

Absence of Long-Range Overhauser Spin-Density Waves in One or Two Dimensions*

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(Received 22 December 1966)

If an Overhauser static spin-density wave is present in an electron gas, the Fourier transform of a certain spin-density correlation function is at least as singular as $(\mathbf{q}-\mathbf{Q})^{-2}$ near the wave vector \mathbf{Q} of the spin-density wave. This rules out long-range spin-density waves in one and two dimensions at finite temperature, since it must be possible to Fourier-transform this correlation function back to position space.

BOGOLIUBOV has shown, using an inequality derived by him, that a singularity of the form q^{-2} occurs in certain correlation functions for superfluids and superconductors. By using similar arguments, we can deduce the existence of an analogous singularity for the case where an Overhauser spin-density wave exists in an electron gas. Bogoliubov¹ finds that, as \mathbf{q} goes to zero, the relation

$$\langle n_{\mathbf{q}} \rangle + \frac{1}{2} \geq k_B T \langle N_0 \rangle m / \hbar^2 q^2 N \quad (1)$$

holds for superfluids, and an analogous relation holds for superconductors. Here $\langle n_{\mathbf{q}} \rangle$ is the boson occupation number of states with wave number \mathbf{q} , $\langle N_0 \rangle$ is the occupation number of the zero momentum state, and the other symbols have their usual meanings.

Hohenberg has applied these relations to show that there can be no superfluidity or superconductivity in one or two dimensions.² For the superfluid case one can integrate both sides of Eq. (1) over a range of \mathbf{q} including $\mathbf{q}=0$. The right-hand side then diverges at small \mathbf{q} as $\int dq/q^2$ or $\int d^2q/q^2$ in one or two dimensions, respectively. However, the integral on the left should not diverge for small \mathbf{q} , since

$$\frac{1}{(2\pi)^3} \int d^3q \langle n_{\mathbf{q}} \rangle = \frac{N - \langle N_0 \rangle}{V}.$$

Hohenberg's conclusion then follows, since we have a divergence on the small side of the inequality, so that (in the superfluid case) we must have $\langle N_0 \rangle = 0$ to save it.

In the form stated by Mermin and Wagner,³ the Bogoliubov inequality reads

$$\begin{aligned} \frac{1}{2} \langle \{A - \langle A \rangle, A^\dagger - \langle A^\dagger \rangle\}_+ \rangle \\ \geq k_B T \frac{|\langle [C, A] \rangle|^2}{\langle [[C, H], C^\dagger] \rangle}. \end{aligned} \quad (2)$$

The brackets $\langle \dots \rangle$ denote thermal expectation values,

* This work was supported by a National Science Foundation postdoctoral fellowship.

¹ N. N. Bogoliubov, *Physik. Abhandl. Sowjetunion* **6**, 1 (1962); **6**, 113 (1962); **6**, 229 (1962).

² P. C. Hohenberg, *Phys. Rev.* (to be published).

³ N. D. Mermin and H. Wagner, *Phys. Rev. Letters* **17**, 1133 (1966); **17**, 1307 (1966).

while $[\dots]$ and $\{\dots\}_+$ refer to commutators and anticommutators, respectively. We will be interested in the case where $\langle A \rangle$ and $\langle A^\dagger \rangle$ vanish, so we drop these terms. We introduce the field operators

$$\begin{aligned} \psi_\sigma(\mathbf{x}) &= V^{-1/2} \sum_{\mathbf{K}} \exp(i\mathbf{K} \cdot \mathbf{x}) a_{\mathbf{K}\sigma}, \\ \psi_\sigma^\dagger(\mathbf{x}) &= V^{-1/2} \sum_{\mathbf{K}} \exp(-i\mathbf{K} \cdot \mathbf{x}) a_{\mathbf{K}\sigma}^\dagger, \end{aligned}$$

and the Fourier components of the density

$$\begin{aligned} \rho_{\mathbf{q}\uparrow} &= \sum_{\mathbf{K}} a_{\mathbf{K}\uparrow}^\dagger a_{\mathbf{K}+\mathbf{q}\uparrow}, & \tilde{\rho}_{\mathbf{q}} &= \sum_{\mathbf{K}} a_{\mathbf{K}\uparrow}^\dagger a_{\mathbf{K}+\mathbf{q}\downarrow}, \\ \rho_{\mathbf{q}} &= \rho_{\mathbf{q}\uparrow} + \rho_{\mathbf{q}\downarrow}. \end{aligned}$$

Here V is the volume of the system. Those Fourier components of the density which are off-diagonal in the spin indices, namely $\tilde{\rho}_{\mathbf{q}}$, are essential for discussing the Overhauser spin-density wave,⁴ since in the Hartree-Fock treatment of this phenomenon the creation operators for the single-particle states are linear combinations of $a_{\mathbf{K}\uparrow}^\dagger$ and $a_{\mathbf{K}+\mathbf{q}\downarrow}^\dagger$. The Hamiltonian which we discuss is the sum of kinetic and potential energies;

$$H = \sum_{\mathbf{K}\sigma} (\hbar^2 K^2 / 2m) a_{\mathbf{K}\sigma}^\dagger a_{\mathbf{K}\sigma} + (2V)^{-1} \sum_{\mathbf{K}} v(\mathbf{K}) [\rho_{\mathbf{K}} \rho_{-\mathbf{K}}^\dagger - N].$$

In order to prove our result^{4a} for the Overhauser spin-density wave, we use Eq. (2) with

$$C = \rho_{\mathbf{q}\uparrow} \quad \text{and} \quad A = \tilde{\rho}_{\mathbf{Q}-\mathbf{q}}.$$

This choice is motivated by an analogy with Hohenberg's treatment of the superconducting case. We compute the commutators which occur in Eq. (2);

$$[C, A] = [\rho_{\mathbf{q}\uparrow}, \tilde{\rho}_{\mathbf{Q}-\mathbf{q}}] = \tilde{\rho}_{\mathbf{Q}},$$

$$[[C, H], C^\dagger] = [[\rho_{\mathbf{q}\uparrow}, H], \rho_{\mathbf{q}\uparrow}^\dagger] = (\hbar^2 q^2 / m) N_{\uparrow}.$$

This second equation is an expression of the f -sum rule,⁵ which holds separately for $\rho_{\mathbf{q}\uparrow}$ and $\rho_{\mathbf{q}\downarrow}$. Then we find

⁴ A. W. Overhauser, *Phys. Rev.* **128**, 1437 (1962).

^{4a} *Note added in proof*: See also, F. Wegner, *Phys. Letters* **24A**, 131 (1967).

⁵ C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 128.

that Eq. (2) reads

$$\frac{1}{2} \langle \{ \tilde{\rho}_{\mathbf{Q}-\mathbf{q}}, \tilde{\rho}_{\mathbf{Q}-\mathbf{q}}^\dagger \}_+ \rangle \geq k_B T |\langle \tilde{\rho}_{\mathbf{Q}} \rangle|^2 m / \hbar^2 q^2 \langle N_\uparrow \rangle. \quad (3)$$

Now we assume that \mathbf{Q} is the wave number of the spin-density wave, of the order of twice the wave number at the Fermi surface. Then $\langle \tilde{\rho}_{\mathbf{Q}} \rangle$ is not zero and is of order N . Let us take the Fourier transform of both sides of Eq. (3). The small side of the inequality

diverges in one or two dimensions, as it did in the superfluid case. However, the Fourier transform of the left-hand side must be finite, due to its physical interpretation as an equal-time spin-density correlation function, which cannot be infinite for all \mathbf{r} .

The physical meaning of the left-hand side of Eq. (3) is more transparent in position space. We have, in three dimensions,

$$\begin{aligned} \frac{1}{(2\pi)^3} \int d^3q \frac{\exp(-i\mathbf{q} \cdot \mathbf{r})}{q^2} &= (4\pi r)^{-1}, \\ \frac{1}{(2\pi)^3} \int d^3q \exp(-i\mathbf{q} \cdot \mathbf{r}) \langle \{ \tilde{\rho}_{\mathbf{Q}-\mathbf{q}}, \tilde{\rho}_{\mathbf{Q}-\mathbf{q}}^\dagger \}_+ \rangle &= \frac{\exp(-i\mathbf{Q} \cdot \mathbf{r})}{(2\pi)^3} \int d^3q \exp(i\mathbf{q} \cdot \mathbf{r}) \langle \{ \tilde{\rho}_{\mathbf{q}}, \tilde{\rho}_{\mathbf{q}}^\dagger \}_+ \rangle, \\ \tilde{\rho}_{\mathbf{q}} &= \int d^3x \exp(-i\mathbf{q} \cdot \mathbf{x}) \psi^\dagger_\uparrow(\mathbf{x}) \psi_\downarrow(\mathbf{x}). \end{aligned}$$

Substituting in Eq. (3), we find the following relation:

$$\exp(-i\mathbf{Q} \cdot \mathbf{r}) \int d^3x \langle \{ \psi^\dagger_\uparrow(\mathbf{x}) \psi_\downarrow(\mathbf{x}), \psi^\dagger_\downarrow(\mathbf{x}-\mathbf{r}) \psi_\uparrow(\mathbf{x}-\mathbf{r}) \}_+ \rangle \geq \frac{mk_B T |\langle \tilde{\rho}_{\mathbf{Q}} \rangle|^2}{4\pi r \hbar^2 \langle N_\uparrow \rangle}. \quad (4)$$

The quantity on the left in Eq. (4) is proportional to the volume, as it should be. To emphasize its physical meaning, we introduce the spin-density components

$$S_x(\mathbf{x}) = \frac{1}{2} (\psi^\dagger_\uparrow(\mathbf{x}) \psi_\downarrow(\mathbf{x}) + \psi^\dagger_\downarrow(\mathbf{x}) \psi_\uparrow(\mathbf{x})), \quad iS_y(\mathbf{x}) = \frac{1}{2} (\psi^\dagger_\uparrow(\mathbf{x}) \psi_\downarrow(\mathbf{x}) - \psi^\dagger_\downarrow(\mathbf{x}) \psi_\uparrow(\mathbf{x})), \quad S^\pm = S_x \pm iS_y.$$

Now Eq. (4) reads

$$\exp(-i\mathbf{Q} \cdot \mathbf{r}) \int d^3x \langle \{ S^+(\mathbf{r}), S^-(\mathbf{x}-\mathbf{r}) \}_+ \rangle \geq \frac{m}{4\pi r} \frac{k_B T}{\hbar^2} \frac{|\langle \tilde{\rho}_{\mathbf{Q}} \rangle|^2}{\langle N_\uparrow \rangle}.$$

In one or two dimensions, then, the amplitude $\langle \tilde{\rho}_{\mathbf{Q}} \rangle$ of the spin-density wave must vanish at finite temperatures, since the Fourier transform from momentum space must exist. The only way to satisfy the inequality (3) is to have the right-hand side vanish. However, we cannot tell anything about what happens at $T=0$, so there is no contradiction with earlier work,⁶ where it was shown that for weak interactions a long-range spin-density wave will occur at $T=0$ only in one dimension. Finally, it has been shown by Fedders and Martin, and by Hamann and Overhauser, that the electron gas in three dimensions probably does not have a spin-density wave instability.⁷

⁶ W. Kohn and S. J. Nettel, Phys. Rev. Letters 5, 8 (1960); J. C. Phillips, Phil. Mag. 5, 1193 (1960).

⁷ P. A. Fedders and P. C. Martin, Phys. Rev. 143, 245 (1966); D. R. Hamann and A. W. Overhauser, *ibid.* 143, 183 (1966).

We can draw an analogy between this behavior as q^{-2} and a similar divergence which arises in the Ornstein-Zernike treatment of critical fluctuations.⁸ There one finds, at the critical point,

$$\langle \rho_{\mathbf{q}} \rho_{-\mathbf{q}}^\dagger \rangle = (k_B T / q^2) \text{ const.},$$

so that the density correlation function in position space is actually infinite at the critical point in one or two dimensions. However, the conclusion from this result is simply that the Ornstein-Zernike treatment is not applicable to the one- or two-dimensional case.

I would like to thank Professor Walter Kohn for proposing this problem and for helpful suggestions.

⁸ M. E. Fisher, J. Math. Phys. 5, 944 (1964), Eq. (4.1).