average in the presence of a fixed (uniform) anomalous field η.

Previous work[3-5] has shown that for a system of restricted dimensionality, the anomalous average Ψ_0 vanishes identically while the spontaneous magnetization M_0^α vanishes for all α in isotropic, spherically symmetric systems, and M_0^x and M_0^y vanish in axially symmetric systems. Answers to the further questions (a) and (b) posed in the Introduction may be provided by considering (with $\eta h_\alpha\equiv 0$) the root-mean-square order parameter[13] $\Psi_\sigma(T)$ defined by

$$(\Psi_\sigma)^2=\lim_{V(\Omega)\to\infty} V(\Omega)^{-2}\int_\Omega d\vec{r}\int_\Omega d\vec{r}'\,\sigma_\Omega(\vec{r},\vec{r}') . \qquad (2.16)$$

The order-order correlation function for a Bose system in a domain Ω is taken as the one-body density matrix[14,15]

$$\sigma_\Omega(\vec{r},\vec{r}')=\langle\psi^\dagger(\vec{r}')\psi(\vec{r})\rangle_\Omega . \qquad (2.17)$$

In the magnetic version of (2.16), sums over the lattice sites of Ω replace the integrals, $\mathfrak{N}(\Omega)$ replaces $V(\Omega)$, and one may take

$$\sigma_\Omega^\alpha(\vec{r},\vec{r}')=\langle S^\alpha(\vec{r})S^\alpha(\vec{r}')\rangle_\Omega , \qquad (2.18)$$

or, in closer analogy to (2.17),

$$\sigma_\Omega(\vec{r},\vec{r}')=\langle S^+(\vec{r}')S^-(\vec{r})\rangle_\Omega,\quad (S^\pm=S^x\pm iS^y). \qquad (2.19)$$

In a fully three-dimensional system one normally expects that $\Psi_0(T)$ is proportional to $\Psi_\sigma(T)$, both being of order unity below a nonzero transition temperature; but general proof of this has never been given. However, for a magnetic system in which the magnetization is a constant of the motion, Griffiths[13] has shown that $\Psi_0\le\Psi_\sigma$.

Of independent interest are the *short long-range order* $\Psi_s(T)$ and the *long long-range order* $\Psi_l(T)$ defined,[16] respectively, by

$$(\Psi_s)^2=\lim_{|\vec{r}-\vec{r}'|\to\infty}\sigma_\infty(\vec{r},\vec{r}')$$
$$\equiv \lim_{|\vec{r}-\vec{r}'|\to\infty}\ \lim_{V(\Omega)\to\infty}\sigma_\Omega(\vec{r},\vec{r}') , \qquad (2.20)$$

where in the thermodynamic limit $\vec{r}$ and $\vec{r}'$ become infinitely distant from the boundary of Ω, and

$$(\Psi_l)^2=\lim_{V(\Omega)\to\infty}\sigma_\Omega(\vec{r},\vec{r}')\big|_{|\vec{r}-\vec{r}'|=R(\Omega)} , \qquad (2.21)$$

where we may suppose that the thermodynamic limit is taken through a sequence of domains self-similar in d dimensions, e.g., cubes ($d=3$), or cylinders of constant height ($d=2$), or of constant cross section ($d=1$), and that $R(\Omega)\propto[V(\Omega)]^{1/d}$ is a characteristic dimension. (As a matter of fact, Ψ_l, even if the limit exists, may well depend on further details of the placement of $\vec{r}$ and $\vec{r}'$ in Ω.)

For the simple nearest-neighbor ferromagnetic square Ising lattice it has been proven[16] that $\Psi_s=\Psi_l$; in addition, one knows[13] that $\sigma_\Omega(\vec{r},\vec{r}')$ is monotonic increasing in $\mathfrak{N}(\Omega)$ [provided $\Omega\supset\Omega'$ whenever $\mathfrak{N}(\Omega)>\mathfrak{N}(\Omega')$]. Suzuki has recently argued[17] that if these conditions hold more generally for a magnetic system in which the magnetization is a constant of the motion, then one also has $\Psi_s\le\Psi_0$.

With these definitions, we will answer question (b) explicitly by proving that $\Psi_\sigma(T)$ vanishes for all $T>0$ for systems of restricted dimensionality ($d\equiv 2$ or 1). [In magnetic systems we require that $J_\alpha(\vec{r})$ does not decay to zero too slowly.] To provide an answer to question (a) we average the correlation function $\sigma_\Omega(\vec{r},\vec{r}')$ over any (reasonably shaped) subdomain $\Gamma\subset\Omega$ which constitutes a "slice" of Ω as indicated in Fig. 1 (see also Sec. III), with a weighting function $f(\vec{r})$, arbitrary except for the condition

$$|f(\vec{r})|=1 . \qquad (2.22)$$

This yields a definition of the corresponding short-range order parameter $\Psi_\Omega\{f|\Gamma\}$ and single-particle occupation number $n_\Omega\{f|\Gamma\}$, namely,

$$[V(\Gamma)\Psi_\Omega\{f|\Gamma\}]^2=V(\Gamma)n_\Omega\{f|\Gamma\}$$
$$=\int_\Gamma d\vec{r}\int_\Gamma d\vec{r}'\,f^*(\vec{r}')f(\vec{r})\,\sigma_\Omega(\vec{r},\vec{r}'), \qquad (2.23)$$

which expression in a Bose system is equal to

$$\langle \,|\int_\Gamma d\vec{r} f(\vec{r})\psi(\vec{r})|^2\rangle_\Omega ,$$

while in a magnetic system it similarly represents the mean-square weighted magnetization of the subdomain. As at least a partial answer to (a) for a Bose system (with $\eta = 0$) we will establish the bounds[7] [see (4.26) and (4.38)]

$$\Psi_\Omega\{f\,|\,\Gamma\} \le \Phi_2\{\ln[V(\Gamma)/v_0]\}^{-1/2} = \Phi_2'\{T\ln[V(\Gamma)/v_0]\}^{-1/2} \quad \text{for } d=2$$

$$\le \Phi_1[V(\Gamma)/v_T]^{-1/4} = \Phi_1'[TV(\Gamma)]^{-1/4} \quad \text{for } d=1 \qquad (2.24)$$

as $V(\Gamma)\to\infty$. Explicit expressions are given for the constants Φ_d [(4.26) and (4.38)], v_0 [(4.39)], and v_T [(4.17) and (4.18)]. The coefficients Φ_d' are then slowly varying functions of intensive parameters, and the main temperature dependence is exhibited in (2.24). These bounds remain valid if the thermodynamic limit $V(\Omega)\to\infty$ is first taken on the left-hand side, and also if a symmetry-breaking field $\eta(\vec{r})$ is imposed everywhere *outside* the subdomain Γ. Roughly speaking, this result proves that $\sigma_\infty(\vec{r},\vec{r}\,')$ must decrease faster than $1/\ln|\vec{r}-\vec{r}\,'|$ for $d=2$ or $|\vec{r}-\vec{r}\,'|^{-1/2}$ for $d=1$. [More precise statements concerning the decrease of $\sigma_\infty(\vec{r},\vec{r}\,')$ are proved in Sec. V.] This is *not* fast enough to ensure that $\sigma_\infty(\vec{0},\vec{r})$ is integrable (over an infinite domain), so that "weak long-range order" or an infinite "anomalous susceptibility" are not ruled out. If, for the case $\Gamma=\Omega$, the domain has sufficiently regular shape so that $f(\vec{r}) = e^{i\vec{K}\cdot\vec{r}}$ can be regarded as a "single-particle state" of a Bose system, then (2.24) asserts that there cannot be macroscopic occupancy of the state $\vec{K}$, i.e., $n_{\vec{K}}/N\to 0$.

For an isotropic or axially symmetric magnetic system, (2.24) is still valid [with appropriately modified definitions (2.23)] provided the exchange interactions decrease sufficiently rapidly with spin separation. [In essence it is sufficient that the $J_\alpha(\vec{r},\vec{r}\,')$ have finite second moments.] If the coupling decreases more slowly, (2.24) has to be modified and, indeed, when the decay is sufficiently slow, no asymptotically decreasing bound can be obtained by our methods (see paper II).

The analysis is based, as in previous arguments,[1,3-5] on Bogoliubov's inequality[2]

$$\tfrac{1}{2}\langle\{\hat{A},\hat{A}^\dagger\}\rangle \ge k_BT\,|\langle[\hat{C},\hat{A}]\rangle|^2/\langle[[\hat{C},\hat{\mathcal{H}}_\Omega],\hat{C}^\dagger]\rangle, \qquad (2.25)$$

which is valid for any Hermitian Hamiltonian and for operators not necessarily Hermitian, but restricted only to the extent that the appropriate thermal averages and commutators must exist. (As usual k_B is Boltzmann's constant.) The reader is referred to the literature[1,3,4] for various proofs of Bogoliubov's inequality.

The first step in the analysis of a Bose system is the introduction of the subdomain $\Gamma\subset\Omega$ and of its "corridor" Δ. In Sec. III a basic inequality is developed by applying Bogoliubov's inequality to Γ with essentially the standard choice for the operator $\hat{C}$ in terms of an arbitrary wave number $\vec{k}$. However, the operator $\hat{A}$ is chosen to be bilinear[6] in $\psi^\dagger(\vec{r})$ and $\psi(\vec{R})$ (the usual choice[3-5] being linear). The inequality is then integrated and summed over a suitable choice of values of $\vec{k}$: The estimation of the resulting integrals is more complex than in the earlier arguments and, at one point, entails the use of the compressibility-fluctuation relation to bound density fluctuations in a subvolume. The final result is (3.37). In Sec. IV this inequality is analyzed in various limiting cases in which $V(\Gamma)$ becomes large in order to establish the results quoted above. Some numerical examples appropriate to superfluid helium illustrate the strength (or weakness) of the basic inequality. Finally, in Sec. V the conclusions that can be drawn about the pointwise behavior of $\sigma_\Omega(\vec{r},\vec{r}\,')$ are discussed. As already mentioned, the analysis for spin systems is reserved for Paper II.

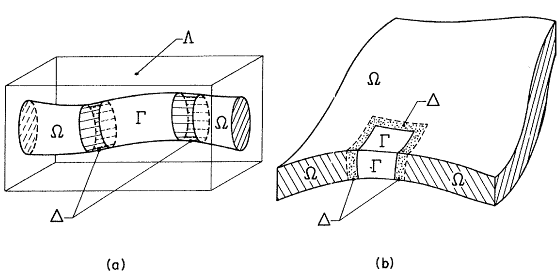

FIG. 1. Sectioned domain Ω showing a "slice" subdomain Γ and surrounding corridor Δ. (a) One-dimensional case showing, in addition, the enclosing "box" Λ. (b) Two-dimensional case; enclosing "box" Λ not shown.

III. BASIC INEQUALTIY FOR BOSE SYSTEMS

A central idea of our analysis is that Bogoliubov's inequality may be usefully applied to a subdomain $\Gamma\subset\Omega$ rather than to the whole system, provided one is able to bound any ordering effects associated with the "surface" of Γ. To discuss these surface effects we construct a "corridor" Δ around Γ which consists of all those points of $\Omega-\Gamma$ which lie within a distance $(1+\delta)b$ ($\delta>0$) of the interior of Γ. The volume $V(\Delta)$ is a measure of the surface of Γ and we will require that

$$V(\Delta)/V(\Gamma)\to 0 \quad \text{when } V(\Gamma)\to\infty . \qquad (3.1)$$

For a system of restricted dimensionality d this means that Γ must be a "slice" domain in the sense, illustrated in Fig. 1, that most of the boundary of Γ is common with part of the boundary of Ω. Simple examples are: (i) if, for $d=1$, the cylinder containing Ω is parallel to the x axis,

$$\Gamma=\{\vec{r}\subset\Omega:\ |x|\leq x_0\};$$

(ii) if, for $d=2$, the planes containing Ω are perpendicular to the z axis,

$$\Gamma=\{\vec{r}\subset\Omega: |x|\leq x_0 |y|\leq y_0\}.$$

To apply Bogoliubov's inequality to a Bose system we choose

$$\hat{C}=\int d\vec{r}\, g(\vec{r})\,\rho(\vec{r})\ , \tag{3.2}$$

with

$$g(\vec{r})=a(\vec{r})\,e^{i\vec{k}\cdot\vec{r}}\ , \tag{3.3}$$

where, as stressed previously, $\vec{k}$ may be quite arbitrary.[5] The smoothly varying real amplitude function $a(\vec{r})$ is constructed to have the following properties:

(i) $a(\vec{r})\equiv 1$ for $\vec{r}\subset\Gamma$,

(ii) $a(\vec{r})\equiv 0$ for $\vec{r}$ outside $\Gamma\cup\Delta$,

(iii) twice continuously differentiable,

(iv) $a(\vec{r})\leq 1$ and $|\nabla a|\leq b^{-1}$ for $\vec{r}\subset\Delta$.

Since the width of the corridor Δ exceeds b by a finite amount, there is no difficulty in satisfying conditions (iii) and (iv).[18]

With this choice of $\hat{C}$, which is the usual one except for the factor $a(\vec{r})$, we obtain

$$\langle\,[[\hat{C},\hat{\mathcal{H}}_\Omega],\hat{C}^\dagger]\rangle=(\hbar^2/m)\int_{\Gamma\cup\Delta}d\vec{r}\,|\nabla g|^2\langle\,\rho(\vec{r})\rangle + \int_{\Gamma\cup\Delta}d\vec{r}\,|g(\vec{r})|^2\,[\eta(\vec{r})\,\langle\,\psi^\dagger(\vec{r})\rangle + \eta^*(\vec{r})\,\langle\,\psi(\vec{r})\rangle\,]. \tag{3.4}$$

For brevity we have dropped the subscript Ω on the expectation brackets $\langle\cdot\rangle$, which will be allowed to denote either canonical ($\eta\equiv 0$) or grand-canonical averages. Now notice that for $\vec{r}$ in Γ the factor $|\nabla g|^2$ reduces simply to k^2, while in Δ it becomes

$$|\nabla g|^2=k^2+|\nabla a|^2\leq k^2+b^{-2}, \tag{3.5}$$

by the assumption (iv) on $a(\vec{r})$. Similarly, we have

$$\begin{aligned}|g(\vec{r})|^2&=1 &&\text{for } \vec{r}\subset\Gamma\\ &=|a(\vec{r})|^2 &&\text{for } \vec{r}\subset\Delta\ .\end{aligned} \tag{3.6}$$

Thus, if

$$N(\Xi)=\int_\Xi d\vec{r}\,\langle\,\rho(\vec{r})\rangle \tag{3.7}$$

denotes the mean number of particles in a subdomain Ξ of Ω, the double commutator is bounded by

$$\langle\,[[\hat{C},\hat{\mathcal{H}}_\Omega],\hat{C}^\dagger]\rangle\leq(\hbar^2/m)\,N(\Gamma\cup\Delta)\,(k^2+\lambda)\ , \tag{3.8}$$

where

$$\lambda=\gamma b_0^{-2}=\gamma b^{-2}+\gamma(m/\hbar^2)\ H\{\eta;\Delta\} + (1-\gamma)\,(m/\hbar^2)\,H\{\eta;\Gamma\}, \tag{3.9}$$

in which

$$\gamma=N(\Delta)/N(\Gamma\cup\Delta)\ , \tag{3.10}$$

and

$$H\{\eta;\Xi\}=2[N(\Xi)]^{-1}\int_\Xi d\vec{r}\,|a(\vec{r})|^2\,|\mathrm{Re}\{\eta(\vec{r})\langle\psi^\dagger(\vec{r})\rangle\}|\ . \tag{3.11}$$

If we choose Γ to be the whole domain Ω [so that $V(\Delta)$ and $N(\Delta)$ vanish], only the third term in (3.9) remains. If, furthermore, the anomalous field $\eta(\vec{r})$ itself is absent, we have simply

$$\lambda\equiv 0\ \text{ for } \Gamma=\Omega,\ \ \eta(\vec{r})\equiv 0. \tag{3.12}$$

More generally, we note that if $V(\Gamma)\to\infty$, we will have $\gamma\to 0$, provided the local density $\langle\,\rho(\vec{r})\rangle$ remains bounded, which we will always assume. If the anomalous field $\eta(\vec{r})$ remains of order unity in Δ, then [noting that $|\langle\,\psi^\dagger(\vec{r})\rangle\,|^2\leq\langle\,\rho(\vec{r})\rangle$, which follows by Schwarz's inequality] the first two terms making up λ will vanish, at least linearly, with γ. On the other hand, the third term might remain of order unity unless the field $\eta(\vec{r})$ *in the subdomain* Γ becomes uniformly small. In the following we will assume, unless especially mentioned, that the anomalous field in Γ itself, if present at all, is always reduced at a rate proportional to γ so that b_0 remains bounded away from zero.

Next we choose[6]

$$\hat{A}=\int d\vec{r}\int d\vec{R}\,f^*(\vec{r})\,e^{-i\vec{k}\cdot\vec{r}}f(\vec{R})\,\psi^\dagger(\vec{r})\,\psi(\vec{R})\ , \tag{3.13}$$

where $f(\vec{r})$ is restricted only by

$$\begin{aligned}|f(\vec{r})|&=1\ \ \text{for } \vec{r}\subset\Gamma\\ &=0\ \ \text{otherwise.}\end{aligned} \tag{3.14}$$

The numerator in the Bogoliubov inequality is then just

$$|\langle\,[\hat{C},\hat{A}]\rangle\,|^2=[V(\Gamma)\,(n\{f\}-n\{fe^{i\vec{k}\cdot\vec{r}}\})]^2, \tag{3.15}$$

where we have written $n\{f\}$ for $n_\Omega\{f|\Gamma\}$, the latter being defined in (2.23).

To find the consequences of the restricted dimensionality of the system we suppose[5] Ω is contained in the rectangular "box" Λ described in Sec. II. Recall that Λ defines the domain between two infinite parallel planes of fixed finite separation D_z ($d=2$), or the region within an infinite cylinder of finite rectangular cross section D_yD_z ($d=1$). Then we may introduce a complete set of wave vectors

$$\vec{k}=(\vec{k}_\parallel;\vec{k}_\perp)=(k_\parallel;2\pi l_y/D_y,\ 2\pi l_z/D_z),\quad d=1$$

$$= (k_{\parallel,x}, k_{\parallel,y}; 2\pi l_z/D_z), \quad d=2 \tag{3.16}$$

with $\vec{k}_\parallel$ a continuous vector, and the integers

$$l_y, l_z = 0, \pm 1, \pm 2, \ldots, \tag{3.17}$$

specifying the discrete vectors $\vec{k}_\perp$ compatible with the box Λ. Defining the fixed "cross section" S_d of Λ to be

$$S_d = D_y D_z \quad \text{for } d=1$$
$$= D_z \quad \text{for } d=2, \tag{3.18}$$

we have

$$S_d^{-1}(2\pi)^{-d}\sum_{\vec{k}_\perp}\int d\vec{k}_\parallel\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')} = \delta(\vec{r}-\vec{r}\,') \quad \text{for } \vec{r} \text{ and } \vec{r}\,' \text{ in } \Lambda. \tag{3.19}$$

The whole inequality (2.25) may now be integrated over all $\vec{k}_\parallel$ subject to

$$\vec{k}_\perp \equiv 0 \quad \text{and} \quad \kappa \le |\vec{k}_\parallel| \le \kappa^\dagger. \tag{3.20}$$

Notice that nonpositive terms on the right-hand side of (2.25) and non-negative terms on the left-hand side can be integrated over all $\vec{k}_\parallel$ without restriction and further summed over all the (allowed) $\vec{k}_\perp$, since these operations will only further strengthen the inequality. If we denote the right-hand side of (2.25) by $R(\vec{k}_\parallel, \vec{k}_\perp)$ and indicate integration subject to (3.20) by a subscript κ, we find

$$R = (2\pi)^{-d}\int d\vec{k}\int_{\kappa_\parallel} R(\vec{k}_\parallel, 0)$$
$$\ge \frac{mk_BT}{\hbar^2}\,\frac{V(\Gamma)^2}{N(\Gamma\cup\Delta)}\,[n^2\{f\}I(\kappa,\lambda) - 2n\{f\}J(\kappa,\lambda)], \tag{3.21}$$

where the inequality results because the positive term involving $n^2\{fe^{i\vec{k}\cdot\vec{r}}\}$ has been discarded. The positive function I is given by

$$I(\kappa,\lambda) = (2\pi)^{-d}\int_\kappa \frac{d\vec{k}_\parallel}{k_\parallel^2+\lambda}$$
$$= (1/\pi\sqrt{\lambda})[\tan^{-1}(\kappa^\dagger/\sqrt{\lambda}) - \tan^{-1}(\kappa/\sqrt{\lambda})], \quad d=1$$
$$= (1/4\pi)\ln[(\kappa^{\dagger 2}+\lambda)/(\kappa^2+\lambda)], \quad d=2 \tag{3.22}$$

so that as $\lambda/\kappa^{\dagger 2}\to 0$ with $\kappa=0$ we have

$$I(0,\lambda) \approx \tfrac{1}{2}\lambda^{-1/2}[(2/\pi)\tan^{-1}(\kappa^\dagger/\sqrt{\lambda})], \quad d=1$$
$$\approx (1/4\pi)\ln(\kappa^{\dagger 2}/\lambda), \quad d=2. \tag{3.23}$$

Conversely, if $\lambda=0$, we have as $\kappa/\kappa^\dagger \to 0$

$$I(\kappa,0) \approx (1/\pi)\kappa^{-1}, \quad d=1$$
$$\approx (1/2\pi)\ln(\kappa^\dagger/\kappa), \quad d=2. \tag{3.24}$$

The second integral J in (3.21) is defined by

$$J(\kappa,\lambda) = (2\pi)^{-d}\int_\kappa d\vec{k}_\parallel \frac{n\{fe^{i\vec{k}\cdot\vec{r}}\}}{k_\parallel^2+\lambda}. \tag{3.25}$$

This can be bounded by (i) using the positivity of $n\{\cdot\}$, (ii) extending the integral to all $\vec{k}_\parallel$ and summing on all $\vec{k}_\perp$, and (iii) applying (3.19). We thus obtain the sequence of inequalities

$$J(\kappa,\lambda) \le (\kappa^2+\lambda)^{-1}\sum_{\vec{k}_\perp}(2\pi)^{-d}\int_\kappa d\vec{k}_\parallel\, n\{fe^{i\vec{k}\cdot\vec{r}}\}$$
$$\le S_d(\kappa^2+\lambda)^{-1}N(\Gamma)/V(\Gamma) = S_d\rho_\Omega(\Gamma)(\kappa^2+\lambda)^{-1}, \tag{3.26}$$

where $\rho_\Omega(\Gamma)$ is the mean density in the subdomain Γ. The resulting estimate can be used to further strengthen the inequality (3.21).

On the left-hand side, $L(\vec{k}_\parallel, \vec{k}_\perp)$ of Bogoliubov's inequality, we write

$$\langle\{\hat{A}^\dagger, \hat{A}\}\rangle = 2\langle\hat{A}\hat{A}^\dagger\rangle + \langle[\hat{A}^\dagger, \hat{A}]\rangle,$$

and extend the integral (and sum) to all $\vec{k}$ on the (positive) first term only. (This decomposition is needed to avoid difficulties with certain singular terms.) On dropping a negative term involving $n\{fe^{i\vec{k}\cdot\vec{r}}\}$ and using the commutation relations, the result can be written

$$L = (2\pi)^{-d}\int_\kappa d\vec{k}_\parallel\, L(\vec{k}_\parallel, 0)$$
$$\le S_d[Q\{f\} + \rho(\Gamma)V(\Gamma)^2 - V(\Gamma)n\{f\}] + \tfrac{1}{2}V(\Gamma)^2 n\{f\}F_d, \tag{3.27}$$

where

$$F_d = (2\pi)^{-d}\int_\kappa d\vec{k}_\parallel = \frac{\kappa^{\dagger d} - \kappa^d}{\pi d^2}, \quad d=1,2 \tag{3.28}$$

and where the functional $Q\{f\}$ is defined by

$$Q\{f\} = \int_\Gamma d\vec{r}\int_\Gamma d\vec{R}\int_\Gamma d\vec{R}'\, f^*(\vec{R}')f(\vec{R}) \times \langle\rho(\vec{r})\psi^\dagger(\vec{R}')\psi(\vec{R})\rangle. \tag{3.29}$$

When $\Gamma=\Omega$, the integral over the operator $\rho(\vec{r})$ in this expression just yields the total number operator $\hat{N}_\Omega$, which, if we employ a *canonical* ensemble, is, as explained, merely proportional to the identity operator. The expectation value in (3.29) thus simplifies, and we obtain the result

$$Q\{f\} = N(\Omega)V(\Omega)n\{f\}$$
$$= V(\Omega)^2\rho_\Omega(\Omega)n\{f\}, \quad \Gamma=\Omega. \tag{3.30}$$

However, when Γ is properly contained in Ω, the functional Q cannot be treated so simply since the number of particles in Γ is not conserved. The point at issue is essentially the size of the natural fluctuations of the number of particles in Γ. This may be estimated via the well-known compressibility sum rule, which, for a finite subdomain, may be written

$$\int_\Gamma d\vec{r}\int_\Gamma d\vec{r}'\,[\langle\rho(\vec{r})\rho(\vec{r}')\rangle-\langle\rho(\vec{r})\rangle\langle\rho(\vec{r}')\rangle]$$
$$=k_BT\rho_\Omega(\Gamma)^2V(\Gamma)K_T[1+\epsilon(\Gamma)], \quad (3.31)$$

where we assume that K_T, the isothermal bulk compressibility of the system, is bounded.[19] The term $\epsilon(\Gamma)$ normally represents a surface-to-volume correction and will vanish as $V(\Gamma)\to\infty$ in the thermodynamic limit. Now the thermal averages admit a Schwarz inequality, which, if

$$L_{XY}=\langle\hat{X}\hat{Y}\rangle-\langle\hat{X}\rangle\langle\hat{Y}\rangle=\langle(\hat{X}-\langle\hat{X}\rangle)(\hat{Y}-\langle\hat{Y}\rangle)\rangle, \quad (3.32)$$

may be written

$$|L_{XY}|^2\le L_{XX}L_{YY}. \quad (3.33)$$

In the Appendix these relations are used with the identifications

$$\hat{X}=\int_\Gamma d\vec{r}\,\rho(\vec{r}), \quad (3.34)$$

$$\hat{Y}=\int_\Gamma d\vec{R}\int_\Gamma d\vec{R}'f^*(\vec{R}')f(R)\psi^\dagger(\vec{R}')\psi(\vec{R}), \quad (3.35)$$

to prove, with the aid of (3.31), that

$$Q\{f\}\le V(\Gamma)^2\rho_\Omega(\Gamma)n\{f\}+V(\Gamma)^{5/2}\rho_\Omega(\Gamma)^2\{k_BTK_T[1+\epsilon(\Gamma)]\}^{1/2}\{1+O[V(\Gamma)^{-1/2}]\}. \quad (3.36)$$

Evidently the first term represents the analog of (3.30) above, while the second and dominant term is the correction due to the finite volume fluctuations.

Finally, on collecting terms and using the definition (2.23), our basic inequality may be written

$$q_0I(\kappa,\lambda)\Psi^4\le\Psi^2\left[q_1+\frac{q_2}{V(\Gamma)[\kappa^2+\lambda]}\right]+\frac{q_3}{[V(\Gamma)]^{1/2}}+\frac{q_4}{V(\Gamma)}, \quad (3.37)$$

where $\Psi=\Psi_\Omega\{f|\Gamma\}$ and q_0 to q_4 are intensive parameters depending on temperature and density. Explicitly, we have

$$q_0=(1-\gamma)[mk_BT/\hbar^2\rho_\Omega(\Gamma)S_d], \quad (3.38)$$

$$q_1=\rho_\Omega(\Gamma)+(\kappa^{\dagger d}-\kappa^d)/2\pi d^2S_d-1/V(\Gamma), \quad (3.39)$$

$$q_2=2(1-\gamma)^2(mk_BT/\hbar^2), \quad (3.40)$$

$$q_3=[\rho_\Omega(\Gamma)]^2\{k_BTK_T[1+\epsilon(\Gamma)]\}^{1/2}, \quad (3.41)$$

$$q_4=\rho_\Omega(\Gamma), \quad (3.42)$$

and, to recapitulate, $I(\kappa,\lambda)$ is defined by (3.22)–(3.24), λ and γ by (3.9)–(3.12), and S_d by (3.18). In the special case $\Gamma=\Omega$ we may set $q_3=0$. We will be mainly interested in the case where $V(\Omega)$ and $V(\Gamma)$ are large so that $\gamma\ll1$, $\epsilon(\Gamma)\ll1$, and $\rho_\Omega(\Gamma)\to\rho_\Gamma$. We may also choose $\kappa^\dagger\gg\kappa$. In these circumstances the q_i approach simple limits q_i^∞ obtained by making the replacements γ, ϵ, κ, $1/V(\Omega)\Rightarrow0$ and $\rho_\Omega(\Gamma)\Rightarrow\rho_\Gamma$.

We may linearize the quadratic inequality (3.37) for $\xi=\Psi^2$ by noting that if ξ_1 is the (positive) root of the corresponding quadratic equality, we must have $\Psi^2\le\xi_1$. If, in addition, the expression for the root ξ_1 is simplified by using the inequality $(1+\zeta)^{1/2}\le1+\frac{1}{2}\zeta$, we finally obtain

$$[\Psi_\Omega\{f|\Omega\}]^2\le\frac{q_1(X)}{q_0I(\kappa,\lambda)}+\frac{1}{q_1(X)}\left(\frac{q_3}{[V(\Gamma)]^{1/2}}+\frac{q_4}{V(\Gamma)}\right), \quad (3.43)$$

where

$$q_1(X)=q_1+q_2/X,\quad X(\Gamma)=V(\Gamma)(\kappa^2+\lambda). \quad (3.44)$$

IV. ANALYSIS OF BOSE INEQUALITY

In this section we derive the results quoted in Sec. II from the basic inequality (3.37) for a Bose system. We consider first the case where Γ is chosen to be Ω in order to prove that $\Psi_\sigma\equiv0$ in the thermodynamic limit and to show how the *long* long-range order vanishes as $V(\Omega)\to\infty$.

A. $\Gamma=\Omega$

In this case q_3 vanishes, and there are two possibilities we may consider.

1. η *Fixed*, $V(\Omega)\to\infty$

In closest analogy with the previous arguments[3,5] we may first suppose that some fixed uniform or periodic field, say,

$$\eta(\vec{r})=\eta_0e^{i\vec{K}\cdot\vec{r}}, \quad (4.1)$$

is imposed so that $\lambda\propto\eta_0$ does not vanish as the thermodynamic limit $V(\Omega)\to\infty$ is taken [see (3.9)–(3.11)]. In this limit we have by (2.23) and (2.16)

$$\Psi=\Psi_\Omega\{f|\Omega\}\to\Psi_{\sigma\{f\}}(\eta_0) \quad (4.2)$$

(with an obvious extension of the previous notation), while with the choice $\kappa=0$ the inequality (3.43) yields

$$[\Psi_{\sigma\{f\}}(\eta_0)]^2\le q_1^\infty/q_0^\infty I(0,\lambda). \quad (4.3)$$

Now, as the field amplitude η_0 vanishes, we have $\lambda\to0$ and $I(0,\lambda)\to\infty$ (for $d=1$ or 2). Hence we conclude that

$$\lim_{\eta\to 0}\Psi_{\sigma\{f\}}\{\eta\}\equiv 0. \tag{4.4}$$

Alternatively, in response to question (b) of the Introduction, we may avoid the use of the symmetry-breaking field altogether.

2. $\eta\equiv 0$

In this case λ vanishes identically and the basic inequality (3.43) becomes

$$\Psi^2\le\frac{q_1}{q_0 I(\kappa,0)}\left[1+\frac{q_2}{q_1 V(\Omega)\kappa^2}\right]+\frac{q_4}{q_1(X)\,V(\Omega)}, \tag{4.5}$$

where, now, $X=V(\Omega)\kappa^2$. Now we are free to choose the cutoff κ as a function of $V(\Omega)$ so as to yield the best inequality. To this end let us consider first $d=1$ when, by (3.24), $I(\kappa,0)\sim\kappa^{-1}$, and then, tentatively, ignore the last term in (4.5). By minimization at fixed $V(\Omega)$ the best choice is seen to be

$$\kappa^2=q_2/q_1 V(\Omega). \tag{4.6}$$

With this value we have $q_1(X)=2q_1$ and we find from (3.24) that for large $V(\Omega)$

$$[\Psi_\Omega\{f\,|\,\Omega\}]^2\le\frac{2\pi(q_1^\infty q_2^\infty)^{1/2}}{q_0^\infty[V(\Omega)]^{1/2}}+\frac{q_4^\infty}{2q_1^\infty V(\Omega)},\quad d=1. \tag{4.7}$$

Asymptotically the second term is negligible, and hence Ψ decreases as $V(\Omega)^{-1/4}$, which is an indication of how the *long* long-range order falls to zero. If the thermodynamic limit is now taken with $f=1$, we find directly that $\Psi_\sigma\equiv 0$, as stated in Sec. II. For more general functions, the result precludes macroscopic occupancy of any "single-particle state" $f(\vec{r})$.

The same choice (4.6) is also quite satisfactory when $d=2$, where, for large $V(\Omega)$, it leads to

$$[\Psi_\Omega\{f\,|\,\Omega\}]^2\le\frac{8\pi(q_1^\infty/q_0^\infty)}{\ln[V(\Omega)\kappa^{\dagger 2}q_1^\infty/q_2^\infty]}+\frac{q_4^\infty}{2q_1^\infty V(\Omega)},\qquad d=2. \tag{4.8}$$

Again the first term dominates asymptotically so that Ψ decreases slowly as $[\ln V(\Omega)]^{1/2}$. This is sufficient, however, to prove that Ψ_σ again vanishes. As a matter of fact, an asymptotically stronger bound [replacing 8π by 4π in (4.8)] may be obtained by taking $\kappa^2\propto[\ln V(\Omega)]/V(\Omega)$, but for the present purpose this is not necessary.

Lastly, we remark that if the field (4.1) acts on Ω but its amplitude is reduced uniformly to zero as $V(\Omega)\to\infty$, then, once again, it follows from arguments similar to those above that $\Psi_\sigma\equiv 0$ in this (special) thermodynamic limit.

B. $\Gamma\subset\Omega$

When Γ is properly contained in Ω, the coefficient q_3 no longer vanishes, and the analysis must be modified. We first note that for large $V(\Gamma)$ and $V(\Omega)$ and *fixed* b, we have from (3.9)–(3.11)

$$\lambda^{-1}=\frac{b_0^2}{\gamma}\approx\frac{b_0^2\rho_\Gamma V(\Gamma)[1+V(\Delta)/V(\Gamma)]}{\rho_\Delta\,V(\Delta)}$$

$$\approx\frac{b_0^2}{c_d b}\left[\frac{V(\Gamma)}{S_d}\right]^{1/d}[1+s(b)],\quad d=1,2 \tag{4.9}$$

where we have assumed that $\rho_{\Gamma\cup\Delta}\approx\rho_\Gamma\approx\rho_\Delta$, and where we write

$$s(b)=V(\Delta)/V(\Gamma)=c_d b\,[S_d/V(\Gamma)]^{1/d},\quad d=1,2 \tag{4.10}$$

where c_1 and c_2 are constants of order unity which depend on the shape of Γ. (If the "side" boundaries of Ω and Γ coincide with those of Λ, we have $c_1\gtrsim 2$ and $c_2\gtrsim 2\sqrt{\pi}$.) Since λ does not vanish for finite $V(\Gamma)$, we may choose $\kappa=0$ with no loss of generality. (Note that the previously optimal value $\kappa^2\propto 1/V$ is now comparable to or less than λ.) We first consider the case $d=1$.

1. $d=1$

From (4.9) and (4.10) we have

$$X=V(\Gamma)\lambda\approx c_1 S_1 b/b_0^2[1+s(b)], \tag{4.11}$$

and the basic inequality (3.43) becomes

$$[\Psi_\Omega\{f\,|\,\Gamma\}]^2\le\frac{2q_1(X)(c_1 bS_1)^{1/2}[1+s(b)]^{-1/2}}{q_0 b_0[(2/\pi)\tan^{-1}(\kappa^\dagger/\sqrt{\lambda})][V(\Gamma)]^{1/2}}+\frac{1}{q_1(X)}\left[\frac{q_3}{[V(\Gamma)]^{1/2}}+\frac{q_4}{V(\Gamma)}\right]. \tag{4.12}$$

Now let us hold b and b_0 fixed so that (4.10) implies $s(b)\to 0$ as $V(\Gamma)\to\infty$. [This is consistent with our assumption $\gamma\to 0$ as discussed after (3.12).] The parameter $\kappa^\dagger$ is still at our disposal and an optimal choice will be discussed below. However, in order to show that (4.12) implies that the short-range order, as measured by $\Psi_\Omega\{f\,|\,\Gamma\}$, decreases like $[V(\Gamma)]^{-1/4}$ (as stated in Sec. II), it is clearly sufficient to choose $\kappa^\dagger$ constant (so that $\kappa^\dagger/\sqrt{\lambda}\to\infty$).

We now restrict attention to the case where $\eta(\vec{r})$ *vanishes in* Γ *and* Δ. We then have $b=b_0$ [see (3.9)]; and the inequality can be optimized with respect to choice of b. One finds that

$$b=b^*(T)\equiv q_1 c_1 S_1/q_2\propto 1/T \tag{4.13}$$

is not too far from optimal.[20] With this choice we find $\gamma\sim 1/V(\Gamma)$ [see (3.9) and (4.9)]. In addition, on using (4.9) and (4.10) we see that for large $V(\Gamma)$

$$q_1(X)\approx 2q_1^\infty s_0,\quad s_0=1+\tfrac{1}{2}s(b^*). \tag{4.14}$$

For fixed cross section S_1 the factor s_0 is asymptotically equal to unity but to see what happens in case S_1 becomes large, it is useful to retain it. Our result can then be written

$$[\Psi_\Omega\{f\,|\,\Gamma\}]^2 \le \rho_\Gamma\,[v_0/V(\Gamma)]^{1/2}, \qquad d=1 \quad (4.15)$$

where the *scale volume* v_0 is given by

$$\rho_\Gamma v_0^{1/2} \simeq \frac{4(q_1^\infty q_2^\infty s_0)^{1/2}}{q_0[(2/\pi)\tan^{-1}(\kappa^\dagger/\sqrt{\lambda})]} + \frac{s_0^{1/2}}{2\rho_\Gamma}\left[q_3^\infty + \frac{q_4^\infty}{[V(\Gamma)]^{1/2}}\right], \quad \eta=0 \quad (4.16)$$

which has been simplified by using $s_0^{-1} \le s_0^{1/2} \le [1+s(b^*)]^{1/2}$ and $\rho_\Gamma \le q_1^\infty$. In order to express this result in more transparent form we introduce a characteristic thermal volume

$$v_T = \Lambda_T D_y D_z\,, \quad (4.17)$$

where the thermal de Broglie wavelength is, as usual,

$$\Lambda_T = (2\pi\hbar^2/mk_BT)^{1/2}\,. \quad (4.18)$$

The mean number of particles in this thermal volume (which is effectively a slice domain of length Λ_T) is just

$$N_T = \rho_\Gamma v_T = \rho_\Gamma \Lambda_T D_y D_z\,, \quad d=1\,. \quad (4.19)$$

In terms of these parameters we find for large $V(\Gamma)$ [using (3.9) and (4.9)]

$$s_0 = 1 + \tfrac{1}{2}s(b^*) = 1 + (c_1^2/8\pi)[N_T v_T/V(\Gamma)] \simeq (1-\gamma)^{-1/2} \quad (4.20)$$

and

$$\lambda \simeq 4\pi/\Lambda_T^2 N_\Gamma, \quad \text{with } N_\Gamma = \rho_\Gamma V_\Gamma\,. \quad (4.21)$$

By (3.38) to (3.42) the only dependence of (4.16) on $\kappa^\dagger$ is through the factor

$$t = (q_1^\infty/\rho_\Gamma)^{1/2}/(2/\pi)\tan^{-1}x \quad \text{with } \kappa^\dagger = x\sqrt{\lambda}. \quad (4.22)$$

For this we find

$$t \simeq [1 + x(\pi N_\Gamma N_T^2)^{-1/2}]^{1/2}\,[1 + 2/\pi x]\,,$$

provided both brackets are close to unity. The optimum choice of x, and thence of $\kappa^\dagger$, is hence found to be close to $2(N_\Gamma N_T^2/\pi)^{1/4}$, so that

$$t \simeq 1 + 2/(\pi^3 N_\Gamma N_T^2)^{1/4}\,. \quad (4.23)$$

Finally, if we define the dimensionless compressibility ratio

$$\chi = K_T/K_T^{\rm ideal} = \rho k_B T K_T\,, \quad (4.24)$$

and use the definitions (3.38), etc., the scale volume is given by

$$v_0 \simeq (16/\pi) N_T v_T s_0^5 t^2\,[1 + (\pi^{1/2}/16N_T)(\chi^{1/2} + N_\Gamma^{-1/2})]^2\,. \quad (4.25)$$

The last factor will be close to unity in most cases of interest ($\chi \ll 1$ for a condensed phase, and $N_\Gamma \gg 1$). If we similarly neglect the deviation of s_0 and t from unity, the result (4.15) becomes

$$\Psi_\Omega\{f\,|\,\Gamma\} \le (2/\pi^{1/4})\,\rho_\Gamma^{1/2} N_T^{1/4}\,[v_T/V(\Gamma)]^{1/4} \le [32 D_y^2 D_z^2 \hbar^2 \rho_\Gamma^3/mk_BTV(\Gamma)]^{1/4}. \quad (4.26)$$

Also, if Γ is a rectangular domain of length L_Γ and sides D_y, D_z, we have

$$\Psi_\Omega\{f\,|\,\Gamma\} \le \rho_\Gamma^{1/2}(16N_T\Lambda_T/\pi L_\Gamma)^{1/4} = \rho_\Gamma^{1/2}(r_0/L_\Gamma)^{1/4}. \quad (4.27)$$

Since we always have $\Psi < \rho^{1/2}$, this inequality has no force until L_Γ exceeds $r_0 = (16/\pi)N_T\Lambda_T$. As an illustration we may consider liquid helium of normal density at, say, 2 °K, which is about 0.2 °K below the bulk Λ point. If the helium is confined in a rectangular channel of width $D_y = D_z = 25$ Å, then $\Lambda_T \simeq 6$ Å and $N_T \simeq 80$. Then the inequality has effect only when L_Γ exceeds $r_0 \simeq 2\times10^3$ Å $= 2\times10^{-5}$ cm. For $L_\Gamma = 1$ cm it would yield $\rho_\Gamma^{-1}\Psi_\Omega^2\{f\,|\,\Gamma\} \le 0.004$. Of course, the inequality is stronger at higher temperatures, lower densities, and for liquids of higher molecular weight.

We may note that the inequality (4.27) contains the factor D_yD_z/L_Γ, which becomes large as the cross section increases. Conversely, we can show generally that $\Psi_\Omega\{f\,|\,\Gamma\}$ vanishes provided that $D_yD_z/L_\Gamma \to 0$. The significance of this factor can be understood as follows. Suppose that owing to some thermal fluctuation, or other agency, the phase φ of the order parameter is twisted uniformly by a half turn over the length of Γ so that the gradient is $\nabla\varphi = \pi/L_\Gamma$. The associated increase in energy density is proportional to $\rho_\Gamma(\hbar^2/2m)(\nabla\varphi)^2$. (For the correct answer one should use the superfluid density, ρ_s, in place of ρ_Γ.) Since $V(\Gamma) = D_yD_zL_\Gamma$, the total increment in energy is just $\Delta E = (h^2/8m) \times \rho_\Gamma(D_yD_z/L_\Gamma)$. The ratio of this to the mean thermal energy k_BT is proportional to

$$\Lambda_T^2 \rho_\Gamma D_y D_z/L_\Gamma = N_T\Lambda_T/L_\Gamma\,.$$

Thus the right-hand side of (4.27) varies as $(\Delta E/k_BT)^{1/4}$, which is a direct measure of the ease of exciting thermally a fluctuation which can destroy the phase coherence along the length of Γ.

2. $d=2$

For a two-dimensional system (4.11) becomes

$$X = V(\Gamma)\lambda \simeq c_2 b\,[S_2 V(\Gamma)]^{1/2}/b_0^2\,[1 + s(b)], \quad (4.28)$$

and on using (3.23) the basic inequality (3.43) yields

$$[\Psi_\Omega\{f\,|\,\Gamma\}]^2 \le \frac{4\pi q_1(X)}{q_0 \ln(\kappa^{\dagger 2}/\lambda)} + \frac{1}{q_1(X)}\left(\frac{q_3}{[V(\Gamma)]^{1/2}} + \frac{q_4}{V(\Gamma)}\right). \quad (4.29)$$

For fixed b and b_0 we see from (4.28) that λ^{-1} diverges as $[V(\Gamma)]^{1/2}$. Thus, if $\kappa^\dagger$ is also fixed $X \to \infty$

and $q_1(X) \to q_1^\infty$ as $V(\Gamma)$ becomes large. The first term in (4.29) then decreases asymptotically as $1/\ln V(\Gamma)$, while the last term decreases much more rapidly. This establishes the result stated in Sec. II: that $\Psi_\Omega\{f\,|\,\Gamma\}$ must decrease at least as fast as $[\ln V(\Gamma)]^{-1/2}$.

To simplify the optimization of (4.29) we again restrict attention to the case where $\eta(\vec{r})$ *vanishes in* Γ *and* Δ. We may simplify the second term as before by replacing $q_1(X)$ by ρ_Γ, since $\rho_\Gamma < q_1 < q_1(X)$ Similarly, in the first term q_2 may be replaced by q_2^∞ [see (3.39)]. Then, if we rewrite (4.29) to display all the dependence on $\kappa^\dagger$ and b explicitly, we obtain

$$\Psi^2 \le \frac{4\pi\rho_\Gamma}{q_0^\infty(1-s_1 b)}\;\frac{1+a_1 b+a_2 b^2+\kappa^{\dagger 2}/8\pi D_z\rho_\Gamma}{\ln[\kappa^{\dagger 2} b(1+s_1 b)\,V(\Gamma)^{1/2}/D_z^{1/2}c_2]} + \rho_\Gamma\left(\frac{\chi^{1/2}}{N_\Gamma^{1/2}}+\frac{1}{N_\Gamma}\right), \qquad (4.30)$$

where, as before, $N_\Gamma = \rho_\Gamma V(\Gamma)$, and where

$$a_1 = q_2^\infty / c_2\rho_\Gamma\,[D_z V(\Gamma)]^{1/2}, \quad a_2 = q_2^\infty/\rho_\Gamma V(\Gamma), \qquad (4.31)$$

and

$$s_1 = c_2 D_z^{1/2}/[V(\Gamma)]^{1/2}\,. \qquad (4.32)$$

If the right-hand side of (4.30) is minimized with respect to $\kappa^\dagger$, one finds the optimal choice is close to

$$\kappa^{\dagger 2} = 8\pi D_z\,\rho_\Gamma(1+a_1 b+a_2 b^2)/\ln\{8\pi b(1+s_1 b)\,\rho_\Gamma\,[D_z V(\Gamma)]^{1/2}/c_2 e\}. \qquad (4.33)$$

When this value for $\kappa^\dagger$ is inserted in (4.30), the thickness b is the only remaining free parameter. Optimization must then be carried out rather carefully, since one discovers that the best choice b^* varies as $V(\Gamma)^{1/2}/\ln V(\Gamma)$, from which it follows that many terms in (4.30) are of comparable order and cannot be neglected. The optimal choice is not far from

$$b = b^*(T) = c_2\,[D_z V(\Gamma)]^{1/2}/[c_2^2 D_z + q_2^\infty/\rho_\Gamma]\,\mathcal{L}[V(\Gamma)]\,, \qquad (4.34)$$

where

$$\mathcal{L}[V(\Gamma)] = \ln\{8\pi D_z\rho_\Gamma V(\Gamma)/e\,[c_2^2 D_z + q_2^\infty/\rho_\Gamma]\}, \qquad (4.35)$$

so that $b^* \sim 1/T\ln T^{-1}$ as $T \to 0$. Then, provided $\mathcal{L}$ is not too small, one obtains

$$[\Psi_\Omega\{f\,|\,\Gamma\}]^2 \le \frac{2\rho_\Gamma N_T}{\mathcal{L} - 2\ln(\mathcal{L}) - 1} + \rho_\Gamma\left[\frac{\chi^{1/2}}{N_\Gamma^{1/2}} + \frac{1}{N_\Gamma}\right]\,, \qquad (4.36)$$

where, now,

$$N_T = \rho_\Gamma \Lambda_T^2 D_z, \quad d=2 \qquad (4.37)$$

is the mean number of atoms in the thermal volume $v_T = \Lambda_T^2 D_z$.

It is clear that the second term will normally be completely negligible compared to the first. On dropping it we may write our result

$$[\Psi_\Omega\{f\,|\,\Gamma\}]^2 \le 2\rho_\Gamma N_T/\ln[V(\Gamma)/v_0] \le 4\pi\rho_\Gamma^2\hbar^2 D_z/mk_B T\ln[V(\Gamma)/v_0], \qquad (4.38)$$

where the scale volume $v_0(\Gamma)$ is given by

$$\rho_\Gamma v_0 \simeq \frac{e^2}{2}\left(\frac{c_2^2}{4\pi}+\frac{1}{N_T}\right)\left[\ln\left(\frac{8\pi N_\Gamma}{e c_2^2}\right)\right]^2, \qquad (4.39)$$

which depends only weakly on $V(\Gamma)$. Alternatively, if we take Γ to be a circular cylinder of radius R_Γ and height D_z we obtain

$$[\Psi_\Omega\{f\,|\,\Gamma\}]^2 \le \rho_\Gamma N_T/\ln(R_\Gamma/r_0)\,, \qquad (4.40)$$

where, using $c_2^2 = 4\pi$, the *scale radius* is

$$r_0(\Gamma) = \frac{e}{(2\pi)^{1/2}}\left(1+\frac{1}{N_T}\right)^{1/2}\ln\left(\frac{2N_\Gamma}{e}\right)\frac{\Lambda_T}{N_T^{1/2}}, \qquad (4.41)$$

where now

$$N_\Gamma(R_\Gamma) = \pi\rho_\Gamma R_\Gamma^2 D_z\,, \qquad (4.42)$$

so that r_0 depends, albeit weakly, on R_Γ. [The numerical coefficient in (4.41) is about 1.08.] At first sight the result (4.40), which shows that Ψ^2 decays as $R \to \infty$ at least as fast as

$$\alpha(R) = \alpha_0/[\ln R - \ln\ln\alpha_1 R]$$

(ignoring inessential parameters), is *weaker* than a decay as $\beta(R) = \beta_0/\ln R$, which would have followed directly from (4.30) without troubling to optimize with respect to b. Closer inspection reveals, however, that the optimized constant α_0 is one-half the original constant β_0. Consequently the bound (4.40) is smaller than the unoptimized result by a factor

$$\alpha(R)/\beta(R) = \tfrac{1}{2}[1-(\ln\ln\alpha_1 R/\ln R)]^{-1} \to \tfrac{1}{2} \quad \text{as} \quad R\to\infty. \qquad (4.43)$$

Evidently a bound varying simply as $1/\ln R$ is included in our results but will be weaker numerically.

Unfortunately, as might be anticipated from the logarithmic dependence on volume or radius, these inequalities are rather weak. Thus, if for example, we consider again liquid helium of normal density at $T = 2\,^\circ$K, we find that the inequality has no force for a film of thickness $D_z = 10$ Å until R_Γ exceeds 10^5 Å. When $R_\Gamma = 1$ cm, it yields a bound of only about $\frac{1}{2}$ for Ψ^2/ρ_Γ. Alternatively, we may ask how thin the film must be to be certain that $\Psi^2 \le 0.1\rho_\Gamma$, say. [Note that with $f(\vec{r}) = 1$ the ratio Ψ^2/ρ_Γ is effectively the condensate density n_0/N.] For a radius of around 1 cm we find that this inequality must hold if the thickness is less than 1.5 Å. Evidently our analysis cannot rule out "effective" Bose condensation in laboratory-sized helium films.

All of the above considerations have referred to subdomains Γ which were "slices" as explained in the previous Sec. III. However, we may obtain bounds for a general subdomain Θ in the case $f(\vec{r}) \equiv 1$ by noting that the one-body density matrix $\sigma(\vec{r}, \vec{r}')$ is never negative.[21] It follows that

$$\Psi_\Omega\{1 \mid \Theta\} \leq \Psi_\Omega\{1 \mid \Gamma\}, \text{ provided } \Theta \subset \Gamma. \qquad (4.44)$$

V. BEHAVIOR OF DENSITY MATRIX

We have obtained bounds on the short-range order parameter $\Psi_\Omega\{f \mid \Gamma\}$, which, by definition, is a double integral of the single-particle density matrix $\sigma_\Omega(\vec{r}, \vec{r}')$ over Γ. It is clearly of interest, however, to obtain more information about $\sigma_\Omega(\vec{r}, \vec{r}')$ itself. To some extent this may be done as follows by using the knowledge[21] that $\sigma_\Omega(\vec{r}, \vec{r}')$ is never negative.

For simplicity we adopt the geometries introduced in Sec. IV; namely, we take

$$d=1: \quad \Omega \equiv \{\vec{r};\ 0 \leq y < D_y,\ 0 \leq z < D_z\},$$
$$\Gamma \equiv \{\vec{r};\ x^2 < R_\Gamma,\ 0 \leq y < D_y,\ 0 \leq z < D_z\},$$
$$V(\Gamma) = 2R_\Gamma D_y D_z = A_1 S_1 \qquad (5.1)$$

and

$$d=2: \quad \Omega \equiv \{\vec{r};\ 0 \leq z < D_z\},$$
$$\Gamma \equiv \{\vec{r};\ x^2 + y^2 < R_\Gamma;\ 0 \leq z < D_z\}, \qquad (5.2)$$
$$V(\Gamma) = \pi R_\Gamma^2 D_z = A_2 S_2 .$$

These formulas define the projected area $A_d(\Gamma)$. Now most interest focuses on $\sigma_\Omega(\vec{r}, \vec{r}')$ in the thermodynamic limit $V(\Omega) \to \infty$. Because of the restricted dimensionality, however, $\sigma_\infty(\vec{r}, \vec{r}')$ will still vary separately with $\vec{r}$ and $\vec{r}'$. Accordingly, we set $\vec{r} = (\vec{r}_\parallel, \vec{r}_\perp)$ and average over the "perpendicular" directions to obtain the "projected" density matrix

$$\bar{\sigma}_\infty(|\vec{r}_\parallel - \vec{r}'_\parallel|) = S_d^{-2} \int d\vec{r}_\perp \int d\vec{r}'_\perp \sigma_\infty(\vec{r}, \vec{r}'), \qquad (5.3)$$

which, as indicated, is a function only of $|\vec{r}_\parallel - \vec{r}'_\parallel|$. Now with $f(\vec{r}) \equiv 1$ we may use the non-negativity of σ_∞ to conclude that

$$[\Psi_\infty\{1 \mid \Gamma\}]^2 = A_d^{-2} \int_{|\vec{r}'_\parallel| < R_\Gamma} d\vec{r}'_\parallel \int_{|\vec{r}_\parallel| < R_\Gamma} d\vec{r}_\parallel \bar{\sigma}_\infty(|\vec{r}_\parallel - \vec{r}'_\parallel|)$$
$$\geq A_d^{-2} \int_{|\vec{r}'_\parallel| < (1/2) R_\Gamma} d\vec{r}'_\parallel \int_{|\vec{R}_\parallel| < (1/2) R_\Gamma} d\vec{R}_\parallel \bar{\sigma}_\infty(|\vec{R}_\parallel|), \qquad (5.4)$$

where the restriction of the ranges of integration to $\frac{1}{2} R_\Gamma$ ensures that $\vec{r}_\parallel = \vec{r}'_\parallel + \vec{R}_\parallel$ always lies in the original domain of integration. Performing the first integration now yields

$$[\Psi_\infty\{1 \mid \Gamma\}]^2 \geq (2^d A_d)^{-1} \int_{|\vec{R}_\parallel| < (1/2) R_\Gamma} d\vec{R}_\parallel \bar{\sigma}_\infty(|\vec{R}_\parallel|)$$
$$\geq \tfrac{1}{2} R_\Gamma^{-d} \int_0^{(1/2) R_\Gamma} \bar{\sigma}_\infty(R) R^{d-1}\, dR, \qquad d = 1, 2. \quad (5.5)$$

Then from the result (4.27) [with N_T defined in (4.19)] we find

$$\int_0^R \bar{\sigma}_\infty(r)\, dr \leq 8\rho_\Gamma (N_T \Lambda_T / \pi)^{1/2} R^{1/2}, \quad d=1 \qquad (5.6)$$

while from (4.40) [with N_T defined in (4.37)] we obtain

$$\int_0^R \bar{\sigma}_\infty(r) r\, dr \leq 8\rho_\Gamma N_T R^2 / \ln(2R/r_0), \quad d=2. \qquad (5.7)$$

These two results demonstrate that $\bar{\sigma}_\infty(r)$ must decrease "on average" at least as fast as $1/r^{1/2}$ for $d=1$ and as $1/\ln(r/r_0)$ for $d=2$. If, as is not implausible, $\bar{\sigma}_\infty(r)$ *decreases monotonically*, we can be more precise. Thus monotonicity implies that

$$\int_0^R \bar{\sigma}_\infty(r) r^{d-1} dr \geq \bar{\sigma}_\infty(R) \int_0^R r^{d-1} dr = \bar{\sigma}_\infty(R) R^d / d, \qquad (5.8)$$

so that from (5.6) and (5.7) we obtain the explicit pointwise bounds

$$\bar{\sigma}_\infty(R) \leq 8\rho_\Gamma (N_T \Lambda_T / \pi)^{1/2} / R^{1/2}, \quad d=1$$
$$\leq 16\rho_\Gamma N_T / \ln(2R/r_0), \qquad d=2 \qquad (5.9)$$

where $r_0(R) \propto \ln R$ is given by (4.41) and (4.42). As explained in connection with (4.44), a bound for $d=2$ with the simpler r dependence $1/\ln(R/r_0')$ can be obtained, but it will be weaker than the above bound, which varies as $1/[\ln(R/r_0') - \ln\ln(R/r_0'')]$.

Asymptotic results similar to (5.9) can still be obtained if it is known only that $\bar{\sigma}_\infty(r)$ is monotonic for $r > r_1$: All that is necessary is to break the range of integration in (5.8) at $r = r_1$. Somewhat more generally, if $\bar{\sigma}_\infty(r)$ is not necessarily monotonic but admits a monotonic *lower* bound $\Sigma(R)$, one can prove the inequalities (5.9) for $\Sigma(R)$. On the other hand, our results cannot yield a pointwise *upper* bound on $\bar{\sigma}_\infty(r)$ if this function is not monotonic, since, for example, tall but sufficiently narrow "spikes" would make a negligible contribution to the integrals over Γ, which is what our basic bounds deal with.

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APPENDIX

In this Appendix the Schwarz inequality is applied to

$$Q\{f\}=\int_{\Xi} d\vec{r} \int_{\Xi} d\vec{R}' \int_{\Xi} d\vec{R} f^*(\vec{R}') f(\vec{R}) \langle \rho(\vec{r}) \Psi^\dagger(\vec{R}') \Psi(\vec{R}) \rangle,$$

$$|f(\vec{r})| = 1 \tag{A1}$$

where the thermal average may be that for the infinite system Ω or for a finite $\Omega \supset \Xi$. We define the average L_{XY} for arbitrary operators X and Y by

$$L_{XY} = \langle XY \rangle - \langle X \rangle \langle Y \rangle , \tag{A2}$$

and in this notation the Schwarz inequality is expressed as

$$|L_{XY}|^2 \le |L_{XX}| \, |L_{YY}| . \tag{A3}$$

For the operators X and Y we choose

$$X = \int_{\Xi} d\vec{r} \rho(\vec{r}) \equiv \hat{N}_{\Xi} ,$$
$$Y = \int_{\Xi} d\vec{r} \int_{\Xi} d\vec{r}' f^*(\vec{r}') f(\vec{r}) \psi^\dagger(\vec{r}') \psi(\vec{r}) , \tag{A4}$$

where we have noted that X is the number operator for the domain Ξ [see (2.8)]. With this choice we have simply

$$Q\{f\} = \langle XY \rangle . \tag{A5}$$

The following operator relations hold for X and Y defined in (A4):

$$X^\dagger = X \ge 0, \quad Y^\dagger = Y \ge 0, \quad [X, Y] = 0. \tag{A6}$$

These relations imply the positivity of XY, so that from (A2) and (A5) we have

$$0 \le Q\{f\} = \langle XY \rangle \le |L_{XY}| + \langle X \rangle \langle Y \rangle . \tag{A7}$$

Now introduce a complete orthonormal set of functions $\varphi_m(\vec{r})$ appropriate to the domain Ξ (say, with vanishing normal derivative at the boundary). With no loss of generality we may choose $\varphi_0(\vec{r}) = [V(\Xi)]^{-1/2}$. Completeness implies

$$\sum_m \varphi_m^*(\vec{r}') \varphi_m(\vec{r}) = \delta(\vec{r} - \vec{r}'), \quad \vec{r}, \vec{r}' \subset \Xi . \tag{A8}$$

Then we define the "occupation number" operators by

$$\hat{n}_m \equiv \int_{\Xi} d\vec{r} \int_{\Xi} d\vec{r}' \varphi_m^*(\vec{r}') \varphi_m(r) f^*(\vec{r}') f(\vec{r}) \psi^\dagger(\vec{r}') \psi(\vec{r}) \ge 0 , \tag{A9}$$

and use (A8) and (A1) to show that

$$\sum_m \hat{n}_m = \int_{\Xi} d\vec{r} \rho(\vec{r}) = \hat{N}_{\Xi} . \tag{A10}$$

Since $\hat{n}_m$ is a non-negative Hermitian operator and $[\hat{n}_m, \hat{n}_{m'}] = 0$, we have $\langle \hat{n}_m \hat{n}_{m'} \rangle \ge 0$, so that

$$\langle X^2 \rangle = \langle \hat{N}_{\Xi}^2 \rangle = \sum_m \sum_{m'} \langle \hat{n}_m \hat{n}_{m'} \rangle \ge \langle \hat{n}_0^2 \rangle . \tag{A11}$$

Now, as explained after (3.31), we may write

$$L_{XX} = \langle (\hat{N}_{\Xi} - \langle \hat{N}_{\Xi} \rangle)^2 \rangle = \rho(\Xi)^2 V(\Xi) k_B T K_T [1 + \epsilon(\Xi)] , \tag{A12}$$

where $\rho(\Xi) = N(\Xi)/V(\Xi)$ is the mean density of particles in Ξ. Furthermore, from (A12) and (A13) we find

$$L_{YY} = V(\Xi)^2 \langle (\hat{n}_0 - \langle \hat{n}_0 \rangle)^2 \rangle$$
$$\le V(\Xi)^2 \langle N_{\Xi}^2 \rangle = V(\Xi)^2 [L_{XX} + N(\Xi)^2]. \tag{A13}$$

The Schwarz inequality then yields

$$|L_{XY}| \le (L_{XX} L_{YY})^{1/2} ,$$
$$\le V(\Xi) \{ L_{XX} [L_{XX} + N(\Xi)^2] \}^{1/2} ,$$
$$= [L_{XX}]^{1/2} V(\Xi) N(\Xi) [1 + L_{XX} N(\Xi)^{-2}]^{1/2} . \tag{A14}$$

Then from (A7), (A13), and (A14), $Q\{f\}$ is bounded by

$$Q\{f\} \le V(\Xi) N(\Xi) n_{\Omega} \{f|\Xi\}$$
$$+ \rho(\Xi)^2 V(\Xi)^2 \{1 + O[1/V(\Xi)]\} , \tag{A15}$$

where $n_{\Omega}\{f|\Xi\}$, which is given by

$$V(\Xi) n_{\Omega} \{f|\Xi\} = \langle Y \rangle , \tag{A16}$$

has essentially been defined in (2.23). The result (A15) is used to bound $Q\{f\}$ in (3.36).

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$$a(x) = \int_{-1}^{x/c} f(x')\,dx' \Big/ \int_{-1}^{1} f(x')\,dx'$$

is, in fact, infinitely differentiable and furthermore, for large enough n the gradient satisfies

$$\nabla a = da/dx = f(x/c)/c \int_{-1}^{1} f(x)\,dx \le b^{-1} \le \tfrac{1}{2} c^{-1},$$

since the normalizing integral approaches 2 as $n \to \infty$.

[19]This might fail at some special critical- or λ-point transition temperature but will be valid for most other cases of interest.

[20]The small correction in the brackets of (4.11) and the effect of the terms involving q_3 and q_4 in (4.12) have been neglected in arriving at (4.13).

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Decay of Order in Isotropic Systems of Restricted Dimensionality. II. Spin Systems

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The ordering of one- and two-dimensional spin systems of finite thickness and cross section is considered in the presence and absence of a symmetry-breaking magnetic field. The exchange interactions are allowed to vary randomly or regularly throughout the lattice. It is shown rigorously by applying Bogoliubov's inequality to a subdomain of the system that, provided the (suitably averaged) exchange interactions do not fall off too slowly, no spontaneous ordering can occur. Explicit bounds on the spin-spin correlation function, summed over the sites in a subdomain, are obtained which indicate how the short-range order decays with distance. Detailed numerical plots for the order as a function of the subdomain size are presented for various realistic values of the temperature. Conditions under which these curves yield bounds on the spatial decay of the spin-spin correlation function are also discussed.

I. INTRODUCTION

This paper represents a continuation of the program begun in the previous one[1] (hereafter referred to as I), which discussed Bose particle systems. Since there is particular interest in spin systems, and since the arguments and numerical analysis will differ somewhat, the magnetic case will be presented in a self-contained fashion (although some allusion will be made to analogous procedures used in the Bose case). The reader should consult the Introduction and Sec. II of I for a general description of notation and strategy[2] (to be summarized briefly below), but those interested solely in spin systems can omit the discussion of second quantization in I [Eqs. (I 2.3)–(I 2.15)].

We consider an anisotropic Heisenberg ferromagnet of $\mathfrak{N}(\Omega)$ localized spins $\vec{S}(\vec{r})$ occupying the sites $\vec{r}$ of a regular lattice contained in a three-dimensional domain Ω. We take the Hamiltonian to be [(I 2.1)]

$$\mathcal{H}_\Omega = -\tfrac{1}{2} \sum_{\vec{r}} \sum_{\vec{r}\,'} \sum_{\alpha = x,y,z} J_\alpha(\vec{r},\vec{r}\,') S^\alpha(\vec{r}) S^\alpha(\vec{r}\,') + \sum_{\vec{r}} \vec{h}(\vec{r}) \cdot \vec{S}(\vec{r}), \tag{1.1}$$

where $\vec{h}(\vec{r})$ is the external field in energy units ($\vec{h} = \frac{1}{2} g \mu_B \vec{H}$), while $J_\alpha(\vec{r},\vec{r}\,')$ is the exchange coupling. We will allow $J_\alpha(\vec{r},\vec{r}\,')$ to be regular or to vary randomly throughout the lattice, subject only to the condition of "planar" isotropy, i.e.,

$$J_x(\vec{r},\vec{r}\,') = J_y(\vec{r},\vec{r}\,') = J(\vec{r},\vec{r}\,') = J(\vec{r}\,',\vec{r}) \quad \text{for} \quad \vec{r},\vec{r}\,' \subset \Omega \ . \tag{1.2}$$