Theory of the $\pi$ state in $^3$He Josephson junctions

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(January 6, 2018)

The flow of superfluid $^3$He-B through a 65 $\times$ 65 array of nanometer size apertures has been measured recently by Backhaus et al. They find in the current–phase relation a new branch, so-called $\pi$ state. We study two limiting cases which show that the $\pi$ state arises from coupling of the phase degree of freedom to the spin-orbit rotation. The $\pi$ state exists in a single large aperture, but is difficult to observe because of hysteresis. A better correspondence with experiments is obtained by assuming a thin wall, where the Josephson coupling between the two sides arises from a dense array of pin-holes.

PACS: 67.57.Np

The flow of superfluid $^3$He-B through a single nanometer-size aperture was studied by Avenel and Varoquaux some time ago \[\textcircled{1}\]. At temperatures near the superfluid transition temperature $T_c$, the current–phase relation is sinusoidal

$$J(\phi) = J_c \sin \phi$$  \hspace{1cm} (1)

as expected for a Josephson junction. Also according to expectation, they find that the sine form (1) gradually becomes tilted when the temperature is lowered. More recently, Backhaus et al. studied a 65 $\times$ 65 array of small apertures [2]. They discovered a new behavior where the current–phase relation acquires a positive slope at phase differences $\phi \approx \pi$. This $\pi$ state develops when the temperature is lowered to approximately 0.6$T_c$.

A few theoretical explanations for the $\pi$ state have been proposed [3,4]. In this letter we present a theory, that is based on the many-component form of the order parameter in $^3$He. It differs from the previous suggestions because it contains no unjustified assumptions and an order-of-magnitude agreement with experiments is obtained without any adjustable parameters.

Unusual current-phase relations occur also in other systems. A $\pi$ junction, where $J_c$ in (1) is negative, can be induced by adding magnetic impurities to a tunneling barrier between two s-wave superconductors [5]. Similar $\pi$ shifts appear in nonmagnetic junctions between d-wave superconductors. In addition, current-phase relations with additional zeros ($J(\phi) = 0$ for $\phi \neq 0$ or $\pi$) can appear for special orientations of the anisotropic crystals [6]. The $\pi$ state in $^3$He differs from these in several respects, most fundamentally because it arises from interplay of two soft modes of the order parameter, the phase $\phi$ and the spin-orbit rotation.

We present calculations in two limiting cases. In the case of a tunneling barrier, the existence of the $\pi$ state can be demonstrated by analytic calculations. The parameters of the tunneling model are estimated using the quasiclassical theory. In the case of a single aperture, the $\pi$ state is obtained by numerical simulations using the Ginzburg-Landau theory of $^3$He.

Tunneling junction.—The simplest case to demonstrate the $\pi$ state is to consider a planar wall through which the $^3$He atoms can tunnel. The energy arising from tunneling between the left ($L$) and right ($R$) sides can be written as \[\textcircled{2}\]

$$F_1 = -\text{Re} \sum_\mu \left[ a A_{L\mu z}^R A_{R\mu z}^L + b (A_{L\mu x}^R A_{R\mu z}^L + A_{L\mu y}^R A_{R\mu y}^L) \right].$$  \hspace{1cm} (2)

Here $A_{\mu j}$ is the 3 $\times$ 3 matrix order parameter where the first index $\mu$ refers to the orientation of the Cooper pair in spin space, and the latter index $j$ in orbital space. The $z$ axis is taken perpendicular to the tunneling wall. Equation (2) is a simple generalization of $F_3 = -\alpha \text{Re}(A^L A^R)$, which describes the Josephson coupling of two s-wave superconductors with order parameters $A^L$ and $A^R$ \[\textcircled{3}\].

In the B phase of $^3$He, the order parameter has the form $A_{\mu j} = \Delta \exp(i\phi) R_{\mu j}$. Here $\Delta$ is the amplitude, $\exp(i\phi)$ a phase factor, and $R_{\mu j}$ a $3 \times 3$ rotation matrix: $\sum_\mu R_{\mu j} R_{\mu k} = \delta_{jk}$. The rotation matrices can be parametrized by an axis $\mathbf{n}$ and an angle $\theta$. Substituting into (3) gives ($\alpha, \beta > 0$)

$$F_3 = -\sum_\mu \left[ a R_{\mu z}^L R_{\mu z}^R + \beta (R_{\mu x}^L R_{\mu z}^R + R_{\mu y}^L R_{\mu y}^R) \right] \cos \phi.$$  \hspace{1cm} (3)

In deriving this expression from (2) one must pay attention to the fact that the order parameter of the p-wave superfluid is strongly suppressed near a wall. As a consequence the parameters $\alpha$ and $\beta$ in (3) are not simply related to the coefficients $a$ and $b$ in (2), but otherwise the dependence of $F_3$ on the soft variables $\phi$ and $R_{\mu j}$ remains the same as obtained by the simple substitution above.

Let us consider the case that the rotation matrices on the left and right sides are the same. This gives rise to the “zero-state” with the critical current $J_c = (2m_3/h)(\alpha + 2\beta) > 0$. This state has lowest energy when $|\phi| < \pi/2$ because it corresponds to the maximum of the expression in square brackets in (3). The
situation changes when $\phi$ exceeds $\pi/2$. There one has to look for a minimum of the expression in the square brackets. This corresponds to the $\pi$ state, which is illustrated by the solid line in Fig. 1a. The critical current $J_c$ in (1) is negative: $J_c = -(2m_3h/\alpha)$ if $\alpha > \beta$ and $J_c = -(2m_3h/2(\beta - \alpha))$ otherwise.

In order to make the tunneling model realistic, we have to consider three additional contributions to the energy. Firstly, there is the magnetic dipole-dipole energy $F_d = 8g_dA^2(\frac{1}{4} + \cos\theta)^2$ [14]. In the bulk it fixes the rotation angle $\theta$ equal to $\theta_0 = \arccos(-\frac{1}{4}) = 104^\circ$. This remains valid also near the junction because both the Josephson energy (3) and the dipole-dipole energy can reach their minima simultaneously: the products of two rotation matrices appearing in the former are not limited by the fact that both matrices have a fixed rotation angle $\theta_0$. Secondly, there is a surface energy that arises from coupling of the dipole-dipole energy to the suppression of the order parameter near walls [1]. It has the form

$$F_s = b_4(\hat{n} \cdot \hat{s})^4 - b_2(\hat{n} \cdot \hat{s})^2,$$

where $\hat{s}$ is the surface normal. The lowest surface energy is achieved when the rotation axis $\hat{n}$ is perpendicular to the wall, $\hat{n} = \pm \hat{s}$, because $b_2 > 2b_4 > 0$. Thirdly, there is a gradient energy associated with spatial bending of the rotation axis $\hat{n}$. It arises because in practice all tunnel junctions are of finite size, and other walls in the container favor a different orientation of $\hat{n}$ than may be the minimum of the Josephson energy. We model the gradient energy by the simple quadratic forms

$$F_s^L = \gamma(\eta^L - \eta^L_\infty)^2, \quad F_s^R = \gamma(\eta^R - \eta^R_\infty)^2,$$

where $\eta$ is the polar angle of $\hat{n}$, i.e., $\cos\eta = \hat{n}_z$. $\eta^L$ and $\eta^R$ denote the polar angles on both sides just at the junction, and we assume that the values $\eta^L_\infty$ and $\eta^R_\infty$ further away are either 0 or $\pi$. In the experimental case the surface energy (4) is important in fixing $\eta^L_\infty$ and $\eta^R_\infty$, but otherwise its contribution is so small that we can neglect it in the following.

The current–phase relations for the tunneling model, (4) and (5), are plotted in Fig. 1. It can be seen that a large value of the gradient energy parameter $\gamma$ suppresses the $\pi$ state. Furthermore, we find two cases where the rotation axes $\hat{n}$ far from the junction are either parallel or antiparallel. The latter has smaller critical current $J_c = (2m_3h/\alpha - \frac{2}{5} \beta)$ but a relatively a more pronounced $\pi$ state. This “bi-stability” was theoretically discussed in Ref. [12] and has recently been observed experimentally [3].

**Evaluation of tunneling parameters.**—The experiment [3] has a square array of apertures of diameter $D = 100$ nm with spacing $S = 3$ nm in a wall of thickness $W = 50$ nm. In order to make the tunneling model to imitate the experiment, we estimate $\alpha$ and $\beta$ by letting all the three lengths to approach zero but keeping their ratios unchanged [8]. The calculation for such “pin-holes” [14] is relatively simple once the self-consistent solution for the order parameter near a wall is known [15]. We assume diffuse scattering of quasiparticles at surfaces. The tunneling form (3) is reproduced in these calculations at temperatures $T \gtrsim 0.5T_c$, and values of $\alpha$ and $\beta$ can be extracted. The parameter $\gamma$ can be estimated using the bending energy of the B phase (4) and assuming a simple form $\gamma(r) - \gamma_\infty \propto r^{-1}$, where $r$ is the radius from the center of the aperture array, and this expression is cut off at the radius of the array. In agreement with experiments, we find that the $\pi$ state appears at low temperatures because $\alpha$ and $\beta \propto (1 - T/T_c)^2$ have stronger temperature dependence than $\gamma \propto 1 - T/T_c$, see Fig. 2. Moreover, the parameters $\alpha$, $\beta$, and $\gamma$ are relatively close within one order of magnitude to those that give an approximate best fit to the experiments (see caption of Fig. 3). This fit reproduces also the absolute magnitude of the critical current, and the same values of the parameters are used for cases of both parallel and antiparallel $\hat{n}$’s.

The tunneling model can be improved trivially by extending the pin-hole calculation to the whole temperature range $0 < T < T_c$. A more ambitious project for the future would be the self-consistent calculation for aperture sizes on the order of the coherence length $\xi_0$. In both cases the resulting Josephson energy $F_3(\phi, R_{\mu^L_J}, R_{\mu^R_J})$ will no more be of the simple form (3).
Single aperture.—The limit opposite to the tunneling barrier is a single large aperture. There the major task is to calculate the order parameter self-consistently. We have done this using the Ginzburg-Landau (GL) theory of $^3$He. The differential equations were solved numerically on a grid in and around the aperture. Our calculations are more general than the previous ones because we use a full a three-dimensional grid. Vanishing $A_{\mu j}$ was assumed at surfaces.

The order parameter of the $\pi$ state is shown in Fig. 3. It is plotted along the axis of a circularly symmetric aperture. For simplicity, we have normalized the order parameter to unit matrix in the bulk, $A_{\mu j}(z = \pm \infty) = \exp(\pm i\phi/2)\delta_{\mu j}$ (assuming the case of parallel $\hat{n}$'s). This is possible because for aperture sizes on the order of the GL coherence length $\xi_{GL}$ the dipole-dipole energy can be neglected. The characteristic property of the $\pi$ state is the components $A_{yx}$ and $A_{zy}$. These are the dominant components in the orifice, and they decay slowly towards the bulk. They imply broken symmetry: the symmetry group of the $\pi$ branch is $m'm2'$ compared to $\infty m\infty$ of the zero branch. (Here prime denotes time-inversion.) This sets rather strong requirement for the calculation because the circular symmetry of the aperture cannot be used to simplify the computation.

The current–phase relations are summarized in Fig. 4. We see that the occurrence of the $\pi$ branch depends sensitively on the diameter of the aperture, whereas the wall thickness is less important. For small apertures no $\pi$ branch is found. When $D$ exceeds approximately $5\xi_{GL}$, the $\pi$ branch appears. In the region (b) the current–phase relation has negative slope. Such a state can be stabilized if the left and right sides are connected, like in a torus...
geometry. Increasing the diameter, the current–phase relation gets a positive slope in region (c). This state is stable also in a piston-driven flow channel. The \(\pi\) state is also the absolute energy minimum at \(\phi = \pi\) in region (c). In region (d) the \(\pi\) state continues to exist but it has higher energy than the zero branch. The calculation assumes the idealized case of flow between two infinite bulk fluids. Any additional hydrodynamic inductance shifts upwards the border between regions (c) and (d) as it increases the energy of current carrying states.

Although the \(\pi\) branch constitutes the absolute energy minimum, it may be difficult to find it experimentally in a single aperture. The reason is that whenever it is locally stable, there always exists a locally stable zero state at the same \(\phi\). Because the order parameters of the \(\pi\) and zero states differ considerably, it may be that the phase slips only take place between two branches of the zero state without ever finding the way to the lower energy \(\pi\) state. This is what we find in the numerical calculations, where the \(\pi\) state was found only if the initial \(A_{ij}\) was chosen close enough to the converged solution. We remind, though, that our calculations are not meant to simulate the correct dynamics of the phase slip.

The dimensions of one aperture in the array at Berkeley are marked on figure 1. This is clearly in the region where no \(\pi\) state is found. Although the Ginzburg-Landau calculation is accurate only at temperatures near \(T_c\), it is unlikely that the \(\pi\) state could be stabilized in a more accurate calculation at lower temperatures. This statement is based on experience gained in previous low-temperature calculations. Thus we conclude that the appearance of the \(\pi\) state in the Berkeley experiment essentially depends on the presence of many apertures.

We have also done two-dimensional calculations that simulate the flow through a long narrow slit. The \(\pi\) state is found and its properties are qualitatively similar to those in a circular aperture. In particular, the transitions from the zero branch to the \(\pi\) branch seem to be absent. This is consistent with the fact that no \(\pi\) branch was found in the experiments by Avenel and Varoquaux.

The \(\pi\) state can be interpreted so that a half-quantum vortex has crossed the orifice. There are no free half quantum vortices in superfluid \(^3\)He-B, but the double-core vortex can be interpreted as a bound pair of two half-quantum vortices. Indeed, the order parameter in Fig. 1 is very similar to that in the double-core vortex on the axis going between the two cores.

**Conclusion.**—The \(\pi\) state was found to occur in both the limits investigated above. Its mechanism is the same in both cases: a lower coupling energy is achieved by producing a spin-orbit rotation that heals slowly in the bulk liquid. The Berkeley experiment is somewhat an intermediate case to the two limits studied, which makes it evident that the \(\pi\) state also there arises from the same mechanism.

The theory above provides several predictions that can be tested experimentally. For example, the \(\pi\) state depends on the linear dimension \(L\) of the aperture array because \(\alpha/\gamma, \beta/\gamma \propto L\). An external magnetic field fixes the surface orientation of \(\hat{n}\), and thus can be used to suppress the \(\pi\) state.

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