Spatial Dependence of the Order Parameter of Superfluid ^{3}He at the A-B Phase Boundary

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Accurate solutions of the Ginzburg-Landau equations describing the A-B phase boundary for a planar interface between ^{3}He-A and ^{3}He-B are calculated near the tricritical pressure and classified in terms of simple discrete symmetries. The order-parameter components of the A-B phase boundary and the interfacial energy $\sigma_{AB}(T)$ deviate considerably from previous variational calculations.

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It is known that in the absence of a magnetic field the two superfluid phases A and B of ^{3}He coexist at a particular temperature T_{AB}, which is a function of pressure.[1] Because the order parameters of the two superfluids are topologically inequivalent there necessarily forms a domain wall separating the A phase from the B phase.

In the following I assume that the A phase is on the left and the B phase is on the right side of this domain wall. The orientation of the order parameter in the A phase is described in terms of a pair of real orthogonal unit vectors $\hat{\boldsymbol{\phi}}_{\rm I}$ and $\hat{\boldsymbol{\phi}}_{\rm II}$ in orbital space and a third unit vector $\hat{\mathbf{w}}$ in spin space.[2] The physical meaning of $\hat{\mathbf{w}}$ is that it fixes the direction along which the triplet Cooper pairs are in the state of total spin $|S=1, m_S=0\rangle$ while the meaning of $\hat{\boldsymbol{\phi}}_{\rm I}$ and $\hat{\boldsymbol{\phi}}_{\rm II}$ is that their cross product $\hat{\mathbf{l}}=\hat{\boldsymbol{\phi}}_{\rm I}\times\hat{\boldsymbol{\phi}}_{\rm II}$ determines the direction along which the pairs are in a state of orbital angular momentum $|L=1, m_L=1\rangle$.

The order parameter in the B phase is characterized by the usual phase variable ϕ and a rotation matrix $R(\theta,\hat{\mathbf{n}})$.[2] In the bulk the nuclear-spin dipole interaction between the ^{3}He particles breaks the spin-orbit symmetry and fixes the angle θ at the Leggett value $\theta=\arccos(-\frac{1}{4})$ in the B phase and also orients $\hat{\mathbf{l}}$ to be parallel to $\hat{\mathbf{w}}$ in the A phase.[2]

In the vicinity of the A-B phase boundary, however, within a layer of thickness smaller than the dipole coherence length $\xi_D\simeq 6$ μm, the bending energy dominates by far the dipole energy and the dipole effects on the local order-parameter components may then be taken into account only perturbatively.

Recently, Yip[3] and Yip and Leggett[4] have pointed out that the spatial dependence of the order parameter at the A-B phase boundary of superfluid ^{3}He induces Andreev reflection of quasiparticles and therefore gives rise to a Kapitza resistance and also a friction force for the moving boundary.[5] The exact spatial dependence of the superfluid order parameter at the A-B phase boundary is then of considerable interest. Following Cross[6] and also Kaul and Kleinert,[7] I apply Ginzburg-Landau theory[8] to describe the energetics of the A-B phase boundary in superfluid ^{3}He for temperature and pressure values near the polycritical point. With the assumption of a planar A-B interface oriented parallel to the y-z plane of the laboratory frame, the superfluid order parameter $\hat{\Delta}=\sum_{j,\lambda}\hat{\mathbf{k}}_j d_{j\lambda}\sigma_\lambda i\sigma_y$ depends on the x coordinate only. Consequently, the Ginzburg-Landau equations reduce to a set of coupled *ordinary* differential equations for the nine complex components $d_{j\lambda}(x)=U_{j\lambda}(x)+iV_{j\lambda}(x)$ of the order parameter $\hat{\Delta}(x)$. Here the nine elements $\hat{\mathbf{k}}_j\sigma_\lambda i\sigma_y$ with $j,\lambda\in\{x,y,z\}$ define a Cartesian basis to span the Hilbert space of triplet Cooper pairs with p-wave symmetry, the unit vector $\hat{\mathbf{k}}$ pointing in the direction of the Fermi wave vector $\mathbf{k}_{\rm F}$ and

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

denoting the Pauli matrices.

It is convenient to normalize the energy in units of the condensation energy f_B^c of the bulk B phase,[8] and the length scale in units of the Ginzburg-Landau coherence length $\xi_{\rm GL}$,[9] and to work with a set[10] of reduced β parameters $\hat{\beta}_j=\beta_j/(\beta_{345}+3\beta_{12})$ reflecting the pressure dependence of the phase diagram of superfluid ^{3}He. At the coexistence temperature T_{AB}, of course, the condensation energies of the bulk B phase and the bulk A phase coincide. Consequently the β parameters fulfill the constraint $2\beta_4+2\beta_5=3\beta_1+\beta_3$, and the ratio of the gap amplitudes Δ_A and Δ_B turns out to be independent of any β parameters: $\Delta_A^2/\Delta_B^2=\frac{3}{2}$. Then the 1D Ginzburg-Landau boundary-value problem to be solved for the order-parameter components $d_{j\lambda}(x)=U_{j\lambda}(x)+iV_{j\lambda}(x)$ is the following:

$$\partial_x^2 d+\Lambda^{-1}(d-C)=0, \tag{1a}$$

and

$$\lim_{|x|\to\infty}\partial_x d=0. \tag{1b}$$

Here Λ denotes the diagonal matrix[11] $\Lambda=\mathrm{diag}\{3,1,1\}$ while the matrix C denotes all the cubic terms in the Ginzburg-Landau equations, weighted with their corresponding β parameters:

$$C=\hat{\beta}_1 d^*\,\mathrm{tr}(dd^{\rm T})+\hat{\beta}_2 d\,\mathrm{tr}(dd^\dagger)+\hat{\beta}_3 d^* d^{\rm T} d+\hat{\beta}_4 dd^\dagger d+\hat{\beta}_5 dd^{\rm T} d^*. \tag{2}$$

Near the A-B transition line either the bulk A phase order parameter

$$d_A = (\tfrac{3}{2})^{1/2}(\hat{\phi}_{\rm I} + i\hat{\phi}_{\rm II}) \otimes \hat{\mathbf{w}}^{\rm T} \tag{3a}$$

or the bulk B-phase order parameter

$$d_B = e^{i\phi} R(\theta, \hat{n}) \tag{3b}$$

solves the boundary-value problem (1).

In fact, I find that straightforward iteration of Eq. (1) apparently always converges to those spatially homogeneous bulk solutions. To find spatially inhomogeneous solutions to Eq. (1) with the properties $\lim_{x\to-\infty} d(x) = d_A$ and $\lim_{x\to\infty} d(x) = d_B$ and with the A-B phase boundary pinned at $x \simeq 0$ the following procedure turned out to be successful. Rather than attempting to solve the Ginzburg-Landau (GL) equation (1) directly, I compute solutions of the heat equation

$$\partial_t d = \partial_x^2 d + \Lambda^{-1}(d - C_t), \tag{4}$$

fulfilling at time $t = 0$ the initial condition $d = d_A$ for $x < 0$ and $d = d_B$ for $x > 0$ and also fulfilling the boundary conditions $\lim_{|x|\to\infty} \partial_x d = 0$ for $t > 0$. The matrix C_t now denotes all the cubic GL terms as defined in Eq. (2) which correspond to a set of specially chosen β parameters favoring the A phase for $x < 0$ and the B phase for $x > 0$. These x- and t-dependent β parameters undergo a jump at $x = 0$ which heals not too rapidly as t increases to infinity; for example, working with the β parameters employed by Sauls and Serene[12] one has at the tricritical point

$$\begin{aligned}
\hat{\beta}_1 &= -0.288 - \epsilon(x,t) \\
\hat{\beta}_2 &= 0.513 + \epsilon(x,t) \\
\hat{\beta}_3 &= 0.504 - \epsilon(x,t) \\
\hat{\beta}_4 &= 0.464 - \epsilon(x,t) \\
\hat{\beta}_5 &= -0.643 - \epsilon(x,t)
\end{aligned} \tag{5}$$

with $\epsilon(x,t) = \mathrm{sgn}(x)/(10 + t^2)$.

In the limit $t \to \infty$ the derivative $\partial_t d$ vanishes, of course, and one obtains a nontrivial solution of the Ginzburg-Landau boundary-value problem Eq. (1). To solve the auxiliary problem Eq. (4) numerically, the standard Cranc-Nicolson discretizing scheme[13] for the heat equation was implemented on a spatial grid with lattice constants as small as $0.025\xi_{\rm GL}$ and up to 1000 grid points were taken into account. The resulting nonlinear difference equations were then iterated until convergence.

As explained in detail in Refs. 3 and 7 it is very convenient to choose the phase and also the orientation of the spin frame of the asymptotic B-phase order parameter such that it approaches a unit matrix for $x \to \infty$:

$$\tilde{d}_B = 1. \tag{6a}$$

Consequently, the A-phase order parameter in this new frame is

$$\begin{aligned}
\tilde{d}_A &= e^{-i\phi} d_A R^{\rm T}(\theta, \hat{\mathbf{n}}) \\
&= \tfrac{3}{2}^{1/2}(\tilde{\phi}_{\rm I} + i\tilde{\phi}_{\rm II}) \otimes \tilde{\mathbf{w}}^{\rm T}
\end{aligned} \tag{6b}$$

with

$$\tilde{\phi}_{\rm I} + i\tilde{\phi}_{\rm II} = e^{-i\phi}(\hat{\phi}_{\rm I} + i\hat{\phi}_{\rm II})$$

and

$$\tilde{\mathbf{w}} = R(\theta, \hat{\mathbf{n}})\hat{\mathbf{w}}.$$

For a geometry with a planar interface described by a normal unit vector $\hat{\mathbf{x}}$ the components of the order parameter $d_{j\lambda}(x) = U_{j\lambda}(x) + iV_{j\lambda}(x)$ are no longer dependent on the coordinates y and z. Consequently, an analysis of the reflection and time-inversion symmetries of the order parameter[14,15] in the asymptotic regime shows that the group $\{1, S_y, KS_z, KS_zS_y\}$ represents possible discrete symmetries of the order parameter. Here, $S_m = 1 - 2\hat{\mathbf{m}} \otimes \hat{\mathbf{m}}^{\rm T}$ denotes reflection at a plane with normal vector $\hat{\mathbf{m}}$ and K means complex conjugation, an operation which is identical to time inversion for triplet Cooper pairs. Table I shows which of the order-parameter components necessarily vanish as a result of each of those discrete symmetries. Of course, inspection of Table I reveals immediately that an order parameter having both symmetries, S_y and KS_z, then only has three nonvanishing real components and just two nonvanishing imaginary components:

$$\begin{pmatrix} U_{xx} & 0 & iV_{xz} \\ 0 & U_{yy} & 0 \\ iV_{zx} & 0 & U_{zz} \end{pmatrix}. \tag{7}$$

It turns out that the solutions of Eq. (1) with minimum interfacial energy σ_{AB} are, indeed, of this symmetry type. The interfacial energy σ_{AB} (near the tricritical point) is determined by subtraction of the free-energy

TABLE I. Symmetry constraints for the order-parameter components.

Symmetry	Order parameter $d = U + iV$
S_y	$\begin{pmatrix} U_{xx} & 0 & U_{xz} \\ 0 & U_{yy} & 0 \\ U_{zx} & 0 & U_{zz} \end{pmatrix} + i \begin{pmatrix} V_{xx} & 0 & V_{xz} \\ 0 & V_{yy} & 0 \\ V_{zx} & 0 & V_{zz} \end{pmatrix}$
KS_z	$\begin{pmatrix} U_{xx} & U_{xy} & 0 \\ U_{yx} & U_{yy} & 0 \\ 0 & 0 & U_{zz} \end{pmatrix} + i \begin{pmatrix} 0 & 0 & V_{xz} \\ 0 & 0 & V_{yz} \\ V_{zx} & V_{zy} & 0 \end{pmatrix}$
KS_zS_y	$\begin{pmatrix} U_{xx} & 0 & 0 \\ 0 & U_{yy} & U_{yz} \\ 0 & U_{zy} & U_{zz} \end{pmatrix} + i \begin{pmatrix} 0 & V_{xy} & V_{xz} \\ V_{yx} & 0 & 0 \\ V_{zx} & 0 & 0 \end{pmatrix}$

density of the homogeneous bulk phase from the Ginzburg-Landau free-energy density corresponding to the solitonlike solution of Eq. (1) describing the A-B phase boundary. After a partial integration and making use of the fact that the spatially varying order parameter solves Eq. (1), the formula

$$\sigma_{AB} = \tfrac{1}{3}\int_{-\infty}^{\infty} dx\,[\mathrm{tr}(d^{\dagger}C) - 3](\tfrac{3}{5})^{1/2}\xi_T f_B^c, \tag{8}$$

is derived, where C denotes all the cubic terms as given in Eq. (2). Using the β parameters from Eq. (5) I obtain the result

$$\sigma_{AB} = 0.71\,\xi_T f_B^c, \tag{9}$$

in excellent agreement with the data of Osheroff and Cross.[1]

It turns out that σ_{AB} is not very sensitive to variations of the β parameters. For example, repeating the calculations for the order parameter $\tilde{d}$ and the interfacial energy σ_{AB} with the same set of β parameters as employed by Kaul and Kleinert in their variational calculation,[7] i.e.,

$$\hat{\beta}_1 = -0.230,\quad \hat{\beta}_2 = 0.461,\quad \hat{\beta}_3 = 0.434,$$
$$\hat{\beta}_4 = 0.384,\quad \hat{\beta}_5 = -0.511, \tag{10}$$

I obtain the slightly different value $\sigma_{AB} = 0.66\,\xi_T f_B^c$. Obviously, this value is significantly lower than the value $\sigma_{AB} = 0.77\,\xi_T f_B^c$ obtained by Kaul and Kleinert.[7] Variational estimates for σ_{AB} would probably have been more accurate with an order-parameter *Ansatz* respecting the symmetries S_y and KS_z as suggested by Eq. (7) and taking into account the possibility of a splitting of all the diagonal components of the order parameter at the interface.

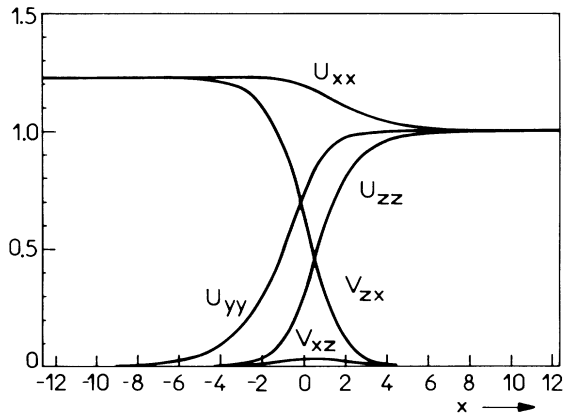

FIG. 1. The spatial variation of the nonvanishing order-parameter components vs distance x from the A-B interface. The unit of length x is ξ_{GL} as defined in Ref. 9. $U_{j\lambda}$ denotes the real part and $V_{j\lambda}$ denotes the imaginary part of the complex order parameter. For $x \to \infty$ the bulk B phase and for $x \to -\infty$ the bulk A phase are approached as discussed in the text. The origin at $x = 0$ coincides with the point of maximum interfacial energy.

The numerical results of the Ginzburg-Landau boundary-value problem Eq. (1) for the order parameter with its components as given by Eq. (7) and with use of the β parameters from Eq. (5) are presented in Fig. 1. In the limit $x \to -\infty$ the order parameter approaches the A-phase order parameter as described in Eq. (6b) with the orientation $\tilde{\phi}_{\mathrm{I}} = \hat{\mathbf{x}}$, $\tilde{\phi}_{\mathrm{II}} = \hat{\mathbf{z}}$, and $\tilde{\mathbf{w}} = \hat{\mathbf{x}}$. Consequently, the vector $\tilde{\mathbf{l}} = \tilde{\phi}_{\mathrm{I}} \times \tilde{\phi}_{\mathrm{II}}$ is pointing perpendicular to the interface normal vector $\hat{\mathbf{x}}$ and the $\tilde{\mathbf{w}}$ vector (also named $\tilde{\mathbf{d}}$ vector in the ^{3}He-A literature) is pointing parallel to the interface normal, always with the assumption of the spin-frame orientation of Eqs. (6a) and (6b). Then, of course, on the B-phase side of the interface the order parameter tends to the unit matrix for $x \to \infty$.

To summarize, one can say that the spin frame of the A phase is oriented in such a way that $\hat{\mathbf{x}} \cdot R(\theta, \hat{\mathbf{n}})\hat{\mathbf{w}} = 1$. This orientation of the asymptotic A phase gives minimal interfacial energy and coincides exactly with the results of Cross[6] and Kaul and Kleinert,[7] who carefully minimized the various bending-energy contributions to the A-phase order parameter in their variational calculations. In fact, upon solution of Eq. (4) and, for example, use of the set of β parameters as given in Eq. (10) almost every initial configuration for $\tilde{d}_A$ rapidly relaxed to this A-phase order parameter or gauge-equivalent ones in the limit $x \to -\infty$. I find, however, also a second solution of Eq. (1) which for $x \to -\infty$ has an asymptotic A-phase order parameter oriented like $\tilde{\phi}_{\mathrm{I}} = \hat{\mathbf{z}}$, $\tilde{\phi}_{\mathrm{II}} = \hat{\mathbf{x}}$, $\tilde{\mathbf{w}} = \hat{\mathbf{z}}$ and also a third one with the orientation $\tilde{\phi}_{\mathrm{I}} = \hat{\mathbf{y}}$, $\tilde{\phi}_{\mathrm{II}} = \hat{\mathbf{z}}$, $\tilde{\mathbf{w}} = \hat{\mathbf{z}}$. These two other configurations probably correspond to saddle-point solutions of the stationarity conditions Eq. (1), the former configuration having the interfacial energy $\sigma_{AB} = 1.0\,\xi_T f_B^c$ and the latter $\sigma_{AB} = 0.76\,\xi_T f_B^c$.

In Fig. 2 the interfacial energy density $\sigma(x) = \frac{1}{3}$

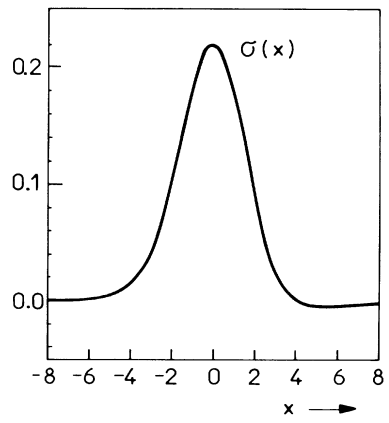

FIG. 2. The interfacial energy density $\sigma(x)$ of the A-B phase boundary vs distance x corresponding to the order-parameter components $d_{j\lambda} = U_{j\lambda} + iV_{j\lambda}$ as plotted in Fig. 1. The unit of length x is ξ_{GL} as defined in Ref. 9.

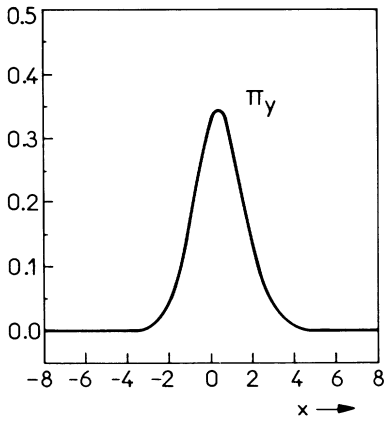

FIG. 3. The spatial variation of the nonvanishing components of the magnetic moment density $\boldsymbol{\pi}$ vs distance x from the A-B interface. The unit of length x is ξ_{GL} as defined in Ref. 9.

$\times \mathrm{tr}(d^{\dagger}C) - 1$ and in Fig. 3 the nonvanishing components of the interfacial magnetic-moment density $\pi_{\mu}(x) = i\epsilon_{\mu\nu\lambda} d_{j\nu} d^{*}_{j\lambda}$ corresponding to the order-parameter components of Fig. 1 are plotted versus distance x; as is clearly seen, the "half width" Λ of the A-B phase boundary is of order $\Lambda \sim 4\xi_{GL} \simeq 3.1\xi_T$, a value which compares favorably with the value employed by the authors of Ref. 4 in their theory of the Andreev-scattering-induced Kapitza resistance.

An important implication of the nonvanishing imaginary components V_{xz} and V_{zx} of the order parameter is that the Tomasch wave numbers $q_T^{\pm} = (\boldsymbol{\Delta}\cdot\boldsymbol{\Delta}^{*} \pm \|\boldsymbol{\Delta} \times i\boldsymbol{\Delta}^{*}\| - \omega^2)^{1/2}$ for quasiparticles traveling along the trajectory $\mathbf{R}(t,\hat{\mathbf{k}}) = \mathbf{R}_0 + v_F t\hat{\mathbf{k}}$ may split at the A-B phase boundary. Here $\Delta_{\mu} = \hat{k}_j d_{j\mu}(\mathbf{R})$ denotes the components of the local order parameter $\boldsymbol{\Delta}$ as seen by those quasiparticles flying in the direction $\hat{\mathbf{k}} = \mathbf{k}_F/\|\mathbf{k}_F\|$ with the energy $\hbar\omega$ and the group velocity v_F, the trajectory parameter t measuring the "time of flight." Note that for $\hat{\mathbf{k}} \| \hat{\mathbf{y}}$ the Tomasch wave numbers $q_T^{\pm}$ remain degenerate while for $\hat{\mathbf{k}} \| \hat{\mathbf{z}}$ there is a substantial spin split. However, also for $\hat{\mathbf{k}} \| \hat{\mathbf{x}}$ there exists a small spin split due to the finite v_{xz} component of the order parameter.

Strictly speaking, therefore, a spatially *constant* equal-spin pairing axis $\hat{\mathbf{x}}_s(\hat{\mathbf{k}})$ for quasiparticles flying through the A-B phase boundary[16] does not exist. It does exist, mathematically, for the trial order parameter of Kaul and Kleinert[4,7] and has been used for an elegant simplification in the calculation of the Kapitza resistance.[3,4] Though, admittedly, the corotation of $\hat{\mathbf{x}}_s(\hat{\mathbf{k}})$ along the trajectory $\mathbf{R}(t,\hat{\mathbf{k}})$ is a small effect in the Ginzburg-Landau regime, because the order-parameter component V_{xz} is small, experience from self-consistent calculations of vortices in ^{3}He-B suggests (making use of the full quasiclassical theory[17]) that small nonunitary components of the order parameter have a tendency to grow at lower temperatures.[18] Whether or not *local* coupling of the spin channels of the Andreev equation should be taken into account in a calculation of the Kapitza resistance depends on the outcome of self-consistent calculations of the order parameter at all temperatures, which are presently under way.

I wish to thank G. Eilenberger, M. Liu, and G. Schön for stimulating discussions.

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