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Absence of Anomalous Averages in Systems of Finite Nonzero Thickness or Cross Section*

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It is shown that doubts concerning the validity of previous proofs that anomalous averages cannot occur in three-dimensional systems of finite cross section or thickness are unfounded. The absence of anomalous averages in Bose systems of finite cross section is explicity demonstrated to illustrate the point.

Two years ago, Hohenberg[1] pointed out that a rigorous inequality due to Bogoliubov could be used to rule out the possibility of anomalous averages (quasiaverages) or broken symmetry in one- and two-dimensional superfluids and superconductors. Similar proofs have since been presented for various kinds of magnetic and crystalline ordering.[2]

Recently, however, some authors[3] have mistakenly questioned the general validity of such conclusions for systems which are not strictly one- or two-dimensional, but have nonzero (but finite) cross section or thickness. These doubts have arisen because the wave functions of a system in a container of finite cross section must vanish on the walls, and hence, even in the ground state, the wave function must have some nonzero curvature and cannot assume a uniform value (as is presumed to correspond to "zero-momentum" $\mathbf{k}=0$). Now the proofs based on Bogoliubov's inequality rest on the divergence of the integral

$$\int_{|\mathbf{k}|<\kappa} \frac{d\mathbf{k}}{k^2} \qquad (1)$$

at the origin in one or two dimensions. An objection is made, however, that such a divergence cannot actually arise, owing to the cutoff imposed at low momentum by the finite cross section (or by the corresponding positive zero-point energy).

Such objections are based on a misunderstanding of Hohenberg's original proof and its several extensions. The essential point is that the wave vectors occurring in the integral (1) can be thought of as auxiliary mathematical variables that need *not* have the physical significance of labeling momentum states of a system with periodic boundary conditions. The wave vectors are in no way restricted by the boundary conditions of the problem or by any confining potentials, but can assume a continuum of values, even when the actual system is confined to a region Ω of volume V_Ω of finite dimensions (and arbitrary shape).

Once this is recognized, it is straightforward to modify Hohenberg's original arguments to yield a rigorous proof that anomalous averages (Ψ_0) must vanish in a system in real, three-dimensional space which, owing to confining potentials or appropriate boundary conditions, remains finite in one or two dimensions in the thermodynamic limit—i.e., in the limit in which the remaining two or one dimensions become infinite. We will consider only the case of a Bose fluid. In the usual fashion, we introduce a symmetry-breaking term

$$\mathcal{S} = -\int_\Omega [\eta\psi^\dagger(r)+\eta^*\psi(r)]d\mathbf{r} \qquad (2)$$

into the Hamiltonian $\mathcal{H}$ to stabilize the anomalous average

$$\Psi_0 = \frac{\langle a_0\rangle}{V_\Omega^{1/2}} = V_\Omega^{-1}\int_\Omega d\mathbf{r}\,\langle\psi(\mathbf{r})\rangle \qquad (3)$$

in a finite system. (Note that Ψ_0 is an intensive quantity.) After taking the thermodynamic limit, we will let the magnitude of the symmetry-breaking field η approach zero.

If the system is strictly confined in the domain Ω, either by virtue of some wall potential which is infinite outside Ω, or by explicit boundary conditions,[4] then the appropriate field operators $\psi(\mathbf{r})$ will vanish identically outside Ω. Since in Bogoliubov's inequality[2]

$$\tfrac{1}{2}\langle\{A,A^\dagger\}\rangle \geq k_BT|\langle[A,C]\rangle|^2/\langle[C^\dagger,[\mathcal{H},C]]\rangle\,, \qquad (4)$$

the operators A and C are arbitrary (provided the relevant traces exist), we can use for A, the operator

$$a_\mathbf{k} = V_\Omega^{-1/2}\int_\Omega d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}\psi(\mathbf{r})\,, \qquad (5)$$

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

[2] N. D. Mermin and H. Wagner, Phys. Rev. Letters **17**, 1133 (1966); N. D. Mermin, J. Math. Phys. **8**, 1061 (1967); Phys. Rev. **176**, 250 (1968).

[3] E. W. Fenton, Phys. Rev. **174**, 517 (1968); see also D. A. Krueger [Phys. Rev. Letters **19**, 563 (1967)] who suggests that Hohenberg's argument may only be valid when periodic boundary conditions are used.

[4] We may suppose that nonadsorbing, impenetrable walls surround the system. Superfluid helium will however cover all experimentally realizable walls with a film, but this merely means that we shall have several films in our container (one on each wall, for example) separated by vapor. The thickness of these films can be controlled by adjusting the over-all density, and the argument goes through as before.

where $\mathbf{k}$ is completely arbitrary and, in particular, is *in no way restricted by the size or shape of* Ω. [The point here is that in constructing the second quantized operators $\psi(\mathbf{r})$ the complete set of single-particle wave *functions* $\varphi_n(\mathbf{r})$ must be taken to satisfy the boundary conditions on the surface of Ω. Once this is done any operator of the form (2) or (5) is an acceptable operator.] We similarly set

$$C=\int_{\Omega} d\mathbf{r}\; e^{-i\mathbf{k}\cdot\mathbf{r}}\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r}). \qquad (6)$$

On using $|\Psi_0|\geq \mathrm{Re}(e^{i\alpha}\Psi_0)$, it is straightforward to derive the basic result

$$n_{\mathbf{k}}=\langle a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\rangle \geq \frac{k_BT|\Psi_0|^2}{(\hbar^2\rho/m)k^2+2|\eta|\,|\Psi_0|}-\frac{1}{2}, \qquad (7)$$

where $\rho=N/V_{\Omega}$ is the density.[5]

Now let us suppose that as the thermodynamic limit is approached, it remains possible to enclose the domain Ω within a rectangular $D\times D\times L$ box Γ (to be concrete we consider the "one-dimensional" case), where L grows without bound in the thermodynamic limit, but D remains finite. (Note that no restriction is placed on the shape of Ω other than that the box Γ can be placed around it.) We may then choose a set of wave numbers $\mathbf{k}$ appropriate to the box Γ, namely,

$$\mathbf{k}=2\pi(l_1/D,\, l_2/D,\, n/L), \qquad (8)$$

where l_1, l_2, and n are positive or negative integers. Next, divide through the inequality (7) by the volume D^2L; sum the right-hand side over all $\mathbf{k}$ of the form (8) with $l_1=l_2=0$ and $|n|<\kappa L/2\pi$ for fixed κ; and sum the left-hand side over all $\mathbf{k}$ of the form (8). Since the left-hand side of (7) is positive for all $\mathbf{k}$, this last step can only strengthen the inequality. Now whenever $\mathbf{r}$ and $\mathbf{r}'$ are in the box Γ, we have

$$(LD^2)^{-1}\sum_{l_1,l_2,n} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}=\delta(r-r'), \qquad (9)$$

so that the left-hand side becomes simply

$$V_{\Omega}^{-1}\int d\mathbf{r}\;\langle\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})\rangle = N/V_{\Omega}=\rho. \qquad (10)$$

On the other hand, in the thermodynamic limit as $L\rightarrow\infty$ the sum over n on the right-hand side of (7) approaches an integral [with, for fixed $|\eta|>0$, an error of relative order $(\kappa L)^{-2}$]. After a slight rearrangement, we thus obtain finally

$$\rho D^2+\frac{\kappa}{2\pi}\geq\frac{k_BT|\Psi_0|^2}{2\pi}\int_{-\kappa}^{\kappa}\frac{dk_z}{(\hbar^2\rho/m)k_z^2+2|\eta|\,|\Psi_0|}. \qquad (11)$$

For small $|\eta|$ the right-hand side diverges as $k_BT \times|\Psi_0|^{3/2}|\eta|^{-1/2}$, which proves that in the thermodynamic limit Ψ_0 must vanish as $|\eta|\rightarrow 0$.

A completely analogous argument goes through for real "two-dimensional" systems which can be enclosed in $D\times L\times L$ boxes with D fixed as the thermodynamic limit is approached.[6] Equally, one can show[7] that $\Psi_{\mathbf{K}}$ [defined from (5) in analogy to (3)] must vanish for all $\mathbf{K}$. Most of the other arguments now in the literature, including Hamilton's exclusion of spin-density waves in one and two dimensions,[8,9] can be similarly generalized.

We conclude with some comments on the physical significance of our results. First, we remark that in the case of a *homogeneous* (uniform) Bose system Hohenberg's results can be interpreted (accepting the physical validity of the method of quasiaveraging) as stating that there cannot be any Bose-Einstein condensation in the zero-momentum state. For such a system, this state is an eigenstate of the single-particle density matrix $\sigma_1(\mathbf{r}_1,\mathbf{r}_1')=\langle\psi^{\dagger}(\mathbf{r}_1)\psi(\mathbf{r}_1')\rangle$. For the inhomogeneous systems with boundaries we are considering, the states of the single-particle density matrix are unknown and are presumably quite complicated in shape. However, if we are willing to extend our belief in quasiaveraging to assert that the thermodynamic limits of $|\Psi_0|^2$ and $V_{\Omega}^{-2}\int_{\Omega}d\mathbf{r}_1\int_{\Omega}d\mathbf{r}_1'\,\sigma_1(\mathbf{r}_1,\mathbf{r}_1')$ are equal, then we can say that our result that $|\Psi_0|$ must vanish in this limit, as $|\eta|\rightarrow 0$, implies that there is no condensation into any eigenstate of $\sigma_1(\mathbf{r}_1,\mathbf{r}_1')$ (with bounded density). This result follows from a lemma due to Penrose and Onsager[10] together with the remark that $\sigma_1(\mathbf{r}_1,\mathbf{r}_1')$ is everywhere non-negative for a Bose system (with real Hamiltonian).[11] Even this result, however, does not exclude the possibility of some more subtle kind of "weak long-range order" in which, in the thermodynamic limit, $\sigma_1(\mathbf{r}_1-\mathbf{r}_1')\rightarrow 0$ as $|\mathbf{r}_1-\mathbf{r}_1'|\rightarrow\infty$, but

$$\int_{|\mathbf{r}|<R}\sigma_1(\mathbf{r})d\mathbf{r}\rightarrow\infty \quad \text{as} \quad R\rightarrow\infty$$

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[5] To obtain this inequality we may assume that the single-particle probability density $n(\mathbf{r})$ tends continuously to zero or the boundaries of Ω. This follows from the fact that all the eigenfunctions of the Hamiltonian vanish continuously as any of their arguments approach the boundary of Ω.

[6] One sets $l_1=0$ but sums on l_2 and n subject to $l_2^2+n^2<\kappa L/2\pi$. The corresponding limiting integral on k_y and k_z diverges, as usual, as $-\ln|\eta|$.

[7] One replaces η by $\eta_{\mathbf{K}}e^{i\mathbf{K}\cdot r}$ in (2) and replaces $\mathbf{k}$ by $\mathbf{k}-\mathbf{K}$ in (6). The right-hand side of (7) is then subject to the changes $\Psi_0\rightarrow\Psi_{\mathbf{K}}$, $\eta\rightarrow\eta_{\mathbf{K}}$, $\mathbf{k}\rightarrow|\mathbf{k}-\mathbf{K}|$. The dimensions D_1 and D_2 of the box Γ are then chosen so that $j_1=K_xD_1/2\pi$ and $j_2=K_yD_2/2\pi$ are integers. Finally, in summing the left-hand side of (7), one sets $l_1=j_1$ and $l_2=j_2$ and sums on n for $|(2\pi n/L)-K_z|<\kappa$.

[8] D. C. Hamilton, Phys. Rev. **157**, 427 (1967).

[9] Contrast with E. W. Fenton, Phys. Rev. Letters **21**, 1427 (1968).

[10] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).

[11] O. Penrose (unpublished); see also G. V. Chester, in *Lectures in Theoretical Physics*, edited by K. T. Mahanthappa (Gordon and Breach, Science Publishers, Inc., New York, 1968), Vol. 11, p. 253.

(corresponding to an infinite "off-diagonal" susceptibility), as has been suggested as a possibility in the analogous case of a two-dimensional Heisenberg ferromagnet.[12]

[12] See H. E. Stanley and T. A. Kaplan, Phys. Rev. Letters **17**, 913 (1966); J. Appl. Phys. **38**, 975 (1967); also G. S. Rushbrooke and P. J. Wood, Proc. Phys. Soc. (London) **A68**, 1161 (1955); Mol. Phys. **1**, 257 (1958).

Note added in proof. A discussion of the asymptotic behavior of the single-particle density matrix in restricted dimensionality has recently been presented by D. Jashow and M. E. Fisher, Phys. Rev. Letters **23**, 286 (1969).

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Surface Spin Waves for the Simple Cubic Antiferromagnet

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The surface spin-wave spectra of a simple cubic two-sublattice antiferromagnet is derived for a {100} surface as a function of the ratio ϵ of the surface exchange to the bulk exchange. The effects of changes in the surface anisotropy are also included. In general, a doubly-degenerate acoustical- or optical-type surface branch is found, depending upon the value of ϵ. For $-0.112<\epsilon<1.107$, an acoustic branch exists over the entire two-dimensional Brillouin zone. If $1.107<\epsilon<1.207$, then the branch is truncated at small values of the propagation vector k parallel to the surface. In the range $1.207<\epsilon<1.25$, no surface states exist for the nearest-neighbor-exchange model. When $1.25<\epsilon<1.854$, a truncated optical-type branch exists. A complete optical branch exists for $\epsilon\geq1.854$. The $k=0$ surface-antiferromagnetic-resonance (SAFMR) mode lies very near the bulk AFMR mode for a wide range of surface perturbation parameters. The SAFMR mode is found to be of very long range when the anisotropy energy is small compared to the exchange energy. For simple cubic $RbMnF_3$, the SAFMR mode is estimated to have a range on the order of 200 μ.

I. INTRODUCTION

A NUMBER of studies of surface spin waves in magnetic systems have been reported recently.[1–7] The first study of the surface states of an antiferromagnet was reported by Mills and Saslow,[4] who investigated the surface magnon spectrum of a free (unperturbed) {100} surface of a body-centered-cubic (bcc) two-sublattice Heisenberg antiferromagnet. They also estimated the effect of small perturbations in the surface parameters. A more recent study by De Wames and Wolfram[7] treats in detail the effects of arbitrary changes in the surface exchange and surface anisotropy fields. In the latter study it was shown that both optical and acoustical spin-wave branches exist.

In this paper we report on a study of the surface spin-wave spectrum of the (100) surface of a two-sublattice simple cubic (sc) antiferromagnet as a function of the "in-plane" surface exchange and the surface anisotropy fields. There are many qualitative differences between this study and the study of the (100) surface of the bcc crystal because the latter surface contains spins of only one of the sublattices, while the sc (100) surface contains spins of both sublattices. This difference in the sublattice configurations leads to quite different results in the two cases for the energies of the surface antiferromagnetic resonance (SAFMR) corresponding to the propagation vector parallel to the surface, **k**, being zero ($k=0$). In the bcc case the SAFMR lies lower than the bulk AFMR mode[4,7] by a factor of approximately $\sqrt{2}$ whenever the anisotropy energy is much less than the exchange energy. This result is relatively insensitive to small perturbations in the surface exchange and anisotropy. The lowering of the SAFMR energy by the factor of $\sqrt{2}$ relative to the bulk mode is characteristic of a surface of a cubic two-sublattice antiferromagnet which has no exchange bonds parallel to the surface (in the nearest-neighbor-exchange approximation). In the case of the sc (100) surface, it is shown that SAFMR mode lies approximately at the sc bulk antiferromagnetic resonance energy under the same conditions as those described for the bcc case. This result is characteristic of surfaces of the cubic two-sublattice antiferromagnet in which the surface contains nearest-neighbor spins of both sublattices. For the sc antiferromagnet both optical and acoustical surface spin waves are found to exist. If the ratio ϵ of the surface exchange to the bulk exchange is less than

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[6] D. L. Mills, in *Localized Excitations in Solids*, edited by R. F. Wallis (Plenum Press, Inc., New York, 1968), p. 426.
[7] R. E. De Wames and T. Wolfram (to be published).