Two-dimensional low-$\kappa$ type-II superconductors are studied numerically within the Eilenberger equations of superconductivity. Depending on the Ginzburg-Landau parameter $\kappa = \lambda/\xi$, vortex-vortex interaction can be attractive or purely repulsive. The sign of interaction is manifested as a first (second) order phase transition from Meissner to the mixed state. Temperature and field dependence of the magnetic field distribution in low-$\kappa$ type-II superconductors with attractive intervortex interaction is calculated. Theoretical results are compared to the experiment.

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Superconductors are divided into two groups, type-I and type-II, based on their behavior in external magnetic field. The underlying physics is especially transparent within the Ginzburg-Landau (GL) model. It can be shown that the difference in thermodynamics originates from the sign of vortex-vortex interaction, which can be attractive or repulsive. The sign of the interaction is controlled by GL parameter $\kappa = \lambda/\xi$, ratio of penetration depth and coherence length near $T_c$. In type-I superconductors ($\kappa < 1/\sqrt{2}$) vortices attract each other. In type-II superconductors ($\kappa > 1/\sqrt{2}$), vortex-vortex interaction is repulsive and the phase transition from Meissner to the mixed state at $H_{c1}$ is of the second order.

It has been verified experimentally since a long time that away from $T_c$ even in type-II superconductors with $\kappa \sim 1$ interaction between vortices can be attractive. Vortex attraction is manifested as a first order phase transition from Meissner to the mixed state. This type of superconductivity we denote as type-IIa to distinguish it from the type-Ib superconductivity with purely repulsive vortex-vortex interaction. Obviously attractive interaction in type-IIa superconductors will turn into repulsive below some critical intervortex distance thus preventing vortices to collapse into the normal state as in type-I superconductors. Evidence for jump in magnetization and mixture of vortex and Meissner domains near $H_{c1}$ is found from many magnetic, calorimetric, decoration and neutron scattering measurements (experimental results are partially reviewed in Ref. [1]). Here we refer just to a nicely performed experiment by Auer and Ullmaier [2], in which all three types (type-I, IIa and IIb) of superconductivity were reproduced in TaN by tuning the value of $\kappa$.

Although low-$\kappa$ type-II superconductors are of less interest from the point of view of potential application, attractive vortex interaction is still a challenging problem not fully understood. Most of the theoretical efforts to understand interaction of vortices as a function of parameter $\kappa$ relied on the extended GL model. Utilization of Bogomolnyi method to treat GL equations for $\kappa$ close to $1/\sqrt{2}$ gave the further impetus for this research direction [3]. However, range of applicability of GL formalism is confined to the region near $T_c$. Therefore to calculate the full temperature dependence of $\kappa_c(T)$, boundary between type-IIa and type-IIb superconductivity, one should rather turn to the microscopic theory of superconductivity. An approximate curve $\kappa_c(T)$ has been calculated by Kramers based on the asymptotic solution of Eilenberger equations of superconductivity. It is argued that the calculated curve is just the lower limit for the true one. Brandt [4] has obtained jumps at $H_{c1}$ by variational approximation of his free energy functional. The only attempt to calculate numerically $\kappa_c(T)$ without approximations besides those immanent to numerical procedure is due to Klein [5]. In this thorough study clean and dirty isotropic 3D superconductors are analyzed.

The purpose of this work is two fold. First, we applied a new method to solve Eilenberger equations for a vortex lattice. It appears to be efficient and faster than the so-called “explosion method” [6]. Second, we extended previous numerical study of 2D superconductors [7] to the low-$\kappa$ case where the interesting attractive vortex-vortex interaction occurs. Though the quantitative results will be different from the 3D case, the qualitative $(\kappa, T)$ phase diagram is quite similar. This is explicitly shown by calculating phase diagram $(\kappa, T)$ of type-I, type-IIa and type-IIb superconductivity. We focused on the magnetic and temperature dependence of calculated magnetic field profiles and compare the result with experimental data.

Eilenberger version of BCS theory of superconductivity is proven to be a good starting point for both analytical and numerical calculations. For the isotropic gap Eilenberger equations are

$$[\omega + u(\nabla + iA)] f = \Psi g, \quad (1)$$

$$[\omega - u(\nabla - iA)] f^\dagger = \Psi^\ast g. \quad (2)$$

These are supplemented by the self-consistency equations for the gap function $\Psi$ and vector-potential $A$

$$\Psi \ln t = 2t \sum_{\omega > 0} \left( f \frac{\Psi - \Psi^\ast}{\omega} \right), \quad (3)$$

$$\nabla \times \nabla \times A = -\frac{4t}{\kappa^2} \text{Im} \sum_{\omega > 0} (ug). \quad (4)$$
Equations are written in following dimensionless units: order parameter is measured in units \(\pi T_c\), length in units \(R = v_0/(2\pi T_c)\), \(v_0\) is Fermi velocity, magnetic field in units \(H_0 = \Phi_0/2\pi R^2\), vector potential in units \(A_0 = \Phi_0/2\pi R\), energy in units \(E_0 = (\pi T_c)^2 N(0) R^3\). Eilenberger parameter \(\kappa\) is

\[
\kappa^{-2} = \frac{2\pi N(0)}{p_0} \left( \frac{\pi}{p_0} \right)^2 \frac{v_0^2}{(\pi T_c)^2}.
\]

It is related to GL parameter \(\kappa\) via \(\kappa^2 = (7\zeta(3)/18)\kappa^2\) in 3D case and

\[
\kappa^2 = \frac{7\zeta(3)}{8} \kappa^2.
\]

in 2D case. Here \(\zeta\) is Riemann’s zeta function. Here, \(\omega = \tau(2\pi + 1)\) is Matsubara frequency with integer \(n\), \(t = T/T_c\) is reduced temperature, \(u\) is unit vector directed along Fermi velocity. Eilenberger Green’s functions \(f, f^\dagger\) and \(g\) are normalized so that \(g = \sqrt{1 - f^\dagger f}\). Average over the isotropic cylindrical Fermi surface \(\langle \ldots \rangle\) reduces to \(1/(2\pi) \int \ldots d\varphi\), average over polar angle \(\varphi\). Expression for the free energy density difference between superconducting and normal state is given by, simplified with the help of Eilenberger and self-consistency equations

\[
F = \kappa^2 (\nabla \times \mathbf{A})^2 - t \sum_{\omega > 0} \frac{1 - g}{1 + g} (\Psi^* f + \Psi f^\dagger).
\]

We use the following notation for spatial average \(\overline{C} = (B/2\pi) \int_C \text{d}ds\), where \(B\) is magnetic induction. Apart from the extreme cases \(H \sim H_{c1}\) and \(H \sim H_{c2}\), which allow for an analytical solution, the only tool at hand is numerical analysis. Standard way to solve Eilenberger equations for a vortex lattice is so-called “explosion” method (for details see Refs. [8]). Here, another approach which takes the advantage of periodicity of the vortex lattice has been adopted. The same approach is used by Brandt[9] to solve numerically GL equations. For this purpose it will be useful to introduce auxiliary functions \(a\) and \(b\) through the following transformation [8]

\[
f = \frac{2a \exp(-i\phi)}{1 + ab}, \quad f^\dagger = \frac{2b \exp(i\phi)}{1 + ab}, \quad g = \frac{1 - ab}{1 + ab},
\]

where \(\phi\) is the phase of the order parameter, \(\Psi = |\Psi| \exp(-i\phi)\). Equations for auxiliary functions \(a\) and \(b\) are decoupled and have the form of Riccati’s differential equation

\[
u \nabla a = -(\omega + iuA_s) a + \frac{|\Psi|}{2} (1 - a^2),
\]

\[
u \nabla b = (\omega + iuA_s) b - \frac{|\Psi|}{2} (1 - b^2).
\]

In new gauge vector-potential \(A_s = A - \nabla \phi\) is proportional to the superfluid velocity. It diverges as \(1/r\) at the vortex center (we put index \(s\) to denote its singular nature). Functions \(a\) and \(b\) are not independent but there is a relationship between them

\[
a^*(r - u, \omega) = b(r, u, \omega).
\]

Therefore it is sufficient to solve only the equation for auxiliary function \(a\). Also, we don’t need to solve equation (8) for all Fermi velocity directions because

\[
a(-r, -u, \omega) = a(r, u, \omega).
\]

Reflection at the \(y\) axis will change the direction of the magnetic field. When combined with time reversal it leaves Hamiltonian of the superconducting system invariant. One can show, at least numerically, that the following equation holds

\[
a(x, y, -ux, uy) = a(-y, -x, ux, uy).
\]

Therefore it is enough to solve Eq. (8) for velocity directions \(0 < \varphi < \pi/2\) to recover \(a\) and \(b\) for all \(u\) via symmetry relations (10), (11), and (12).

Singular vector-potential has the following property

\[
\nabla \times A_s = B(r) - 2\pi e_s \sum_{r_i} \delta(r - r_i),
\]

where \(r_i\) are positions of vortices and \(\delta(r)\) is 2D Dirac function. For an ideal vortex lattice \(z\)-component of the magnetic field \(B(r) = \nabla \times A\) and modulo of the gap function \(|\Psi|\) has the periodicity of the vortex lattice. The same is not true for \(\Psi\) and \(A\). However, superfluid velocity, i.e. \(A_s\), is invariant under the translation from one to another vortex lattice cell. Therefore one must assume that auxiliary functions \(a\) and \(b\) are also periodic functions. Then we expand \(a\) in Fourier series

\[
a(r) = \sum_Q a(Q) \exp(iQr),
\]

where summation goes over reciprocal vortex lattice vectors \(Q\). Fourier transform of a periodic function \(f(r)\) is defined as

\[
[f(r)]_{FT} = \frac{B}{2\pi} \sum_{\text{cell}} \int f(r) \exp(-iQr) \, d^2r.
\]

We split the local magnetic field \(B(r)\) into constant part, magnetic induction \(\overline{B}\), and periodic part \(B'(r)\) with zero average over the vortex lattice cell. Similarly, vector-potential is splitted into two parts

\[
B(r) = \overline{B} + B'(r) = \nabla \times \overline{A} + \nabla \times A'.
\]

We will assume that \(A'(r)\) is periodic with \(\nabla \cdot A' = 0\), so that all uncertainty of the gauge is in \(\overline{A}\). Therefore \(A'\) is periodic solution of the self-consistency equation (13).
From the equation (13) one can construct singular vector-potential $A$ through the periodic solution $A' = A - \nabla \phi'$ where

$$\nabla \phi' = \sum_{\mathbf{r}_i} \frac{(y - y_i)e_x + (x - x_i)e_y}{(x - x_i)^2 + (y - y_i)^2}.$$

(18)

Sum converges very slowly and the rate of convergence can be improved by Ewald construction

$$\nabla \phi' = B \sum_{\mathbf{Q} \neq 0} \frac{-Q_x e_x + Q_y e_y}{Q^2} \exp (-\gamma Q^2) \sin (\mathbf{Qr}) +$$

$$\sum_{\mathbf{r}_i} \frac{(y - y_i)e_x + (x - x_i)e_y}{(x - x_i)^2 + (y - y_i)^2} \exp \left[ - \frac{(\mathbf{r} - \mathbf{r}_i)^2}{4\gamma} \right].$$

(19)

Parameter $\gamma$ is in principle arbitrary; we choose $\gamma = \pi$ to assure good convergence for both sums.

Self-consistency equations are solved by iteration. For a given vector-potential $A'$ and gap function $\Psi$, Eq. (8) is solved numerically. We start the iteration procedure with $A' = 0$ and $\Psi = \text{const}$. Functions $a$ and $b$ are then used to calculate new values of $A'$ and $\Psi$ with help of self-consistency equations, and the whole process is repeated until the self-consistency is achieved. Equation (8) is also solved by iteration. We solved it in Fourier space where unknown are coefficients $a$. Iterative procedure for unknown coefficients $a$ is

$$a(Q) = \frac{[\Psi((1 - a^2)/2 - i\mathbf{u}A_x a)]_{\Omega T}}{\omega + iQ\mathbf{u}}.$$

(20)

Maximum summation frequency was set as $\omega_c = 20t$ ($h\omega_c = 20\pi k_B T_c$ in physical units). Vortex lattice unit cell is divided into $N \times N$ mesh which turns into approximating auxiliary functions $a$ and $b$ by sum over $N \times N$ harmonics. We set $N = 128$. Integration over polar angle $\varphi$ in each quadrant is performed by 30-points Gauss-Legendre integration. Iteration procedure fails for extremely small $\omega$, i.e. for very low temperatures $t \leq 0.05$.

In all other cases it is recommended to damp the iteration process via $a_{new} = (c_1 a_{new} + c_2 a_{old})/(c_1 + c_2)$ with $c_1 \leq c_2$. To manipulate with eqs. (14) and (15), fast Fourier transform algorithm should be used.

Now we concentrate on type-II superconductors with $\kappa \sim 1$. For a particular value of $\kappa$ and $t$ set of Eilenberger equations are solved numerically for various values of magnetic induction $B$, so we can construct free energy density $F(B)$. However, in the experiment we actually control applied field $H$ and not induction $B$. For a given applied filed $H$ proper thermodynamic potential is Gibbs energy $G(\mathbf{B},T)$ which is at minimum when the thermodynamic equilibrium is achieved, $\partial G/\partial B = 0$. This condition is rewritten via Helmholtz free energy $F(B,T)$

$$H(B) = \frac{1}{2\kappa^2} \frac{\partial F}{\partial B}.$$

(21)

If there are meta-stable states, as we expect in type-IIa superconductors, function $H(B)$ is multi-valued and to find a true magnetic induction one should look for global minimum of Gibbs energy. In Fig. 2 we plotted typical example of magnetization curve with meta-stable states, i.e. for some values of $H$ there are three different values of magnetic induction that correspond to the extrema of Gibbs energy. To find $B$ which corresponds to the minimum energy one has to construct Gibbs energy density:

$$G = F - 2\kappa^2 BH.$$

(22)

For example, we found that the minimum Gibbs energy for $H = 0.34$ correspond to the highest value of induction $B = 0.20$. Therefore from the behavior of Gibbs energy we can reconstruct the $B(H)$ curve. From $H = 0$ up to $H = H_{c1}^*$ magnetic induction is zero and we have Meissner state. Note that $H_{c1}^*$ is less than $H_{c1} = \lim_{B \to 0} H(B)$. At $H = H_{c1}^*$ there is first order phase transition from the Meissner state $B = 0$ to the mixed state $B = B_0$ (jump in
magnetization. It means that energy of well separated vortices is bigger than vortex-lattice energy at \( B = B_0 \), due to attraction of vortices. For a fixed temperature the value of induction jump \( B_0 \) decreases with increasing \( \kappa \) and at some critical value \( \kappa_c, B_0 = 0 \). Then for all \( \kappa > \kappa_c \) we have a second order phase transition from the Meissner to mixed state, i.e. type-IIb superconductivity.

Calculations are performed for various temperatures \( t = 0.2 - 0.9 \) to find the critical parameter \( \kappa_c \) that separates type-IIa and type-IIb superconductivity. The results are shown on Fig. 2. Boundary line is qualitatively similar to the 3D case obtained by different numerical scheme. Boundary between type-I and type-II superconductivity can be obtained from the condition \( H_c = H_{c2} \). Calculation itself is trivial and we did it merely to show the quantitative difference between 3D (shown by dashed line in Fig. 2) and 2D case. Compared to 3D case, boundary between type-I and type-II superconductivity in 2D superconductors is almost constant and changes only few percent down to \( T = 0 \). In 3D case there is possibility for cross-over from type-I to type-II superconductivity as one goes from \( T_c \) to \( T = 0 \).

We obtained selfconsistent solution for the order parameter \( \Psi(r, t) \) and field distribution \( A(r, t) \) for various \( \kappa, B \) and temperature \( T \). Only one interesting aspect will be presented: magnetic field profile as viewed via nuclear magnetic resonance (NMR) and muon spin rotation (\( \mu \)SR). These are standard experimental techniques that probe the magnetic field profile in the mixed state. NMR absorption intensity in a small frequency interval \( \Delta \omega \) of the ac field is proportional to the fraction of the VL cell area where the field value is in the corresponding interval \( \Delta \omega \propto \Delta H \), i.e. signal is proportional to \( \int \delta(H - H(r))dr \). NMR line shape has the logarithmic singularity at the saddle point of magnetic field. In s-wave superconductor from the relative position of the NMR peak one can make conclusion about the VL structure.

Kung measured NMR profile in V foil as a function of temperature. The applied field was perpendicular to the foil plane. In this geometry magnetic induction was fixed and almost temperature independent. It was found that the maximum magnetic field (field at the vortex center) is linear in \( T \) down to the lowest attainable temperature 0.1\( T_c \) in that experiment. Delrieu calculated magnetic field profile in the limit \( T = 0 \) and small magnetization. He found singularities at the positions of field maximum and minimum which have conical shape compared to parabolic shape near \( T_c \). It was shown that the slope \( dH_{max}/dT \) is finite at \( T = 0 \).

We calculated temperature dependence of \( H_{max} \) in superconductor with \( \kappa = 0.8 \) for fixed magnetic induction \( B = 0.16 \). The result is shown in Fig. 2. Overall behavior \( H_{max}(T) \) resemble the linear behavior reported in Kung. The result is in agreement with the calculation of Delrieu if the curve is extrapolated to \( T = 0 \). We note that in Ref. 1\( H_{max} \) has a more pronounced convex curvature. Therefore, in spite the value of magnetic penetration depth is saturated already below 0.4\( T_c \), magnetic field distribution is temperature dependent down to very low temperatures.

In summary, we presented the new method to solve selfconsistently Eilenberger equations in the mixed state. Its efficiency is demonstrated in the problem of low-\( \kappa \) 2D superconductors. Being faster then previous techniques, we hope it will stimulate further numerical studies of type-II superconductors.

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