Phase Fluctuations and Vortex Lattice Melting in Triplet Quasi-One-Dimensional Superconductors at High Magnetic Fields

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Assuming that the order parameter corresponds to an equal spin triplet pairing symmetry state, we calculate the effect of phase fluctuations in quasi-one-dimensional superconductors at high magnetic fields applied along the y (b’) axis. We show that phase fluctuations can destroy the theoretically predicted triplet reentrant superconducting state, and that they are responsible for melting the magnetic field induced Josephson vortex lattice, above a magnetic field dependent melting temperature $T_m$.

The upper critical field $H_{c2}$ of quasi-one-dimensional superconductors for perfectly aligned magnetic fields along the y (b’) axis has been calculated (at the mean field level) for both singlet and triplet states [1]. In the case of triplet pairing, these studies predicted a remarkable reentrant superconducting phase, for magnetic fields precisely aligned along the y (b’) axis. New experiments performed in these systems lead to the observation of unusual superconductivity, for instance, in quasi-one-dimensional superconductors (of the Bechgaard salts family with chemical formula (TMTSF)$_2$X, where X = ClO$_4$, PF$_6$, ...), the experimental upper critical field exceeds substantially the Pauli paramagnetic limit [2]. This indicates that high magnetic field superconductivity in these systems is most likely triplet. More recently, it has been argued by Lebed, Machida, and Ozaki (LMO) that the spin-orbit coupling must be strong in order to explain the observed experimental upper critical fields [3] and the absence of the Knight shift for fields parallel to the y (b’) axis. However, estimates of the value of spin-orbit coupling are several orders of magnitude smaller [4] than the values required to fit the critical temperature of (TMTSF)$_2$PF$_6$ [5]. In fact, at low magnetic fields. Very recently, the present authors [6] have analysed the angular dependence of $H_{c2}$ for magnetic fields applied along the yz plane, where weak spin-orbit coupling and equal spin triplet pairing were assumed. There, it was found that a strong suppression of the critical temperature $T_c(H)$ occurred for very small angular deviations from the y (b’) axis. This result is in qualitative agreement with the rapid drop of the putative upper critical in (TMTSF)$_2$ClO$_4$ [7]. However, all these theoretical works [8, 9, 10] used a mean field approach, where the effects of fluctuations were completely ignored. Thus, the main point of the present paper is to discuss the effects of phase fluctuations on the field versus temperature phase diagram of quasi-one-dimensional superconductors at high magnetic fields parallel to the y (b’) axis. For that purpose, we study phase fluctuation effects in the weak spin-orbit, equal spin triplet state (ESTP) proposed by one us [11] as a possible candidate state for triplet superconductivity in the (TMTSF)$_2$X family. In particular, we show that phase fluctuations melt the predicted magnetic field induced Josephson vortex lattice at high magnetic fields [3] at a melting temperature $T_m(H) < T_c(H)$. Furthermore, we show that the curvature of $T_m(H)$ is opposite to that of $T_c(H)$ at high magnetic fields (range from 5 to 20 T), and that the superconducting state still exists at high magnetic fields for temperatures $T < T_m(H)$.

We model quasi-one-dimensional systems via the energy relation

$$\varepsilon_{\alpha}(k) = \varepsilon_{\alpha}(k) - \sigma \mu_B H, \quad (1)$$

with the $\alpha$-branch dispersion

$$\varepsilon_{\alpha}(k) = v_F (\alpha k_x - k_F) + t_y \cos(k_y b) + t_z \cos(k_z c), \quad (2)$$

corresponding to an orthorombic crystal with lattice constants $a, b$ and $c$ along the $x, y$ and $z$ axis respectively. In addition, since $E_F = v_F k_F \gg t_y \gg t_z$, the Fermi surface of such systems is not simply connected, being open both in the $xz$ plane and in the $xy$ plane. Furthermore, the electronic motion can be classified as right-going ($\alpha = +$) or left-going ($\alpha = -$).

In this paper, we consider only magnetic field applied along the y (b’) direction for simplicity, since quantum confinement along the transverse z direction occurs when $t_z/\omega_{cz} \ll 1$, where $\omega_{cz} = v_F G_z$ with $G_z = |e| H_y c$. Throughout the paper, we work in units where the Planck’s constant and the speed of light are equal to one, i.e., $\hbar = c = 1$, and use the gauge $A = (H_y z, 0, 0)$, where $\alpha$ and $k_x, k_y$ are still conserved quantities (good quantum numbers) while $k_z$ is not.

In the presence of the magnetic field $H$, the non-interacting Hamiltonian is

$$H_0(k - eA) = \varepsilon_{\alpha}(k - eA) - \sigma \mu_B H \quad (3)$$
in the gauge $A = (H_y z - H_z y, 0, 0)$. The eigenfunctions of $H_0(k - eA)$ are

$$\Phi_{qn}(r) = \exp[i(k_x x + k_y y)], J_{N_z - n_z} \frac{\alpha t_z}{\omega_{cz}}, \quad (4)$$

where $r = (x, y, z)$, $z = n_z c$ with associated quantum numbers $qn = \alpha, k_x, k_y, N_z, \sigma$ and eigenvalues

$$\varepsilon_{qn} = \varepsilon_{\alpha, \sigma}(k_p) + \alpha N_z \omega_{cz}. \quad (5)$$
The function $J_{\nu}(u)$ is the Bessel function of integer order $p$ and argument $u$, while now

$$
\varepsilon_{\alpha, \sigma}(k) = v_F (\alpha k_x - k_F) + t_y \cos(k_y b) - \sigma \mu_B H \tag{6}
$$

is a 2D dispersion. Notice that the electronic wavefunction in Eq. (6) is confined along the $z$ direction when $t_z/\omega_{cz} \ll 1$, thus limiting the electronic motion to a nearly two dimensional situation. Furthermore, notice that the eigenvalues in Eq. (6) involve many magnetic subbands labeled by quantum numbers $N_z$ and that the eigenvalue $\varepsilon_{\alpha n}$ is invariant under the quantum number transformation $(\alpha, k_x, k_y, N_z, \sigma) \rightarrow (-\alpha, -k_x, -k_y, -N_z, \sigma)$, for the same spin state $\sigma$. Since, these magnetic subbands are spin-split into spin-up and spin-down bands, Cooper pairs can be easily formed in an ESTP pairing state, involving electrons with quantum numbers $(\alpha, k_x, k_y, N_z, \sigma)$ and $(-\alpha, -k_x, -k_y, -N_z, \sigma)$, provided that the pairing interaction $\lambda_\sigma$ conserves spin (which seems to be the case for the (TMTSF)$_2$X family, except for very small spin-orbit and dipolar couplings). Thus, in the ESTP state the order parameter vector

$$
\Delta(r) = [\Delta_+(r), 0, \Delta_z(r)] \tag{7}
$$

has components only in the $m_x = +1$ ($\mu = \uparrow\uparrow$) and $m_x = -1$ ($\mu = \downarrow\downarrow$) channels, only.

Now we turn our attention to the construction of the effective free energy, where we assume that the interaction $\lambda_\mu = \lambda$ and the density of states $N_\nu = N$ are independent of the spin channel, which implies that $\Delta_\mu(r) = \Delta(r)$. Following the functional integral formulation of the ESTP discussed by Sá de Melo [11], we derive the effective free energy functional $F$ in the limit where the magnetic field is exactly pointing along the $y$ direction and where it nearly confines the electronic motion to a two dimensional regime ($t_z/\omega_{cz} \ll 1$). In this case, $\Delta(r) = \Delta_n(x, y)$, where $n$ now labels the planes $z = nc$, and the effective free energy takes the form

$$
F = \sum_{mn} \int \! dr \left( F_1 + F_2 + F_3 + F_4 + F_m \right) \tag{8}
$$

The first term is the local quadratic form

$$
F_1 = a_1 |\Delta_n|^2, \tag{9}
$$

where the critical temperature can be derived from the coefficient

$$
a_1 = N \left[ \ln \left( \frac{T}{T_{c2d}} \right) - \frac{(t_z/\omega_{cz})^2 \ln (\omega_{cz} / \pi T)}{2} \right], \tag{10}
$$

The second term has the form

$$
F_2 = a_{2z} |\partial \Delta_n / \partial x|^2 + a_{2y} |(\partial / \partial y - i 2 G_y x / b) \Delta_n|^2, \tag{11}
$$

and corresponds to the spatial variation of $\Delta_n(x, y)$, with coefficients $a_{2z} = N^3 \beta \mu_B T^2$ and $a_{2y} = N^3 C (t_y b)^2 / 2 T^2$, with $C = 7 \zeta(3) / 16 \pi^2$. The third term corresponds to the contribution of the magnetic field induced Josephson coupling

$$
F_3 = a_3 |\Delta_n|^2 \exp (-i 2 G_y x / c) - |\Delta_n|^2, \tag{12}
$$

with coefficient $a_3 = N (t_z / \omega_{cz})^2 \ln (\omega_{cz} / \gamma / 2 \pi T)$. While the fourth term corresponds to the non-local fourth order contribution

$$
F_4 = a_{41} |\Delta_n|^2 + a_{42} |\Delta_n|^2 |\Delta_{n+1}|^2, \tag{13}
$$

where $a_{41}$ and $a_{42}$ are complicated functions of $t_y$, $t_z$, $\omega_{cz}$, and $\omega_{cz}$. The last term

$$
F_m = \int d^3 r \frac{B^2}{8 \pi} \tag{14}
$$

is just the magnetic energy. Using $\Delta_n = |\Delta_n| \exp (i \phi_n)$, it is easy to show that the terms in Eqs. (13) do not contribute to the phase fluctuation free energy,

$$
F_p = \sum_n \int \! dr \left( F_{px} + F_{py} + F_{pz} + F_{pm} \right). \tag{15}
$$

Using units where $\hbar = e^* = 1$, the first two contributions to the phase fluctuation free energy are

$$
F_{p_{\mu}} = E_{\mu} \left| \frac{\partial}{\partial \mu} \phi_n - i 2 e A_n \right|^2, \tag{15}
$$

where the characteristic energies in the $xy$ plane are

$$
E_\mu = |a_{2x}| |\Delta_n|^2, \tag{16}
$$

with $\mu = x, y$. The third contribution is

$$
F_{p_x} = J_z \cos (\phi_{n+1} - \phi_n - 2 G_z x - 2 e \bar{A}_{nz}), \tag{17}
$$

where $\bar{A}_{nz} = \int_{nc}^{(n+1)c} d z A_z / \bar{c}$, with the Josephson energy term being

$$
E_z = e^2 J_z = a_3 |\Delta_n| |\Delta_{n+1}|. \tag{18}
$$

The last contribution to the phase only fluctuation free energy is

$$
F_{p_m} = \frac{1}{8 \pi} \int d^3 r \left( \nabla \times A \right)^2, \tag{19}
$$

where $\mathbf{A}$ is the fluctuation vector potential. The saddle point amplitude of the order parameter has the form

$$
|\Delta_n| = \Delta_0 \left[ 1 + (t_z / \omega_{cz})^2 \cos (2 G_z x) \right], \tag{20}
$$

where the prefactor is $\Delta_0 = \delta \left[ 1 + (t_z / \omega_{cz})^2 \right]$, (for $E_F \gg \omega_{cz}$), with $\delta = \sqrt{T_c (H / T_c - H / 2 C) / 4 C}$. The saddle point phase $\phi_n^{(0)} = 2 G_z n x - (8 \pi a_3 \Delta_0^2 / H)^2 n \sin (2 G_z x)$. This corresponds to a rectangular Josephson vortex lattice with periodicity $l_x = \pi / G_z$ ($G_z$ is the inverse magnetic length) and $l_z = \bar{c}$ ($\bar{c}$ is the unit cell along
the z direction) holds a flux quantum $\phi_0$ inside the plaquette $(l_x, l_y)$, i.e., $H_{1x}l_y = \phi_0$. In what follows we use similar methods to those developed by Horovitz and Korshunov and Larkin to study the vortex lattice melting in layered superconductors. Writing down the phase of the order parameter as

$$\phi_n(x, y) = \phi_0 + \chi_n(x, y),$$

and integrating over the fluctuating vector potential we obtain the effective non-local sine-Gordon “Hamiltonian”

$$H = \int d\mathbf{r} (H_1 + H_2)$$

$$H_1 = \sum_{\mu} \left( E_{\mu} \sum_{n, n'} \frac{\partial \chi_n}{\partial \mu} \frac{\partial \chi_{n'}}{\partial \mu} \right)$$

$$H_2 = -\Gamma \sum_n \cos(\chi_{n+1} - 2\chi_n + \chi_{n-1}),$$

where the co-sinusoidal coupling constant is

$$\Gamma = J^2/4\sqrt{E_x E_y} \sqrt{\tilde{\gamma}_x(\pi) \tilde{\gamma}_y(\pi) h_z^2}$$

with the function

$$\tilde{\gamma}_\mu(q) = \frac{\lambda(q)}{\lambda(q) + 16\pi^2 E_\mu d/\phi_0^2}$$

being the discrete Fourier transform of $\gamma(n, n')$, where $\lambda(q) = [1 - \cos(q)]$. When $\Gamma \to 0$, the effective Hamiltonian given in Eq. (21) reduces to a layered anisotropic XY model, where phase fluctuations between layers $n$ and $n'$ are still coupled via the function $\gamma_n(n, n')$. Scaling the integration variables $x \to \tilde{x} \sqrt{E_x}$ and $y \to \tilde{y} \sqrt{E_y}$, and defining the charges $q_n = \int d\mathbf{r} \chi_n(x)/2\pi$, which correspond to the vorticities at position $r_i$ in the $n$-th plane, leads to a partition function identical to the anisotropic quasi-two-dimensional Coulomb gas, when an expansion in powers of the very small parameter $\Gamma$ and Gaussian integration over $\chi_n$ are performed, i.e.,

$$Z = \sum_m \left\{ \prod_{i=0}^{2m} \left( \int d\mathbf{r}_i \sum_{n_i} \right) \right\} \left( \frac{\Gamma}{2\gamma} \right)^{2m} \exp(A),$$

where the exponent in the partition function is

$$A = -\frac{1}{2} \sum_{i,j} q_{n_i} M(\mathbf{r}_{ij}, n_{ij}) q_{n_j}$$

where the charges $q_{n_i} = +1$ for $i = 1, \ldots, m$ and $q_{n_i} = -1$ for $i = m + 1, \ldots, 2m$. In addition, $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ and $n_{ij} = n_j - n_i$, and the correlation function

$$M(\mathbf{r}_{ij}, n_{ij}) = \int \frac{d^2 k}{(2\pi)^2} \frac{d q}{2\pi} \tilde{M}(k, q) \exp \left[ i(\mathbf{k} \cdot \mathbf{r}_{ij} + n_{ij} q) \right]$$

has as Fourier transform the function $\tilde{M}(k, q) = T/\sqrt{E_x E_y} k^2 \tilde{\gamma}(q)$, with $\tilde{\gamma}(q) = \sqrt{\gamma_x(q) \gamma_y(q)}$. Upon integration over $k$ and proper core regularization, the relevant part of the interaction term becomes

$$M(\mathbf{r}_{ij}, n_{ij}) \approx \frac{\alpha(n_{ij}) T}{2\pi \sqrt{E_x E_y}} \ln(|r_{ij}|/a_0)$$

where $\alpha(n_{ij}) = \int dq \exp(i n_{ij} q)/[2\pi \tilde{\gamma}(q)]$. Notice that the charges interact logarithmically whether they are in the same layer or not; however, the strength of the logarithmic interaction is larger when they are in the same layer. This means that in the limit where $\Gamma \to 0$ there is a phase transition which belongs to the same universality class of the Kosterlitz-Thouless-Berezinskii transition and, correspondingly, in the present problem, to the melting of the magnetic field induced rectangular Josephson vortex lattice. The transition here occurs when

$$T_m = \frac{\pi \sqrt{E_x(T_m) E_y(T_m)}}{1 + \sqrt{E_x(T_m) E_y(T_m)} 16\pi^3 \tilde{c}/\phi_0^2}$$

Notice that the right hand side of Eq. (29) is also dependent on temperature via $E_x(T)$. Using the expressions for $E_x(T)$ defined in Eq. (11) and solving equation Eq. (29) for the melting temperature at infinite field results in

$$T_m(\infty) = \frac{T_c(\infty)}{1 + \eta}$$

where $\eta = 2\pi \sqrt{2} T_c(\infty)/\tilde{c}$. Since $\eta > 0$, the melting temperature $T_m(\infty)$ is smaller than the saddle point (mean field) critical temperature $T_c(\infty)$, thus indicating that classical phase fluctuations reduce the transition temperature from $T_c(\infty)$ to $T_m(\infty)$. However, this reduction is small for Bechgaard salts since $\eta \ll 1$. When the condition $H \to \infty$ is relaxed the first order correction to $T_m$ can be computed using a perturbative renormalization group method since $E_x$ is much smaller than $T_c(\infty)$ and $T_m(\infty)$. This standard procedure leads to

$$T_m(H) = T_m(\infty) \left[ 1 + \epsilon \left( \frac{\ell_0^2 \Gamma}{2T_m(\infty)} \right)^2 \right]$$

where $\epsilon = \pi/2$, $\ell_0 = \pi/\omega_{cz}$ and the magnetic field dependent coefficient

$$\Gamma = \pi^2 \frac{\tilde{c} \tilde{v}_F}{\zeta(3) \tilde{t}_y b} \left( \frac{\Delta_0^2 \tilde{c}}{\omega_{cz}} \right) \ln^2 \left( \frac{\gamma \omega_{cz}}{2\pi T_c(\infty)} \right).$$

Notice the explicit magnetic field dependence of $\Gamma \sim H^{-6} \ln^2(H)$, such that the correction to $T_m(\infty)$ increases with decreasing magnetic field as $T_m(H) - T_m(\infty) \sim H^{-6} \ln^2(H)$ in the high field regime where $t_z/\omega_{cz} \ll 1$. This behavior has the following interpretation: a reduction of the magnetic field increases the magnetic field.
induced Josephson coupling $E_z$ and the system starts to become less two-dimensional, so that phase fluctuations become less efficient and $T_m(H)$ increases with decreasing field. However, the increase in $T_m(H)$ with decreasing field is very slow, and it looks quite flat when $T_c(H)$ and $T_m(H)$ are plotted in the same scale (See Fig. 1). This is in sharp contrast with what happens with the saddle point (mean field) critical temperature, which at high magnetic fields decreases from $T_c(\infty)$ as the magnetic field is lowered. The difference in behavior between $T_c(H)$ and $T_m(H)$ is illustrated in Fig. 1.

![FIG. 1. This figure shows the (mean field) critical temperature $T_c(H)$ and the melting temperature $T_m(H)$, in the regime $t_z/\omega_{c_2} \ll 1$ for applied fields $H$ precisely aligned with the $y$ ($b'$) axis. The ratio $t_z/\omega_{c_2} \approx 1/3, 1/18$ for fields $H = 5, 30$ Teslas, respectively. Temperatures are in Kelvin, and fields are in Teslas. The parameters used were $T_c(\infty) = 1.5K$, $t_y = 100K$, $t_z = 5K$ with lattice constants characteristic of Bechgaard salts.]

In summary, we have assumed an ESTP state as a plausible candidate for triplet superconductivity in quasi-one-dimensional systems \[\ldots\], and we have presented analytical results for the effects of phase fluctuations in the magnetic field versus temperature phase diagram of quasi-one-dimensional superconductors. We discussed for simplicity just the case of perfect alignment with the $y$ ($b'$) direction, and showed that phase fluctuations destroy the reentrant superconducting phase when $t_z/\omega_{c_2} \ll 1$. This loss of phase coherence corresponds to the melting of the magnetic field induced Josephson vortex lattice above the melting temperature $T_m(H)$. At very large fields $T_m(H)$ is only slightly smaller than the mean field critical temperature $T_c(H)$, however $T_m(H)$ has the opposite curvature of $T_c(H)$. This means that $T_m(H)$ decreases with increasing field while $T_c(H)$ increases with increasing field, provided that the condition $t_z/\omega_{c_2} \ll 1$ is satisfied. Furthermore, $T_m(H) - T_m(\infty) \sim H^{\frac{1}{16}} \ln^4(H)$ in this high field regime, and $T_m(H)$ looks quite flat when plotted in the same scale as $T_c(H)$. Finally, it is important to emphasize that we have discussed here the effects of classical phase fluctuations for perfect alignment along the $b'$ direction only.\[\ldots\]

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[1] A. G. Lebed, JETP Lett. 44, 114 (1986).
[2] L. N. Burlachkov, L. P. Gorkov, and A. G. Lebed, Europhys. Lett. 4, 941 (1987).
[3] N. Dupuis, G. Montambaux, and C. A. R. Sá de Melo, Phys. Rev. Lett. 70, 2613 (1993).
[4] I. J. Lee, et. al., Synth. Metals 70, 747 (1995).
[5] I. J. Lee, et. al., Phys. Rev. Lett. 78, 3555 (1997).
[6] A. G. Lebed, K. Machida, M. Ozaki, Phys. Rev. B 62 R795 (2000).
[7] I.J, Lee, et. al., cond-mat/0001332,(2000).
[8] I. J. Lee and M. J. Naughton, “The Superconducting State in Magnetic Fields: Special Topics and New Trends”, Ed. C. A. R. Sá de Melo, Ch. 14, pp. 272-295, World Scientific, Singapore (1998).
[9] X. Huang and K. Maki, Phys. Rev. B 39, 6459 (1989).
[10] C. D. Vaccarella and C. A. R. Sá de Melo, cond-mat/0010297, (2000).
[11] C. A. R. Sá de Melo, Physica C 260, 224 (1996).
[12] C. A. R. Sá de Melo, “The Superconducting State in Magnetic Fields: Special Topics and New Trends”, Ed. C. A. R. Sá de Melo, Ch. 15, pp. 296-324, World Scientific, Singapore (1998).
[13] C. A. R. Sá de Melo, J. Supercond. 12, 459 (1999).
[14] The Bechgaard salt family (TMTSF)$_2$X is truly triclinic, however, many of the qualitative results discussed in this paper can be easily generalized to the triclinic case.
[15] The Josephson vortex lattice (calculated in mean field theory) is rectangular, instead of triangular as considered in Ref. 8. The assumed orthorhombic symmetry of the underlying lattice imposes serious restrictions on the boundary conditions for the spatial profiles of the magnetic field, and thus frustrates the triangular solution in favor of the rectangular.