

Cooper pairs versus Bose condensed molecules: The ground-state current in superfluid ³He-A

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We present a new calculation of the current \bar{g} flowing in a ground state of the Bardeen-Cooper-Schrieffer (BCS) form for a weakly inhomogeneous superfluid with the symmetry of ³He-A. When the structure of the order parameter not determined by symmetry is appropriate to ³He-A and when the mass density ρ of the helium is essentially uniform, our current reduces to that calculated by Cross. If the mass density is allowed to vary, we find a generalization of the Cross current which shows that when $\bar{v}_s = 0$ and the anisotropy axis \bar{l} is uniform, then the current is simply $(\hbar/4M) \bar{\nabla} \rho \times \bar{l}$. We show that this property of the BCS ground state, which taken with the Cross definition leads to an "intrinsic angular momentum density" of $\rho\hbar/2M$ at zero temperature, also follows directly from the Gor'kov equations. If the range of the order parameter is taken to be small compared with the interatomic separation, then the ground state does not describe ³He-A, but a Bose-Einstein condensate of tightly bound diatomic molecules. In this limit our current reduces to the form calculated by Ishikawa *et al.* We indicate why their analysis is only valid in this limit, and offer some rather more general remarks on the differences between Cooper pairing and the Bose-Einstein condensation of diatomic molecules.

I. INTRODUCTION

Using the Gor'kov formulation of weak-coupling (BCS) theory, Cross has shown that the mass current density in weakly inhomogeneous superfluid ³He-A in local equilibrium is accurately given at zero temperature by¹

$$\bar{g} = \rho \bar{v}_s + \frac{\hbar}{4M} \rho \bar{\nabla} \times \bar{l} - \frac{\hbar}{2M} \rho \bar{l} (\bar{l} \cdot \bar{\nabla} \times \bar{l}) \quad (1.1)$$

where \bar{v}_s is the superfluid velocity, \bar{l} is the local anisotropy axis, and ρ is the total mass density of the helium. There are small corrections to Eq. (1.1) due to the fact that particle-hole symmetry is not exact.

Recently, however, Ishikawa *et al.*² have described a calculation of the zero-temperature mass current based on the configuration space form of the BCS ground state,³

$$\Psi_N(12 \cdots N) = \alpha \phi(12) \cdots \phi(N-1, N) \quad (1.2)$$

They find that

$$\bar{g} = \rho \bar{v}_s + \frac{\hbar}{4M} \bar{\nabla} \times \rho \bar{l} \quad (1.3)$$

No assumption of particle-hole symmetry is made, and Eq. (1.3) is said to be an exact consequence of Eq. (1.2) to linear order in the gradient expansion.

The discrepancy between the results of Cross and Ishikawa *et al.* casts doubt not only on the form for the low-temperature current in ³He-A, but also, more generally, on the equivalence between calculations based on the Gor'kov equations and calculations

based on the configuration-space wave function Ψ_N . We wish to resolve these uncertainties by describing a third calculation of the ground-state current density. We find

$$\bar{g} = \rho \bar{v}_s + \frac{\hbar}{4M} \bar{\nabla} \times \rho \bar{l} - \frac{\hbar}{2M} c_0 \bar{l} (\bar{l} \cdot \bar{\nabla} \times \bar{l}) \quad (1.4)$$

where

$$c_0 = M \int_{-\infty}^{\infty} \frac{dk_z}{2\pi^2} \bar{k}_z^2 n(0, 0, \bar{k}_z) \quad (1.5)$$

$n(\bar{k})$ is the local equilibrium single-particle k -space occupation number (for either spin population), and the z -axis is along the direction of $\bar{l}(\bar{r})$.

Our calculation is also based on the ground state Ψ_N , and our current does indeed reduce to that of Ishikawa *et al.*, provided the range of the pair wave function ϕ in the relative coordinate is small compared with the interatomic spacing.⁴ In this limit, however, the state Ψ_N is describing the Bose-Einstein condensation of diatomic molecules, and *not* Cooper pairing.

The current (1.3) is precisely what one would have expected without any elaborate calculation for a condensate with a number density $N(\bar{r}) = \rho(\bar{r})/2M$ of molecules each possessing an intrinsic angular momentum $\bar{L}(\bar{r}) = \hbar \bar{l}(\bar{r})$. The first term in Eq. (1.3) gives the contribution to the current from molecular center-of-mass motion, while the second term gives the bound current produced by the internal motion. Such internal motion can produce a macroscopic current at constant density if the direction

of \bar{L} varies or at uniform \bar{L} if there is a variation in the mass density. The bound current density $\frac{1}{2}\bar{\nabla} \times [N(\bar{r})\bar{L}(\bar{r})]$ is quite analogous to the bound electric current density $\bar{j} = c\bar{\nabla} \times \bar{M}$ of macroscopic electrodynamics, and its meaning can be fully elucidated by simple classical models.

In ${}^3\text{He-A}$, on the other hand, the range of ϕ is large compared with the interatomic spacing. Because the energy gap vanishes along the direction of \bar{T} , $n(0, 0, \bar{k}_z)$ is identical to the normal-state zero-temperature Fermi distribution. Hence the coefficient c_0 in Eq. (1.4) becomes just $Mk_F^3/3\pi^2$, which is identical to the mass density in a paired system with particle-hole symmetry. Thus the third term of Eq. (1.4) reduces to the third term of the Cross current (1.1) in the pairing limit. We believe that the analysis of Ref. 2 fails to include this case because a nonvanishing $n(0, 0, \bar{k}_z)$ is necessarily accompanied by singular behavior in the pair wave function ϕ (Appendix A). This singularity can be allowed for, but if it is not explicitly taken into account the third term in the current (1.4) can easily be overlooked.

Note also that in ${}^3\text{He-A}$ the mass density is virtually uniform, although states of the form (1.2) need not be so restricted. Thus in the physically relevant case the second term of the current (1.4) reduces to the second term of the Cross current (1.1). More precisely, however, even at uniform (in this case zero) temperature and uniform chemical potential and in the absence of external fields, the local equilibrium mass density in ${}^3\text{He-A}$ can still have very slight spatial variations provided the amplitude of the local energy gap varies and provided that particle-hole symmetry is not exact. If this possibility is allowed for, the second term of Eq. (1.4) will give, in addition to the second term of Eq. (1.1), a small correction

$$\frac{\hbar}{4M}\bar{\nabla} \times \rho\bar{T} = \frac{\hbar}{4M}\rho\bar{\nabla} \times \bar{T} + \frac{\hbar}{4M}\left(\frac{\partial\rho}{\partial|\Delta|^2}\right)_{\mu,T}\bar{\nabla}|\Delta|^2 \times \bar{T} \quad (1.6)$$

The additional term is precisely the small term which breaks particle-hole symmetry that Cross identifies as the contribution to the current from a very small intrinsic pair angular momentum.

Thus both forms (1.1) and (1.3) for the current density are limiting cases of the more general form (1.4). The form (1.3) of Ishikawa *et al.* holds in the molecular limit; the Cross form (1.1) emerges in the pairing limit, when nonuniformities in the mass density are negligibly small.

Before proceeding to our calculation, we add a cautionary remark and succumb to an irresistible temptation:

The fields \bar{T} and \bar{v} , appearing in Eqs. (1.1), (1.3), and (1.4) are defined by assuming that a certain

quantity has locally the A -phase symmetry. Cross takes the quantity to be the gap Δ , we take it to be the order parameter ψ , and Ishikawa *et al.* assume both ψ and the pair wave function ϕ have this form. In the uniform case if one quantity has the required form, so will the other two. In the nonuniform case this is often true to linear order in the gradient expansion, but it need not be (Appendix C). In the event of a disagreement, the correct quantity is almost certainly the order parameter.

We cannot resist adding a few remarks on the old and, by now, somewhat metaphysical question of "intrinsic pair angular momentum". It seems indisputable that in the molecular limit where the current assumes the form (1.3), the term $(\hbar/4M)\bar{\nabla} \times (\rho\bar{T})$ describes the contribution to the current from a density $\rho/2M$ of carriers of angular momentum $\hbar\bar{T}$. Precisely this term continues to be present in the pairing limit. Its structure is obscured by the fact that the mass density is virtually uniform in this limit and its significance is rendered uncertain by the appearance of another term in the derivatives of \bar{T} . Under such conditions it is wisest to abandon the concept of intrinsic pair angular momentum and ask only questions with specific calculable answers.

If, however, one does identify an intrinsic angular momentum using the criterion given by Cross, then we maintain that, when properly applied, that criterion gives an intrinsic angular momentum of $\frac{1}{2}\hbar$ per atom at $T=0$. The Cross criterion is to identify the intrinsic angular momentum from the form of the current when only the amplitude of the energy gap varies. Under such conditions he finds a current numerically equal to

$$\frac{\hbar}{4M}\left(\frac{\partial\rho}{\partial|\Delta|^2}\right)_{\mu,T}\bar{\nabla}|\Delta|^2 \times \bar{T} \quad (1.7)$$

Because $\rho(\mu, T, |\Delta|^2=0)$ is uniform at uniform μ and T , this term can equally well be written

$$\frac{\hbar}{4M}\bar{\nabla}[\rho(\mu, T, |\Delta|^2) - \rho(\mu, T, |\Delta|^2=0)] \times \bar{T} \quad (1.8)$$

and it is $[\rho(\mu, T, |\Delta|^2) - \rho(\mu, T, |\Delta|^2=0)]/2M$ that Cross identifies with the density of carriers of angular momentum $\hbar\bar{T}$.⁵

The ambiguity permitting this subtraction can be removed by the device of applying an external field U as an additional source of nonuniform density at uniform μ and T . In Appendix B we demonstrate directly from the Gor'kov equations that at uniform \bar{T} and \bar{v} , such a potential gives rise to an additional term which at $T=0$ assumes the form

$$\frac{\hbar}{4M}\left(\frac{\partial\rho}{\partial U}\right)_{\mu,T,|\Delta|^2}\bar{\nabla}U \times \bar{T} \quad (1.9)$$

precisely as Eq. (1.4) requires. Thus the term $(\hbar/4M)\vec{\nabla}\rho \times \vec{1}$ is not an artifact of possible pathologies in the configuration-space ground state Ψ_N , but is also implied by the orthodox formalism.

In Sec. II we derive the mass current (1.4) from the N -particle wave function (1.2), indicating where we believe Ishikawa *et al.* lost the third term. The calculation itself might be of some additional interest because of the way in which the distinction between Bose-Einstein condensed diatomic molecules and Cooper pairs can be followed through successive steps.

Several more technical points are relegated to the Appendices: In Appendix A we examine in somewhat more detail the conditions under which the state Ψ_N describes tightly bound Bose-Einstein condensed molecules. We also examine the singularities that must arise in the pair wave function ϕ in the limit of Cooper pairing.

In Appendix B we generalize the Cross calculation to the case in which a slowly varying external potential U is present to demonstrate directly that the Gor'kov equations also give a term in $\vec{\nabla} \times (\rho \vec{1})$ rather than $\rho \vec{\nabla} \times \vec{1}$, when ρ is permitted to vary.

In Appendix C we examine the relation between the pair wave function ϕ and the order parameter ψ for spatially nonuniform systems.

In Appendix D we discuss some further problems raised by a recent paper of McClure and Takagi.⁶

In Appendix E we derive an important relation between the one-particle density matrix and the order parameter [Eq. (2.9)] directly from the weak-coupling Gor'kov equations at zero temperature.

II. COMPUTATION OF THE MASS CURRENT DENSITY

We compute the mass current density in the state Ψ_N by computing the one-particle density matrix,⁷

$$\rho(11') = N \Psi_N(12 \cdots N) \Psi_N^*(1'2 \cdots N) \quad (2.1)$$

The calculation is most simply performed by relating the one-particle density matrix to the order parameter.⁸ The order parameter ψ (1,2) is found from the asymptotic behavior of the two-particle density matrix

$$\begin{aligned} \rho^{(2)}(12, 1'2') &= N(N-1) \Psi_N(123 \cdots N) \\ &\quad \times \Psi_N^*(1'2'3 \cdots N) \quad , \quad (2.2) \end{aligned}$$

when the pair of points \vec{r}_1, \vec{r}_2 is far removed from the pair \vec{r}'_1, \vec{r}'_2 . In this limit

$$\rho^{(2)}(12, 1'2') \sim \psi(12)\psi^*(1'2') \quad (2.3)$$

It can be shown⁹ that when Ψ_N is of the form (1.2) there is a nonvanishing order parameter. Furthermore, the one-particle density matrix is related to the

order parameter by¹⁰

$$\rho(11') - \rho(12)\rho(21') = \psi(12)\psi^*(1'2) \quad (2.4)$$

We express both ρ and ψ in terms of the center-of-mass variable $\vec{r} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ and the difference variable $\vec{r} = \vec{r}_1 - \vec{r}_2$. We shall compute¹¹

$$\rho(\vec{r}, \vec{p}) = \int d^3\vec{r}' e^{-i\vec{p}\cdot\vec{r}'} \rho(12) \quad , \quad (2.5)$$

in terms of which the mass current density is given by

$$\vec{g}(\vec{r}) = \int \frac{d^3p}{(2\pi)^3} \vec{p} \text{tr} \rho(\vec{r}, \vec{p}) \quad (2.6)$$

(where the trace is over the spin variables).

It is convenient to introduce the functional product notation

$$f \cdot g(1, 2) = f(13)g(32) \quad (2.7)$$

and the notation f^+ for the function

$$f^+(12) = f^*(21) \quad (2.8)$$

With this notation we can write Eq. (2.4) in the form

$$\rho - \rho \cdot \rho = \psi \cdot \psi^+ \quad (2.9)$$

We wish to evaluate the current when ρ and ψ are slowly varying functions of the center-of-mass variable. For this purpose we use the gradient expansion¹²

$$f \cdot g = f(\vec{r}, \vec{p})g(\vec{r}, \vec{p}) + \frac{1}{2}i[f(\vec{r}, \vec{p}), g(\vec{r}, \vec{p})] \quad (2.10)$$

corrections to which are of second order in the center-of-mass gradients. Here $f(\vec{r}, \vec{p})$, $g(\vec{r}, \vec{p})$, and $f \cdot g(\vec{r}, \vec{p})$ are 2×2 , (spin) matrix functions of \vec{r} and \vec{p} , and the spin structure of the Poisson bracket $[f, g]$ is given by

$$[f, g]_{s_1 s_2} = \sum_{s_3, i} \left(\frac{\partial}{\partial r_i} f_{s_1 s_3} \frac{\partial}{\partial p_i} g_{s_3 s_2} - \frac{\partial}{\partial p_i} f_{s_1 s_3} \frac{\partial}{\partial r_i} g_{s_3 s_2} \right) \quad (2.11)$$

To zeroth order in center-of-mass gradients, the relation between density matrix and order parameter is given by ignoring the Poisson bracket in the gradient expansion (2.10). Equation (2.9) then gives

$$\rho^{(0)}(\vec{r}, \vec{p}) - \rho^{(0)}(\vec{r}, \vec{p})^2 = \psi(\vec{r}, \vec{p})\psi^+(\vec{r}, \vec{p}) \quad (2.12)$$

[where $\psi^+(\vec{r}, \vec{p})$ is the adjoint of the 2×2 matrix $\psi(\vec{r}, \vec{p})$]. This gives a $\text{tr} \rho^{(0)}$ which is even in \vec{p} and yields no current.

To find the current induced by a nonuniform order parameter to leading nonvanishing order in the center-of-mass gradients, we write

$$\rho = \rho^{(0)} + \rho^{(1)} \quad (2.13)$$

where $\rho^{(1)}$ is linear in the gradients. The term in ρ^2 in Eq. (2.9) gives

$$\begin{aligned} (\rho \cdot \rho)(\vec{r}, \vec{p}) &= \rho^{(0)2}(\vec{r}, \vec{p}) + \rho^{(0)}(\vec{r}, \vec{p})\rho^{(1)}(\vec{r}, \vec{p}) \\ &+ \rho^{(1)}(\vec{r}, \vec{p})\rho^{(0)}(\vec{r}, \vec{p}) \\ &+ \frac{1}{2}i[\rho^{(0)}(\vec{r}, \vec{p}), \rho^{(0)}(\vec{r}, \vec{p})] , \end{aligned} \quad (2.14)$$

to first order in the gradients. The term in ψ gives

$$\begin{aligned} (\psi \cdot \psi^+)(\vec{r}, \vec{p}) &= \psi(\vec{r}, \vec{p})\psi^+(\vec{r}, \vec{p}) \\ &+ \frac{1}{2}i[\psi(\vec{r}, \vec{p}), \psi^+(\vec{r}, \vec{p})] . \end{aligned} \quad (2.15)$$

In the A phase of ${}^3\text{He}$ (and in any of the so-called "unitary" phases) $\psi\psi^+$ and hence $\rho^{(0)}$ are diagonal in spin. Consequently the second and third terms of Eq. (2.14) are the same, and the Poisson bracket vanishes. Assembling Eqs. (2.13)–(2.15) into Eq. (2.9), and using the defining relation (2.12) for $\rho^{(0)}$, we find^{13,14}

$$\rho^{(1)} = \frac{1}{1-2\rho^{(0)}} \frac{i}{2}[\psi, \psi^+] . \quad (2.16)$$

The other relevant features of the A -phase order parameter are contained in the general form¹⁵

$$\psi(\vec{r}, \vec{p}) = (\vec{d}(\vec{r}) \cdot \vec{\sigma}) i \sigma_y c(\vec{r}, \vec{p}) f(\vec{r}, \vec{p}) . \quad (2.17)$$

Here \vec{d} is a real unit vector and c is a complex polynomial in \vec{p} of the form

$$c(\vec{r}, \vec{p}) = \frac{1}{\sqrt{2}}[\vec{\phi}^{(1)}(\vec{r}) + i\vec{\phi}^{(2)}(\vec{r})] \cdot \vec{p} , \quad (2.18)$$

where the $\vec{\phi}^{(i)}$ are a pair of orthogonal unit-vector fields. The function $f(\vec{r}, \vec{p})$ is real and has cylindrical symmetry as a function of \vec{p} about the axis $\vec{l}(\vec{r}) = \vec{\phi}^{(1)}(\vec{r}) \times \vec{\phi}^{(2)}(\vec{r})$.

Using the form (2.17) we find that Eq. (2.16) gives

$$\text{tr}\rho^{(1)} = \frac{1}{1-2\rho^{(0)}} \text{Im}[c^* f, c f] , \quad (2.19)$$

where the bracket is now just the ordinary Poisson bracket of the two functions $c^* f$ and $c f$. Because f is real, elementary Poisson bracket identities permit one to cast Eq. (2.19) in the form

$$\text{tr}\rho^{(1)} = \frac{1}{1-2\rho^{(0)}} \text{Im} \frac{1}{c} [|c f|^2, c] . \quad (2.20)$$

Now Eq. (2.17) gives

$$\psi(\vec{r}, \vec{p})\psi^+(\vec{r}, \vec{p}) = |c f|^2 \quad (2.21)$$

and therefore we have from Eq. (2.12)

$$\vec{\nabla} |c f|^2 = (1-2\rho^{(0)}) \vec{\nabla} \rho^{(0)} \quad (2.22)$$

for either the r derivatives or the p derivatives of

$|c f|^2$. Consequently Eq. (2.20) can be simplified to¹⁶

$$\text{tr}\rho^{(1)} = \text{Im} \frac{1}{c} [\rho^{(0)}, c] = \text{Im} \left[\frac{\rho^{(0)}}{c}, c \right] . \quad (2.23)$$

Since $\rho^{(0)}$ does not contribute to the mass current (2.6), the leading terms in the current are given by

$$\vec{g}(\vec{r}) = \int \frac{d^3 p}{(2\pi)^3} \vec{p} \text{tr}\rho^{(1)} = \int \frac{d^3 p}{8\pi^3} \vec{p} \text{Im} \left[\frac{\rho^{(0)}}{c}, c \right] . \quad (2.24)$$

We can rewrite this in the form

$$\begin{aligned} g_i(\vec{r}) &= \int \frac{d^3 p}{8\pi^3} p_i \left\{ \frac{\partial}{\partial r_j} \text{Im} \left[\frac{\rho^{(0)}}{c} \frac{\partial c}{\partial p_j} \right] \right. \\ &\quad \left. - \frac{\partial}{\partial p_j} \text{Im} \left[\frac{\rho^{(0)}}{c} \frac{\partial c}{\partial r_j} \right] \right\} . \end{aligned} \quad (2.25)$$

It is convenient to deal separately with the two terms in Eq. (2.25). This can be done provided one attends to the following somewhat delicate point¹⁷:

Should the polynomial c vanish anywhere, then although this leads to no singularities in the original integral¹⁸ it might produce divergences in each piece if Eq. (2.25) is treated as two separate integrals. This possibility can be dealt with by removing from the range of integration small regions containing the zeros of c . Since these are not singular regions of the original integrand the value of the integral is unaffected by their removal, provided the volume of the removed regions is taken to zero after the integral is evaluated. In this way one can control any artificial divergences that might arise when the integral is split. The removal is accomplished by inserting into the integrand of Eq. (2.25) a function $\theta(|c|^2)$ with

$$\theta(x) = 1, \quad x \geq \lambda , \quad (2.26)$$

$$\theta(x) = 0, \quad \lambda > x \geq 0 .$$

The limit $\lambda \rightarrow 0$ is to be taken after the pieces of the integral are evaluated.

With the θ function installed in the integrand we may separate the two pieces of Eq. (2.25) with impunity. We may take the r derivative outside of the first piece provided we subtract the resulting derivative of the θ function; we may integrate by parts in the second piece, provided we take account of the resulting p derivative of the θ function. The result is

$$\begin{aligned} g_i(\vec{r}) &= \frac{\partial}{\partial r_j} \int \frac{d^3 p}{8\pi^3} \rho^{(0)} p_i \text{Im} \left[\frac{1}{c} \frac{\partial c}{\partial p_j} \right] \theta(|c|^2) \\ &+ \int \frac{d^3 p}{8\pi^3} \rho^{(0)} \text{Im} \left[\frac{1}{c} \frac{\partial c}{\partial r_i} \right] \theta(|c|^2) \\ &+ \int \frac{d^3 p}{8\pi^3} \rho^{(0)} p_i \text{Im}[c, c^*] \theta'(|c|^2) , \end{aligned} \quad (2.27)$$

where the contributions from the neighborhood of the zeros of c produced by the derivatives of the θ function are grouped together in the third term.

The three terms in Eq. (2.27) are all easily evaluated when c has the form (2.18), and taking the limit $\lambda \rightarrow 0$ causes no difficulty. The first term in Eq. (2.27) gives $\frac{1}{4} \vec{\nabla} \times (\rho \vec{\Gamma})$, where $\rho(\vec{r})$ is the mass density

$$\rho(\vec{r}) = \int \frac{d^3 p}{4\pi^3} \rho^{(0)}(\vec{r}, \vec{p}) \quad (2.28)$$

and

$$\vec{\Gamma}(\vec{r}) = \vec{\phi}^{(1)}(\vec{r}) \times \vec{\phi}^{(2)}(\vec{r}) \quad (2.29)$$

The second term gives $\rho \vec{v}_s$, where¹⁹

$$\vec{v}_s = \frac{1}{2} \phi_i^{(1)} \vec{\nabla} \phi_i^{(2)} \quad (2.30)$$

To evaluate the third term,²⁰ note that c vanishes if and only if \vec{p} lies along the direction of $\vec{\Gamma}$. Taking this direction as the z axis, one finds a contribution to the mass current of

$$-\vec{\Gamma}(\vec{\Gamma} \cdot \vec{\nabla} \times \vec{\Gamma}) \int_{-\infty}^{\infty} \frac{dp_z}{(2\pi)^2} \rho^{(0)}(\vec{r}, 0, 0, p_z) p_z^2 \quad (2.31)$$

which gives the third term in Eq. (1.4) with the value (1.5) for the coefficient c_0 .

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APPENDIX A

We examine some pertinent features of the pair wave function ϕ , the order parameter ψ , and the density matrix ρ in the two limiting cases of Cooper pairing and the Bose-Einstein condensation of diatomic molecules.

The order parameter is related to the pair wave function by²¹

$$\psi = \lambda \phi - \lambda^2 \phi \cdot \phi^+ \cdot \psi \quad (A1)$$

where λ is a normalization constant fixed by the condition

$$N = \rho(11) \quad (A2)$$

The relation (2.9) between density matrix and order parameter can be expressed in any of the following equivalent forms²¹:

$$\begin{aligned} \rho &= \lambda \psi \cdot \phi^+ = \lambda \phi \cdot \psi^+ \\ &= \lambda^2 \phi \cdot \phi^+ - \lambda^2 \phi \cdot \phi^+ \cdot \rho \end{aligned} \quad (A3)$$

If the quadratic term in ρ were absent from Eq. (2.9) then in view of the normalization condition (A2) the relation between density matrix and order parameter would be simply

$$\rho(11') = \frac{N}{2} \left[\frac{2\psi(12)\psi^*(1'2)}{\psi(34)\psi^*(34)} \right] \quad (A4)$$

This is just $\frac{1}{2}N$ times the one-particle density matrix for a two-particle system whose wave function is proportional to ψ —i.e., the one-particle properties of the system are precisely those of a Bose condensate of $\frac{1}{2}N$ diatomic molecules, each with wave function ψ .

It follows from the third of the forms (A3) that $\rho \cdot \rho$ will be negligible compared with ρ provided $\lambda^2 \phi \cdot \phi^+$ is negligible compared with unity. When the latter condition holds, Eq. (A1) gives $\psi = \lambda \phi$. Thus in the molecular limit the order parameter is simply proportional to the pair wave function.

Note also that the condition $\rho \cdot \rho \ll 1$ requires all eigenvalues of the integral operator $\rho(12)$ to be small compared with unity. Since these eigenvalues are the one-particle occupation numbers, the molecular limit is only attained if the N -fermion system described by the state Ψ_N is completely nondegenerate.

For a uniform system to be in the molecular limit we must have

$$\lambda^2 \phi(\vec{k}) \phi^+(\vec{k}) \ll 1 \quad (A5)$$

for all wave vectors \vec{k} . With $\rho = \lambda^2 \phi \cdot \phi^+$, the normalization condition (A2) gives²²

$$\lambda^2 = \frac{N}{V} / \int \frac{d^3 k}{4\pi^3} \phi(\vec{k}) \phi^+(\vec{k}) \quad (A6)$$

Equations (A6) and (A5) give the condition

$$\int \frac{d^3 k}{4\pi^3} \phi(\vec{k}) \phi^+(\vec{k}) / [\phi(\vec{k}) \phi^+(\vec{k})]_{\max} \gg \frac{N}{V} \quad (A7)$$

for the molecular limit to hold.

The left-hand side of Eq. (A7) is proportional to the volume of k space over which the nonvanishing part of the pair wave function is spread. By the uncertainty principle it is therefore proportional to the inverse cube of the spatial range of that wave function. We therefore find the expected condition that Eq. (1.2) will describe a Bose-Einstein condensate of fermion pairs, provided the range of the pair wave function is small compared with the mean interparticle spacing.

When $\rho(\vec{k})$ is not small compared with unity, the uniform system is described by the more general relations

$$\psi(\vec{k}) = \frac{\lambda\phi(\vec{k})}{1 + \lambda^2\phi(\vec{k})\phi^+(\vec{k})} \quad (\text{A8})$$

and

$$\rho(\vec{k}) = \frac{\lambda^2\phi(\vec{k})\phi^+(\vec{k})}{1 + \lambda^2\phi(\vec{k})\phi^+(\vec{k})} \quad (\text{A9})$$

with the normalization condition

$$n = \int \frac{d^3k}{4\pi^3} \frac{\lambda^2\phi(\vec{k})\phi^+(\vec{k})}{1 + \lambda^2\phi(\vec{k})\phi^+(\vec{k})} \quad (\text{A10})$$

Since $\phi\phi^+$ is a non-negative real number, the right-hand side of Eq. (A10) varies monotonically from zero at $\lambda=0$ to $(1/4\pi^3)\Omega$ as $\lambda \rightarrow \infty$, where Ω is the volume of k space in which $\phi\phi^+$ is nonzero. The normalization condition can thus be satisfied at a unique value of λ if and only if the volume Ω is larger than $\frac{4}{3}\pi k_F^3$ (where k_F is defined in terms of the number density n : $n = k_F^3/3\pi^2$). With this restriction on ϕ , there is no difficulty in normalizing the state Ψ_N .

Note, though, that with λ finite (A9) implies that values of \vec{k} at which there is complete degeneracy [i.e., $\rho(\vec{k}) = 1$] can only occur where the pair wave function diverges. Since the simplest cutoff models of pairing give perfect degeneracy and hence a divergent pair wave function for most of the interior of the Fermi sphere, the state (1.2) would appear to be disastrously ill suited to describe the pairing limit. In fact this pathology can be dealt with by the device of softening the cutoff to allow a minute but nonzero amplitude of the energy gap all the way down to $\vec{k}=0$. There are then no values of \vec{k} at which degeneracy is perfect (for s -wave pairing) and a manageable set of measure zero on which ϕ becomes singular (in the general case of anisotropic pairing).

At the end of the calculation, one must take the limit of vanishing "softening" and demonstrate that the final results are independent of the particular regularization procedure followed. This can be insured by working from the start not with the pair wave function ϕ , but the order parameter ψ , which Eq. (A8) requires to vanish harmlessly at points where ϕ diverges. If this is done no explicit regularization procedure need be introduced at all. This is the approach we have followed here.

It is important to recognize, however, that symmetry-determined values of \vec{k} at which $\psi(\vec{k})$ vanishes [and hence at which $\rho(\vec{k}) = 1$] cannot be dealt with by such a regularization procedure. In the case of $^3\text{He-A}$, the order parameter vanishes for \vec{k} along the direction of $\vec{\Gamma}$, and therefore ϕ is necessarily singular at such \vec{k} below the Fermi surface. This singularity leads to a very long-range term in the

dependence of ϕ on the components of the relative coordinate perpendicular to $\vec{\Gamma}$. To avoid difficulties produced by this term, gradient expansions should only be applied to expressions involving the density matrix and order parameter.

Note finally, that if $\phi(\vec{k})$ is of the A -phase form

$$\phi = (k_x + ik_y)f(k_\perp, k_z) \quad (\text{A11})$$

(with z along $\vec{\Gamma}$), then unless f diverges as $k_\perp \rightarrow 0$, ϕ will vanish on the z axis. But if $\phi(\vec{r})$ is short ranged, one can easily show that $f(k_\perp, k_z)$ is bounded as $k_\perp \rightarrow 0$. Hence $\rho(0, 0, k_z)$ must vanish identically in the molecular limit, according to Eq. (A9).

APPENDIX B

We introduce an external potential $U(\vec{r})$ as a device for inducing an appreciable density gradient at constant (zero) temperature and chemical potential. We then extend the Cross analysis to calculate the term in the current proportional to $\vec{\nabla}U$. It suffices to calculate at constant $\vec{\Gamma}$ and zero \vec{v}_s . We start with the fact that any change in the one-particle Green function G can be computed from the identity

$$\delta G = -G_0 \delta G^{-1} G_0 \quad (\text{B1})$$

where G^{-1} is given by

$$G^{-1} = \omega - \epsilon - \Delta \frac{1}{\omega + \epsilon} \Delta^+ \quad (\text{B2})$$

and G_0 is the zeroth-order Green function,

$$G_0 = \frac{\omega + \epsilon}{\omega^2 - E^2} = \frac{E + \epsilon}{2E} \frac{1}{\omega + E} + \frac{E - \epsilon}{2E} \frac{1}{\omega - E} \quad (\text{B3})$$

We first evaluate Eq. (B1) when the changes in G are the first order terms in $\vec{\nabla}U$. In the presence of U , the operator ϵ is given in the rp representation by $\epsilon(\vec{p}) + U(\vec{r})$, and the operator $(\omega + \epsilon)^{-1}$ is given by $1/[\omega + \epsilon(\vec{p}) + U(\vec{r})]$ with no corrections linear in the gradient of U . Applying the gradient expansion (2.10), we find

$$G^{(1)}(\vec{r}, \vec{p}) = -\frac{G_0^2}{(\omega + \epsilon)^2} \frac{i}{2} \{[\Delta, U]\Delta^+ + \Delta[U, \Delta^+]\} \quad (\text{B4})$$

or

$$\begin{aligned} \vec{p} \text{tr} G^{(1)}(\vec{r}, \vec{p}) &= \frac{1}{(\omega^2 - E^2)^2} \text{Im} \left[\Delta \vec{\nabla} U \cdot \frac{\partial \Delta^+}{\partial \vec{p}} \right] \vec{p} \\ &= \frac{1}{(\omega^2 - E^2)^2} f^2(\vec{p} \cdot \vec{\Gamma} \times \vec{\nabla} U) \vec{p} \quad (\text{B5}) \end{aligned}$$

where we have used the fact that in the A phase Δ

has the form

$$\Delta = \vec{d} \cdot \vec{\sigma} (i\sigma_y) (\vec{\phi}^{(1)} + i\vec{\phi}^{(2)}) \cdot \vec{p} f(p^2, (\vec{p} \cdot \vec{T})^2) ,$$

$$f, d \text{ real} . \quad (\text{B6})$$

We next compute the form of $\partial\rho/\partial U$, to zeroth order in the gradients. This also follows from Eq. (B1), which gives

$$\frac{\partial G}{\partial U} = G_0^2 \left[1 - \Delta \frac{1}{(\omega + \epsilon)^2} \Delta^+ \right]$$

$$= \frac{(E - \epsilon)^2}{(2E)^2} \frac{1}{(\omega - E)^2} + \frac{(E + \epsilon)^2}{(2E)^2} \frac{1}{(\omega + E)^2}$$

$$+ \frac{\Delta\Delta^+}{2E^2} \frac{1}{\omega^2 - E^2} - \frac{\Delta\Delta^+}{(\omega^2 - E^2)^2} . \quad (\text{B7})$$

To construct the mass current from Eq. (B5) or $\partial\rho/\partial U$ from Eq. (B7) we must do the frequency sums and integrate over momenta. The first two terms in Eq. (B7) have vanishing frequency sums at $T=0$, while the frequency sum of the third gives precisely the same contribution as the frequency sum of the last at $T=0$. Since

$$\Delta\Delta^+ = f^2 p_i p_j (\delta_{ij} - l_i l_j) , \quad (\text{B8})$$

if we write the current that results from Eq. (B5) in the form

$$g_i = \int d^3 p F(\vec{p}) p_i p_j (\vec{T} \times \vec{\nabla} U)_j , \quad (\text{B9})$$

then the $\partial\rho/\partial U$ that results from Eq. (B7) will have the form

$$\frac{\partial\rho}{\partial U} = -2 \int d^3 p F(\vec{p}) p_i p_j (\delta_{ij} - l_i l_j) . \quad (\text{B10})$$

The same function F appears in Eqs. (B9) and (B10). It depends only on the magnitude p and on $(\vec{p} \cdot \vec{T})^2$, so that $\int d^3 p (p_i p_j) F$ has the form

$$\int d^3 p p_i p_j F = A \delta_{ij} + B l_i l_j . \quad (\text{B11})$$

Substituting this into Eqs. (B9) and (B10) we find

$$g_i = A (\vec{T} \times \vec{\nabla} U)_i , \quad (\text{B12})$$

$$\frac{\partial\rho}{\partial U} = -4A , \quad (\text{B13})$$

and therefore²³

$$\vec{g} = -\frac{1}{4} \frac{\partial\rho}{\partial U} (\vec{T} \times \vec{\nabla} U) = \frac{1}{4} (\vec{\nabla}\rho)_{T, \mu|\Delta|^2} \times \vec{T} . \quad (\text{B14})$$

APPENDIX C

We show here that if a gradient expansion is valid for the integral equation relating the order parameter

ψ to the pair wave function ϕ , then to linear order in the gradients the order parameter $\psi(\vec{r}, \vec{p})$ will have the A -phase form specified by Eqs. (2.17) and (2.18) if the pair wave function $\phi(\vec{r}, \vec{p})$ has that form.

We stress that in many cases of interest (and, in particular, in the case of ${}^3\text{He-A}$ —see Appendix A) the pair wave function may well have too long a range to permit a gradient expansion at all. Note also that even when a gradient expansion can be performed, the result is by no means a foregone conclusion. For example (see below) a pair wave function of the B -phase form gives an order parameter that deviates from the B -phase form to linear order in the gradients.

We start with the relation (A1) between ψ and ϕ ,

$$\psi = \lambda\phi - \lambda^2\phi \cdot \phi^+ \cdot \psi . \quad (\text{C1})$$

If $\phi(\vec{r}, \vec{p})$ is of the general "unitary" form

$$\phi(\vec{r}, \vec{p}) = (\vec{\phi}(\vec{r}, \vec{p}) \cdot \vec{\sigma}) (i\sigma_y) , \quad (\text{C2})$$

with

$$\vec{\phi}(\vec{r}, \vec{p}) = g(\vec{r}, \vec{p}) \vec{d}(\vec{r}, \vec{p}) , \quad (\text{C3})$$

and $\vec{d}(\vec{r}, \vec{p})$ a real unit vector, then the zeroth-order solution to Eq. (C1) is

$$\psi^{(0)}(\vec{r}, \vec{p}) = \frac{\lambda\phi(\vec{r}, \vec{p})}{1 + \lambda^2|g(\vec{r}, \vec{p})|^2} , \quad (\text{C4})$$

which is easily seen to be of the form given by Eqs. (2.17) and (2.18) if ϕ is of that form.

We now show that the first-order corrections to ψ in a gradient expansion of Eq. (C1) vanish. The gradient expansion (2.10) gives

$$\psi^{(1)} = \frac{-\lambda^2}{(1 + \lambda^2|g|^2)} \frac{1}{2i} \{ [\phi, \phi^+] \psi^{(0)} + [\phi\phi^+, \psi^{(0)}] \}$$

$$\text{or} \quad (\text{C5})$$

$$\psi^{(1)} = \frac{-\lambda^3}{(1 + \lambda^2|g|^2)^2} \frac{1}{2i} \{ [\phi, \phi^+] \phi + [\phi\phi^+, \phi] \} . \quad (\text{C6})$$

Using the forms (C2) and (C3) for ϕ and exploiting the fact that \vec{d} is real, one finds that

$$[\phi, \phi^+] \phi + [\phi\phi^+, \phi] = |g|^2 g \epsilon_{ijk} [d_i, d_j] d_k . \quad (\text{C7})$$

In the A -phase form, however, the vector \vec{d} is independent of \vec{p} , and therefore $\psi^{(1)}$ vanishes.

We emphasize that in nonuniform configurations one cannot take it for granted that a local symmetry of the pair wave function will be inherited by the order parameter, even to first order in a valid gradient expansion. For example the pair wave function is locally of the form characterizing ${}^3\text{He-B}$ if

$$d_i(\vec{r}, \vec{p}) = R_{ij}(\vec{r}) p_j \quad (\text{C8})$$

and R is a real orthogonal matrix. In this case (C7)

does not vanish identically, leading to the rather surprising conclusion that a pair wave function of the (triplet) B -wave form gives an order parameter with a *singlet* piece in linear order of the gradient expansion.

APPENDIX D

In a recent letter McClure and Takagi⁶ compute the angular momentum for a class of states of the form (1.2) for which the order parameter is locally of the A -phase form, with a spatial inhomogeneity that is constrained to have cylindrical symmetry about a given line (taken to be in the z direction). They find that L_z has the mean value $\frac{1}{2}N\hbar$ independent of the detailed form of the inhomogeneity. Their result is also independent of whether the inhomogeneity is weak; no gradient expansion is made.

Since the total angular momentum is the volume integral of $\vec{r} \times \vec{g}$, it is natural to ask whether our form (1.4) leads to this result. We find that the first two terms of Eq. (1.4) by themselves give precisely the McClure-Takagi angular momentum for all configurations satisfying their symmetry conditions. In demonstrating this we adopt the McClure and Takagi boundary condition that the density should vanish at the surface of the container. It is then essential that the second term in the current (1.4) is $\vec{\nabla} \times (\rho \vec{l})$ and not $\rho \vec{\nabla} \times \vec{l}$. Thus provided the twist $\vec{l} \cdot \vec{\nabla} \times \vec{l}$ vanishes [so that the third term of Eq. (1.4) is absent] and provided the Cross "intrinsic angular momentum" is interpreted as a manifestation of the term in $\vec{l} \times \vec{\nabla} \rho$, there is no contradiction between the McClure-Takagi result and any of the textural calculations they mention of Cross and Brinkman,⁵ or Mermin and Ho.¹⁹

There are, however, within the class of order parameters considered by McClure and Takagi, configurations of nonvanishing twist for which the third term in the current (1.4) gives a nonvanishing contribution to $\int \vec{r} \times \vec{g} d^3r$, thereby contradicting their general result.

The fact that a pair wave function leading to a nonvanishing third term in Eq. (1.4) must necessarily be very long ranged (see Appendix A) might make one wonder whether McClure and Takagi inadvertently discard important terms in apparently innocent analytical manipulations. However there is a slightly different way to formulate their result, which sharpens the paradox. If one takes the function carrying the symmetry to be not the order parameter ψ but the pair wave function ϕ then the entire N -particle state can be shown to be an *eigenstate* of L_z . The value of the angular momentum is then an immediate consequence of simple symmetry arguments, and the source of the discrepancy with the gradient expansion must be sought elsewhere.

The resolution is not to be found in the delicate

distinction between symmetries of ψ and ϕ discussed in Appendix C, for it is easily shown²⁴ that if ϕ has the McClure-Takagi symmetry so does ψ . Nor do we believe that higher-order terms in the gradient expansion will make significant contributions to the volume integral of $\vec{r} \times \vec{g}$.

We suspect that the difficulty can be traced to the condition that Ψ_N , and hence the pair wave function ϕ , must vanish at the surface of the cylindrical vessel. This means that the range of ϕ is in fact bounded by the radius of the cylinder. Our conclusion (Appendix A) that a ϕ of finite range led to a vanishing coefficient c_0 in the current (1.4) was based on an analysis of the infinite system. Whether or not c_0 must vanish when the range is of the order of the size of the system is an open question. Quite aside from this unresolved point, it is possible that the gradient expansion itself may break down in the rather peculiar surface layer through which the density must drop *slowly* to zero. Such a model of the surface region is, of course, quite unphysical, but it is worth investigating in the attempt to resolve the discrepancy.

We believe that it is important to find the origin of this paradox, whether it be physical or mathematical, because until it is found it is difficult to exclude another possible explanation with definite physical consequences: that the entire third term in the current (1.4) is nothing but an unphysical manifestation of a subtle failure of the bulk gradient expansion. We regard this as unlikely, but it must be kept in mind until the McClure-Takagi paradox is settled.

APPENDIX E

We show here that the relation (2.4) [or (2.9)] between the one-particle density matrix and the order parameter is a general consequence of the weak-coupling Gor'kov equations at zero temperature, being unaltered by the presence of (not necessarily slowly varying) external fields.

We take the Gor'kov equations in the form

$$\begin{aligned} (\omega - \epsilon)G &= 1 + \Delta F, \\ (\omega + \epsilon)F &= \Delta^+ G. \end{aligned} \quad (E1)$$

It is easily verified that these are solved by

$$\begin{aligned} G &= \sum_{\alpha} \frac{|\alpha 1\rangle \langle \alpha 1|}{\omega - \epsilon_{\alpha}}, \\ F &= \sum_{\alpha} \frac{|\alpha 2\rangle \langle \alpha 1|}{\omega - \epsilon_{\alpha}}, \end{aligned} \quad (E2)$$

where the sets of ket vectors $|\alpha 1\rangle$ and $|\alpha 2\rangle$ solve

the Hermitian eigenvalue

$$\begin{pmatrix} \epsilon & \Delta \\ \Delta^+ & -\epsilon \end{pmatrix} \begin{pmatrix} |\alpha 1\rangle \\ |\alpha 2\rangle \end{pmatrix} = \epsilon_\alpha \begin{pmatrix} |\alpha 1\rangle \\ |\alpha 2\rangle \end{pmatrix}, \quad (\text{E3})$$

and the eigenkets satisfy the orthonormality and completeness relations

$$\sum_{\mu=1,2} \langle \alpha \mu | \alpha' \mu \rangle = \delta_{\alpha\alpha'}, \quad (\text{E4})$$

$$\sum_{\alpha} |\alpha \mu\rangle \langle \alpha \nu| = \delta_{\mu\nu} 1. \quad (\text{E5})$$

In weak coupling Δ is independent of frequency and there is therefore no frequency dependence to G and F beyond that explicit in Eq. (E2). The frequency sums can therefore be performed to construct the density matrix ρ from G and the order parameter ψ^+

from F ,

$$\rho = \sum_{\alpha} f(\epsilon_{\alpha}) |\alpha 1\rangle \langle \alpha 1|, \quad (\text{E6})$$

$$\psi^+ = \sum_{\alpha} f(\epsilon_{\alpha}) |\alpha 2\rangle \langle \alpha 1|, \quad (\text{E7})$$

where f is the Fermi function.

If we square the form (E6) for ρ , use the orthonormality condition (E4), and identify one of the resulting terms with the aid of (E7), we find,

$$\rho^2 + \psi\psi^+ = \sum_{\alpha} f(\epsilon_{\alpha})^2 |\alpha 1\rangle \langle \alpha 1|. \quad (\text{E8})$$

At zero temperature f is either zero or unity, so the sum on the right-hand side of (E8) reduces back to ρ [cf. Eq. (E6)], which yields Eq. (2.9).

- ¹M. C. Cross, *J. Low Temp. Phys.* **21**, 525 (1975); and Ph.D. thesis (Cambridge University, 1975) (unpublished). There are no Fermi-liquid corrections to Eq. (1.1). Strong-coupling corrections have not been computed.
- ²M. Ishikawa, K. Miyake, and T. Usui, in *Physics at Ultralow Temperatures*, edited by T. Sugawara *et al.* (Physical Society of Japan, Tokyo, 1978), p. 159.
- ³See, for example, V. Ambegaokar, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969), Vol. 1, p. 259 (Sec. IIC). Here 1, 2, ... stand for the space and spin indices $\bar{r}_1 s_1, \bar{r}_2 s_2, \dots$ and the operator \mathcal{Q} antisymmetrizes and normalizes.
- ⁴This is shown in Appendix A, where we demonstrate that if ϕ is short ranged, then $n(0, 0, \bar{k}_z)$ is identically zero.
- ⁵According to Brinkman and Cross [W. K. Brinkman and M. C. Cross, in *Progress in Low Temperature Physics*, edited by D. F. Brewer (North-Holland, Amsterdam, 1978), Vol. VII A, p. 105]. Combescot pointed out that the Cross intrinsic term had this structure, but offered an (unreported) interpretation they claimed not to understand. Since Combescot is on record [Roland Combescot, *Phys. Rev. B* **18**, 6071 (1978)] as favoring an intrinsic angular momentum density of zero, his interpretation would evidently not be the same as ours. See also R. Combescot, *Phys. Rev. B* **18**, 3139 (1978).
- ⁶M. G. McClure and S. Takagi, *Phys. Rev. Lett.* **43**, 596 (1979).
- ⁷We use the convention that repeated indices are integrated over space and summed on spin.
- ⁸Aside from being simple algebraically, this approach avoids many of the difficulties arising from the possible singular behavior of the pair wave function. Details of the relation between the order parameter and the pair wave function are examined in Appendices A and C.
- ⁹For this and other properties of the state Ψ_N see V. Ambegaokar, in Ref. 3.
- ¹⁰This follows from Eqs. (148)–(151) of Ref. 3. The relation is also derived from the conventional BCS ground

state of an inhomogeneous system by J. G. Valatin, *Phys. Rev.* **122**, 1012 (1961), Eq. (8a). In Appendix E we show that the relation follows directly from the weak-coupling Gor'kov equations at zero temperature, in the presence of arbitrary spatial inhomogeneities. Note that if the term quadratic in ρ were absent, Eq. (2.4) would, to within a normalization constant, be the expression for the one-particle density matrix of a two-particle system with wave function ψ . Aspects of this limiting case, in which the state (1.2) describes a Bose-Einstein condensate of diatomic molecules, are examined in Appendix A. It is interesting to bear in mind, while reading Sec. II, that it is only this quadratic term in ρ that distinguishes diatomic molecules from Cooper pairs.

- ¹¹Except where we wish to emphasize the role played by the Planck constant or the ³He atomic mass, we shall use units in which \hbar and M are both equal to unity. (The reader is warned that an equally common convention is to set M equal to one-half.)
- ¹²See, for example, N. R. Werthamer, *Phys. Rev.* **132**, 663 (1963), Eqs. (7) and (8).
- ¹³Note that the nonlinear term in $\rho^{(0)}$ responsible for the difference between diatomic molecules and Cooper pairs is manifested only through the prefactor $1/(1-2\rho^{(0)})$.
- ¹⁴Note that to establish on the level of the gradient expansion the equivalence between Eq. (2.16) and the density matrix calculated from the Gor'kov equations, it is essential to take into account terms coming from the gradient expansion of the nonlocal relation between the order parameter and the energy gap.
- ¹⁵See, for example, A. J. Leggett, *Rev. Mod. Phys.* **47**, 331 (1975). See Appendix C for the conditions under which the pair wave function is also of this form.
- ¹⁶Note that the factor $1-2\rho^{(0)}$ distinguishing between Cooper pairs and diatomic molecules no longer appears explicitly in Eq. (2.23). Thus the gradient expansion of the one-particle density matrix for a two-particle system with wave function of the form (2.17) is also precisely of the form (2.23). At this level of the gradient expansion

the distinction between Cooper pairs and diatomic molecules is entirely contained within the structure of the density matrix $\rho^{(0)}$.

- ¹⁷We suspect that the failure of Ishikawa *et al.* to find the third term in Eq. (1.4) characteristic of Cooper pairing is due to their not having allowed for this difficulty.
- ¹⁸This follows from the fact that in the form (2.19) c appears explicitly only in the numerator while $\rho^{(0)}$, according to Eqs. (2.12) and (2.21) is either zero or unity at the zeros of c .
- ¹⁹N. D. Mermin and T. -L. Ho, Phys. Rev. Lett. **36**, 594 (1976).
- ²⁰This is the only term in which features of the density matrix other than the value of the total mass density play a role. It is therefore the only term that distinguishes between diatomic molecules and Cooper pairs. Since Eqs. (2.12) and (2.17) require $\rho^{(0)}$ to be either zero or unity at

the zeros of c , the term must vanish in the molecular limit (cf. Appendix A). It would be nice to have a simple picture for the origin of this term. We suspect that the manner in which it arises here entirely from the zeros of the energy gap below the Fermi sea is offering an important clue to its significance, but that significance continues to elude us.

²¹See Ref. 3.

²²For simplicity we consider only the "unitary" case in which $\phi\phi^+$ and ρ are diagonal in spin.

²³If U varies then so, in general, will the overall amplitude of the energy gap. The contribution from this variation is precisely the term (1.7) already calculated by Cross.

When added to Eq. (B14) this simply converts $(\partial\rho/\partial U)_{\mu,T,|\Delta|}$ to $(\partial\rho/\partial U)_{\mu,T}$.

²⁴S. Takagi (private communication, via M. G. McClure).