Thermodynamics and excitation spectrum of a quasi-one-dimensional superconductor in a high magnetic field

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(Received 8 April 1994)

At high magnetic field, the semiclassical approximation which underlies the Ginzburg-Landau theory of the mixed state of type-II superconductors breaks down. In a quasi-one-dimensional superconductor with an *open Fermi surface*, a high magnetic field stabilizes a cascade of superconducting phases which ends in a strong reentrance of the superconducting phase. From a microscopic mean-field model, we determine the thermodynamics and the excitation spectrum of these quantum superconducting phases.

It has recently been proposed that quasi-one-dimensional (quasi-1D) superconductors should exhibit an unusual phase diagram in a high magnetic field.[1,2] In a quasi-1D conductor (weakly coupled chains system) with an *open Fermi surface*, the magnetic field does not quantize the semiclassical orbits which are *open* but it induces a dimensional crossover in the sense that it tends to confine the wave functions along the chains. This quantum effect of the field strongly modifies the phase diagram predicted by the Ginzburg-Landau-Abrikosov-Gor'kov (GLAG) theory which is based on the semiclassical phase integral (or eikonal) approximation.[3] The usual Ginzburg-Landau (GL) regime is followed, when the field is increased, by a cascade of superconducting phases separated by first-order transitions which ends in a strong reentrance of the superconducting phase where the chains interact by Josephson coupling. The superconducting state evolves from an Abrikosov vortex lattice in the GL regime towards a Josephson vortex lattice in the reentrant phase. Between these two limits, the amplitude of the order parameter and the current distribution show a symmetry of a laminar type while the vortices still describe a triangular lattice. The cascade of phase transitions originates in commensurability effects between the periodicity of the order parameter and the crystalline lattice spacing. This high-field superconductivity can survive even in the presence of Pauli pair breaking because the quasi-1D Fermi surface allows one to construct a Larkin-Ovchinnikov-Fulde-Ferrell state which can exist far above the Pauli limited field. A very important aspect is that the temperature and magnetic field scales are determined by the coupling between chains.[2] This means that the temperature and magnetic field ranges where high-field superconductivity is expected can be experimentally accessible if appropriate (i.e., sufficiently anisotropic) materials are chosen.

In this paper, we derive the thermodynamics and the excitation spectrum of these quantum superconducting phases from a microscopic model in the mean-field approximation. We consider a strongly anisotropic superconductor described by the dispersion law ($\hbar = k_B = 1$ throughout the paper) $E(\mathbf{k}) = v(|k_x| - k_F) + t_z \cos(k_z c)$ where the Fermi energy is chosen as the origin of the energies. v is the Fermi velocity for the motion along the

chains and t_z is the coupling between chains separated by the distance c. For a linearized dispersion law, the y direction parallel to the magnetic field does not play any role (as long as the Cooper pairs are formed with states of opposite momenta in this direction) so that we restrict ourselves to a 2D model. We assume that the zero-field critical temperature T_{c0} is smaller than t_z so that the superconductor is really 3D: In the GLAG description, there is no Josephson coupling between chains even at $T = 0$. We consider singlet pairing but we neglect the Zeeman term (i.e., we put the g factor equal to zero). The Pauli pair breaking effect can easily be incorporated in the present description.

In the gauge $\mathbf{A}(Hz, 0, 0)$, the one-particle Hamiltonian obtained from the Peierls substitution $\mathcal{H}_0 = E(\mathbf{k} \rightarrow -i\nabla - e\mathbf{A})$ is given by

$$\mathcal{H}_0^\alpha = v(-i\alpha\partial_x - k_F) + \alpha \hat{m}\omega_c + t_z \cos(-ic\partial_z), \quad (1)$$

where $\alpha = + (-)$ labels the right (left) sheet of the Fermi surface and $\hat{m}$ is the (discrete) position operator in the z direction. We have introduced the energy $\omega_c = Gv$ where $G = -eHc$ is a magnetic wave vector and H the external magnetic field perpendicular to the system. $\mathcal{H}_0$ can easily be diagonalized by noting that the momentum along the chains is a good quantum number and by taking the Fourier transform with respect to m. The eigenstates and the corresponding eigenenergies are

$$\phi_{k_x,l}^\alpha(\mathbf{r}) = \frac{1}{\sqrt{cL_x}} e^{ik_x x} J_{l-m}(\alpha \tilde{t}), \quad (2)$$

$$\epsilon_{k_x,l,\sigma}^\alpha = v(\alpha k_x - k_F) + \alpha l \omega_c, \quad (3)$$

where $\mathbf{r} = (x, m)$, $\tilde{t} = t_z/\omega_c$, $\alpha = \text{sgn}(k_x)$, and J_l is the lth-order Bessel function. L_x is the length of the system in the x direction. The spectrum consists in a discrete set of 1D spectra. The state $\phi_{k_x,l}^\alpha$ is localized around the lth chain with a spatial extension in the z direction of the order of $\tilde{t}c$ which corresponds to the amplitude of the semiclassical orbits.[2] Note that the states $\phi_{k_x,l}^\alpha$ can be obtained from the localized states introduced by Yakovenko[4] by a gauge transformation. The superconducting instability can be qualitatively understood from the spectrum (3). In zero field, time-reversal symmetry ensures that $E_\uparrow(\mathbf{k}) = E_\downarrow(-\mathbf{k})$ so that the pairing at zero

total momentum presents the usual (Cooper) logarithmic singularity which results in an instability of the metallic state at a finite temperature T_{c0}. A finite magnetic field breaks down time-reversal symmetry. Nonetheless, we still have $\epsilon^{\alpha}_{k_x,l_1,\uparrow} = \epsilon^{-\alpha}_{q_x-k_x,l_2,\downarrow}$ for $q_x = -(l_1 + l_2)G$. Thus, whatever the value of the field, some pairing channels will present the Cooper singularity $\sim \ln(2\gamma\Omega/\pi T)$ ($\gamma \sim 1.781$ and Ω is the cutoff energy of the attractive interaction) if the total momentum along the chain q_x is a multiple of G. This results in logarithmic divergences at low temperature in the linearized gap equation which destabilize the metallic state at a temperature $0 < T_c < T_{c0}$.[1,2] Besides the most singular channels which present the Cooper singularity, there exist less singular channels with singularities $\sim \ln|\Omega/n\omega_c|$ ($n \neq 0$) for $T \ll \omega_c$. In this high-field limit ($\omega_c \gg T$), a natural approximation consists in retaining only the most singular channels. Such an approximation has been used previously in the mean-field theory of the field-induced spin-density-wave phases observed in some organic conductors (single gap approximation) (Ref. 5) and in the mean-field theory of isotropic superconductors in a high magnetic field where it is known as the quantum limit approximation (QLA).[6] In the following, we shall adopt this latter designation.

In order to obtain the critical temperature when $\omega_c \gg T$, we consider the two-particle vertex function in the representation of the eigenstates of $\mathcal{H}_0$. In the chosen gauge, the total momentum q_x along the chains is a constant of motion. Since in the QLA we consider only the most singular pairing channels, the center of gravity of the Cooper pair in the perpendicular direction is related to the total momentum q_x by $L_{12} = (l_1 + l_2)/2 = -q_x/(2G)$ as explained above, and therefore becomes also a constant of motion. Thus the two-particle vertex function can be written as $\Gamma^{\alpha\alpha'}_{q_x(L),L}(l_{12},l'_{12})$ with $q_x(L) = -2LG$, where $l_{12} = l_1 - l_2$ and $l'_{12} = l'_1 - l'_2$ describe the relative motion of the pair in the z direction. In the ladder approximation, the integral equation for Γ then reduces to ($l \equiv l_{12}$, $l' \equiv l'_{12}$)

$$\Gamma^{\alpha\alpha'}_{q_x(L),L}(l,l') = -\lambda V^{\alpha\alpha'}_{l,l'}$$
$$+ \frac{\lambda}{2}\chi(0) \sum_{\alpha'',l''} V^{\alpha\alpha''}_{l,l''} \Gamma^{\alpha''\alpha'}_{q_x(L),L}(l'',l'), \quad (4)$$

where $V^{\alpha\alpha'}_{l,l'} = \alpha^l \alpha'^{l'} V_{l,l'}$ and

$$V_{l,l'} = \int_0^{2\pi} \frac{dx}{2\pi} J_l(2\tilde{t}\cos x) J_{l'}(2\tilde{t}\cos x). \quad (5)$$

$-\lambda V^{\alpha\alpha'}_{l,l'}$ is the matrix element of the local electron-electron interaction $-\lambda\delta(\mathbf{r}_1 - \mathbf{r}_2)$ ($\lambda > 0$) in the representation of the states $\phi^{\alpha}_{k_x,l}$. Note that $V^{\alpha\alpha'}_{l,l'}$ is independent of the center of gravity of the Cooper pair. $\chi(0) = N(0)\ln(2\gamma\Omega/\pi T)$ is the pair susceptibility at zero total momentum in zero field and $N(0)$ is the density of states per spin at the Fermi level. The preceding integral equation is solved by introducing the orthogonal transformation $U_{l,l'}$ which diagonalizes the matrix $V_{l,l'}$. One obtains

$$\Gamma^{\alpha\alpha'}_{q_x(L),L}(l,l') = -\lambda\alpha^l\alpha'^{l'} \sum_{l''} \frac{U_{l,l''}\bar{V}_{l'',l''}(U^{-1})_{l'',l'}}{1 - \lambda\chi(0)\bar{V}_{l'',l''}}, \quad (6)$$

where $\bar{V}$ is the diagonal matrix $U^{-1}VU$. The metallic state becomes instable when a pole appears in the two-particle vertex function which leads to the critical temperature

$$T_c = \frac{2\gamma\Omega}{\pi} e^{\frac{-1}{\lambda N(0)\bar{V}_{l_0,l_0}}}, \quad (7)$$

where $\bar{V}_{l_0,l_0}$ is the highest eigenvalue of the matrix V. The critical temperatures are shown in Fig. 1 for the two highest eigenvalues of V. This clearly indicates that there are two lines of instability competing with each other and leading to a cascade of first-order transitions in agreement with the exact mean-field calculation of T_c.[2] Except for the last phase, T_c calculated in the QLA is several orders of magnitude below the exact critical temperature: It has been pointed out previously that the QLA strongly underestimates the critical temperature.[7] The existence of two lines of instability results from the fact that $V_{l,l'} = 0$ if l and l' do not have the same parity. Diagonalizing the matrix $V_{l,l'}$ is then equivalent to separately diagonalizing the matrices $V_{2l,2l'}$ and $V_{2l+1,2l'+1}$. In the following, we label these two lines by $l_0 = 0,1$ so that $\bar{V}_{l_0,l_0} = \max_l \bar{V}_{2l+l_0,2l+l_0}$. Since $2L = l_1 + l_2$ and $l_1 - l_2$ have the same parity, L is integer (half-integer) for $l_0 = 0$ ($l_0 = 1$) and can be written as $L = -l_0/2 + p$ with p integer. Correspondingly, we have $q_x(L) = (l_0 - 2p)G$. It is clear that the instability line l_0 corresponds to the instability line $Q = l_0 G$ which was previously obtained in another approach.[2] From Eq. (6), one can see that the superconducting condensation in the channel $q_x(L), L, l_0$ corresponds to the following spatial dependence for the order parameter:

$$\Delta_{q_x(L),L,l_0}(\mathbf{r}) \sim \sum_{\alpha,l} \alpha^l U_{l,l_0} \phi^{\alpha}_{k_x,L+\frac{l}{2}}(\mathbf{r}) \phi^{\bar{\alpha}}_{q_x(L)-k_x,L-\frac{l}{2}}(\mathbf{r}),$$
$$(8)$$

where we note $\bar{\alpha} = -\alpha$. Noting that the matrices V and U have a range of the order of $\tilde{t}$ (i.e., $V_{l,l'}$, $U_{l,l'}$ are important for $|l|$, $|l'| < \tilde{t}$), one can see that $\Delta_{q_x(L),L,l_0}$ has the form of a strip extended in the direction of the chains and localized in the perpendicular direction on a length
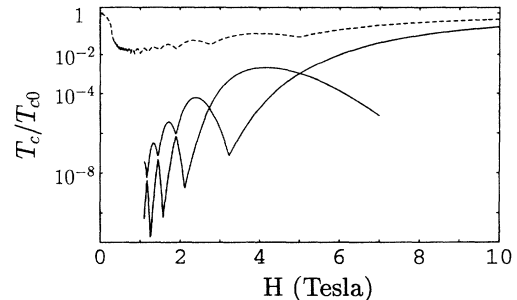

FIG. 1. Solid lines: critical temperature vs magnetic field for $l_0 = 0$ and $l_0 = 1$ in the QLA. Dashed line: exact mean-field critical temperature.

of the order of $c\tilde{t}$. This is not surprising since $\Delta_{q_z(L),L,l_0}$ results from pairing between the localized states $\phi^\alpha_{k_x,l}$.

Following the original approach proposed by Abrikosov,[3] we construct the order parameter for $T < T_c$ as a linear combination of the solutions (8): $\Delta(\mathbf{r}) = \sum_L \gamma(L)\Delta_{q_x(L),L,l_0}(\mathbf{r})$ where $2L$ must have the parity of l_0. Since $\Delta_{q_x(L),L,l_0}$ is localized in the z direction with an extension of the order of $c\tilde{t}$, a natural choice for the coefficients $\gamma(L)$ is to take $\gamma(L) \neq 0$ if $L = -l_0/2 + pN'$ (p integer) where the unknown integer N' is expected to be of the order of $\tilde{t}$. In order to correctly describe the triangular Josephson vortex lattice in the last phase ($\tilde{t} \ll 1$),[2] we choose $\gamma(L) \equiv \gamma(p) = 1$ (i) for p even (odd) which leads to (noting $N = 2N'$)

$$\Delta_{l_0,N}(\mathbf{r}) = \Delta \sum_{l,p} U_{2l+l_0,l_0}\gamma_p e^{i(l_0-pN)Gx} J_{p\frac{N}{2}+l-m}(\tilde{t})$$

$$\times J_{p\frac{N}{2}-l-l_0-m}(-\tilde{t}), \qquad (9)$$

where the amplitude Δ is chosen real. Equation (9) defines a variational order parameter where the two unknown parameters Δ and N have to be determined by minimizing the free energy. It can be seen that $|\Delta(\mathbf{r})|$ has periodicity $a_x = 2\pi/NG$ and $a_z = Nc$ so that the unit cell contains two flux quanta: $Ha_x a_z = 2\phi_0$ (when a triangular lattice is described with a square unit cell, the unit cell contains two flux quanta). In Ref. 2, the order parameter was constructed by imposing that it describe both the triangular Abrikosov vortex lattice in a weak field ($\omega_c \ll T$) and the triangular Josephson vortex lattice in a very strong field ($\omega_c \gg t_z$). Both approaches lead to the same order parameter when only the Cooper singularities are retained.

In order to derive the thermodynamics and the excitation spectrum in the superconducting phases, it is necessary to determine the normal and anomalous Green's functions from the Gor'kov equations

$$(i\omega - \mathcal{H}^\alpha_0)G^\alpha_\sigma(\mathbf{r},\mathbf{r}',\omega) - \Delta_\sigma(\mathbf{r})F^{\overline{\alpha}\dagger}_{\overline{\sigma}}(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}'),$$

$$(-i\omega - \mathcal{H}^{\overline{\alpha}\dagger}_0)F^{\overline{\alpha}\dagger}_{\overline{\sigma}}(\mathbf{r},\mathbf{r}',\omega) + \Delta^*_\sigma(\mathbf{r})G^\alpha_\sigma(\mathbf{r},\mathbf{r}',\omega) = 0, \quad (10)$$

with the self-consistency equation $\Delta^*_\sigma(\mathbf{r}) = \lambda T \sum_{\alpha,\omega} F^{\alpha\dagger}_\sigma(\mathbf{r},\mathbf{r},\omega)$. Here $\Delta_\sigma(\mathbf{r}) = \lambda \sum_\alpha \langle \psi^\alpha_\sigma(\mathbf{r})\psi^{\overline{\alpha}}_{\overline{\sigma}}(\mathbf{r})\rangle$ where the $\psi^\alpha_\sigma(\mathbf{r})$'s are fermionic operators for particles moving on the sheet α of the Fermi surface. $\Delta_\uparrow(\mathbf{r}) = -\Delta_\downarrow(\mathbf{r})$ is the variational order parameter defined by (9). G^α_σ and $F^{\alpha\dagger}_\sigma$ are the Fourier transforms with respect to the imaginary time τ of the correlation functions $-\langle T_\tau \psi^\alpha_\sigma(\mathbf{r},\tau)\psi^{\alpha\dagger}_\sigma(\mathbf{r},0)\rangle$ and $-\langle T_\tau \psi^{\alpha\dagger}_\sigma(\mathbf{r},\tau)\psi^{\overline{\alpha}\dagger}_{\overline{\sigma}}(\mathbf{r},0)\rangle$. In (10), it is assumed that the magnetization $\mathbf{M} = (\mathbf{B} - \mathbf{H})/4\pi$ is equal to zero. This approximation is justified in the last phase ($\tilde{t} \ll 1$) where $\mathbf{M}$ is of the order of $\tilde{t}^2$ and its contribution to the Gibbs free energy $G(T,H)$ of the order of $\tilde{t}^4$. In the other phases, we expect that the approximation $\mathbf{B} = \mathbf{H}$ will give reliable results at least not too far from the reentrant phase.

In order to have a simple description of the superconducting state, we introduce the magnetic Bloch states

$$\phi^\alpha_{\mathbf{q},l} = \sqrt{\frac{N}{N_z}}\sum_p e^{-ipq_z a_z}\phi^\alpha_{q_x+pNG,l-pN}, \qquad (11)$$

where N_z is the number of chains. The eigenenergies are $\epsilon^\alpha_{\mathbf{q},l,\sigma} = \epsilon^\alpha_{q_z,l,\sigma}$. $\mathbf{q}$ is restricted to the first magnetic Brillouin zone: $|q_x| - k_F \in] - \pi/a_x, \pi/a_x]$ and $q_z \in] - \pi/a_z, \pi/a_z]$. There are N branches ($-N/2 < l \leq N/2$) at the Fermi level. The order parameter (9) is entirely described by the pairing between the states $\phi^\alpha_{\mathbf{q},l}$ and $\phi^{\overline{\alpha}}_{l_0 G-\mathbf{q},-l_0-l}$ where $\mathbf{G} = (G,0)$. Consequently, the Gor'kov equations (10) become diagonal in the representation of the magnetic Bloch states and their solutions are

$$G^\alpha_\sigma(\mathbf{q},l,\omega) = \frac{-i\omega - \epsilon^\alpha_{\mathbf{q},l,\sigma}}{\omega^2 + {\epsilon^\alpha_{\mathbf{q},l,\sigma}}^2 + |\Delta^\alpha_\sigma(\mathbf{q},l)|^2},$$

$$F^{\alpha\dagger}_\sigma(\mathbf{q},l,\omega) = \frac{\Delta^\alpha_\sigma(\mathbf{q},l)^*}{\omega^2 + {\epsilon^\alpha_{\mathbf{q},l,\sigma}}^2 + |\Delta^\alpha_\sigma(\mathbf{q},l)|^2}, \qquad (12)$$

where the pairing amplitude $\Delta^\alpha_\sigma(\mathbf{q},l)$ is defined by

$$\Delta^\alpha_\sigma(\mathbf{q},l) = \int d^2\mathbf{r}\, \phi^\alpha_{\mathbf{q},l}(\mathbf{r})^*\phi^{\overline{\alpha}}_{l_0 G-\mathbf{q},-l_0-l}(\mathbf{r})^*\Delta_\sigma(\mathbf{r})$$

$$= \Delta_\sigma \alpha^{l_0}\overline{V}_{l_0,l_0}\sum_p \gamma_p e^{-ipq_z a_z}U_{2l+l_0+pN,l_0}. \qquad (13)$$

Here $\Delta_\uparrow = -\Delta_\downarrow = \Delta$. The functions G^α_σ and $F^{\alpha\dagger}_\sigma$ appearing in (12) are the Fourier transforms of the correlation functions $-\langle T_\tau b^\alpha_{\mathbf{q},l,\sigma}(\tau)b^{\alpha\dagger}_{\mathbf{q},l,\sigma}(0)\rangle$ and $-\langle T_\tau b^{\alpha\dagger}_{\mathbf{q},l,\sigma}(\tau)b^{\overline{\alpha}\dagger}_{l_0 G-\mathbf{q},-l_0-l,\overline{\sigma}}(0)\rangle$ where $b^\alpha_{\mathbf{q},l,\sigma}$ ($b^{\alpha\dagger}_{\mathbf{q},l,\sigma}$) are annihilation (creation) operators of a particle with spin σ in the state $\phi^\alpha_{\mathbf{q},l}$.

From the knowledge of the Green's functions, we can calculate the free energy of the system. Close to T_c, the difference between the free energies of the superconducting and normal states can be obtained in a GL expansion $F_N[\Delta] = A\Delta^2 + B\Delta^4/2$ where

$$A = \frac{\lambda^{-1}}{S}\int d^2\mathbf{r}\left|\frac{\Delta(\mathbf{r})}{\Delta}\right|^2 - \frac{T}{S}\sum_{\mathbf{q},l,\omega}\frac{|\Delta^\alpha_\sigma(\mathbf{q},l)/\Delta|^2}{\omega^2 + {\epsilon^\alpha_{\mathbf{q},l,\sigma}}^2},$$

$$B = \frac{T}{S}\sum_{\mathbf{q},l,\omega}\frac{|\Delta^\alpha_\sigma(\mathbf{q},l)/\Delta|^4}{(\omega^2 + {\epsilon^\alpha_{\mathbf{q},l,\sigma}}^2)^2}, \qquad (14)$$

where $S = L_x N_z c$ is the area of the system. The two preceding equations can be further simplified by using (13). Minimizing the free energy $F_N[\Delta]$ with respect to Δ, we obtain $F_N = -A^2/2B$. In the reentrant phase where the approximation $\mathbf{B} = \mathbf{H}$ is justified, we find that the minimum of F_N is obtained for $N = 2$.[8] When the field is decreased from its value in the reentrant phase, the system undergoes a first-order phase transition and the minimum of F_N is then obtained for $N = 4$. This result is in agreement with Ref. 2 where it is argued that the first-order phase transitions are due to commensurability effects between the crystalline lattice spacing and the periodicity of the order parameter. Unlike what was expected,[2] the best value of N switches to 6 before reaching the next first-order transition. This indicates the importance of the screening of the external field in calculating the free energy in the phases $N \geq 4$.

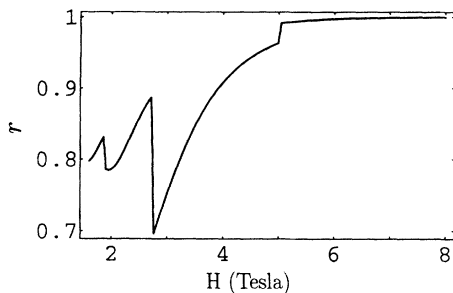The specific heat jump at the transition is obtained

FIG. 2. Ratio $r = (\Delta C/C_N)/(\Delta C/C_N)_{\rm BCS}$ vs magnetic field.
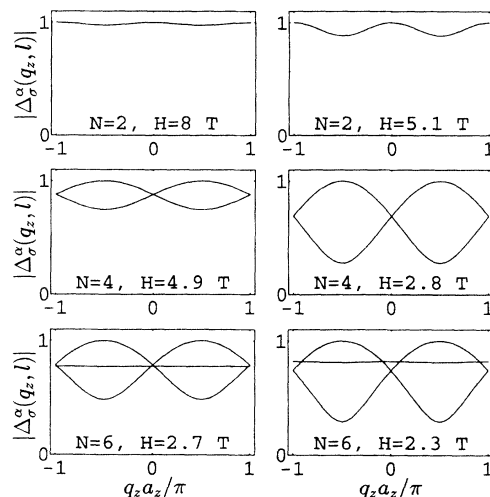

FIG. 3. Excitation spectrum in the phases $N = 2$, $N = 4$, and $N = 6$. The units are chosen so that $\max |\Delta_\sigma^\alpha(q_z, l)| = 1$. In the phase N, there are $N/2$ distinct branches.

from $\Delta C = -T\partial^2 F/\partial T^2$. The ratio $\Delta C/C_N$ where C_N is the specific heat of the normal state is found to be always smaller than the (BCS) zero-field value and discontinuous at the first-order phase transitions (Fig. 2). The discontinuity can be related to the slope $\Delta T/\Delta H$ of the first-order transition line:[9] The slope is positive for the last transition and negative for the other transitions. The magnetization is obtained from $M = -\partial F_N/\partial H$. Since T_c is determined by $F_N = 0$, M has the sign of dT_c/dH.[10] Each phase will therefore first be paramagnetic and then diamagnetic for increasing field, except the reentrant phase which is always paramagnetic.[11]

From the Green's functions (12), we deduce the quasiparticle excitation spectrum $E_{\mathbf{q},l,\sigma}^\alpha = \pm[\epsilon_{\mathbf{q},l,\sigma}^{\alpha\,2} + |\Delta_\sigma^\alpha(\mathbf{q},l)|^2]^{1/2}$. A gap $2\Delta_\sigma^\alpha(\mathbf{q},l)$ opens at the Fermi level in each branch l. The spectrum is shown in Fig. 3 for the last three phases $N = 2$, $N = 4$, and $N = 6$. In the very-high-field limit ($\tilde{t} \ll 1$), the spectrum is almost flat, the dispersion of the quasiparticle band being of the order of $\tilde{t}^2$. When the field is decreased within a given phase, the dispersion increases. The minimum excitation energy decreases when N increases. Thus Fig. 3 clearly

shows how the system evolves from a quasi-1D (quasi-2D if the magnetic field direction is taken into account) behavior in very high magnetic field ($\tilde{t} \ll 1$) towards the GL regime ($\omega_c \ll T$) where the spectrum is known to be gapless.[3]

In conclusion, we have solved the BCS theory for a quasi-1D superconductor in a high magnetic field. The theory can easily be extended to include the pairing channels which are not considered in the QLA: The results presented in this paper are not qualitatively modified.

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