Superconducting phase boundary - square vs. disc

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The interest was triggered by an experimental paper in Nature (V.V. Moshchalkov, L. Gielen, C. Strunk, R. Jonckheere, X. Qiu, C. van Haesendonck and Y. Bruynseraede, Nature 373 (1995) 319). These authors measured the superconducting phase boundary for a square piece of superconductor, whose size is smaller than the Landau-Ginzburg coherence length. One thus expects to see signs of flux quantization. The experiments were compared to a disc geometry. Although the agreement was reasonable, small deviations naturally made one ask the question what the influence of the geometry is. To find the phase boundary one needs to solve for the groundstate energy of the Schrödinger equation (acting on the order parameter of the superconductor) in a magnetic field.

$$(-i\hbar\vec{\partial}-e^*\vec{A}/c)^2\psi=\hbar^2\xi^{-2}(T)\psi \quad , \quad \vec{A}=\tfrac{1}{2}H(-x_2,x_1)$$

The dependence of Landau-Ginzburg coherence length ξ on the temperature is related to the phase boundary by $\xi^2(0)/\xi^2(T)=(T_c-T)/T_c$ (see the paper mentioned above), $T\equiv T_c(H)$. The normal component of the **covariant** derivative vanishes at the boundary

$$\vec{n}\cdot(-i\hbar\vec{\partial}-e^*\vec{A}/c)\psi=0$$

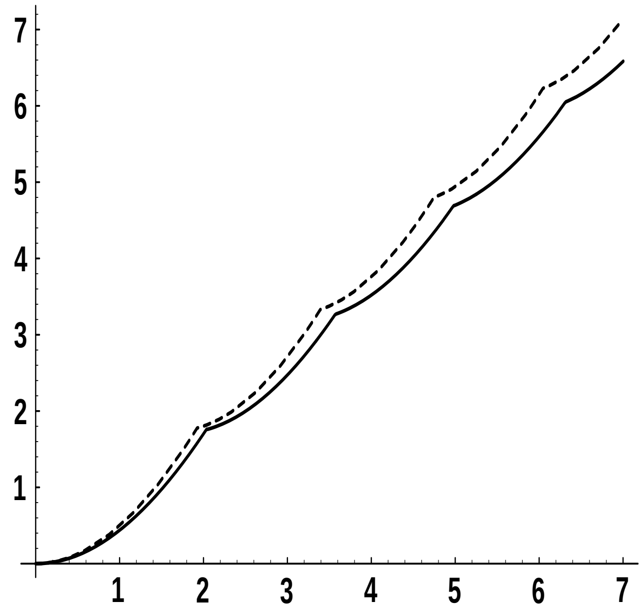

Figure 1: The superconducting phase boundary for a square (full line) and a disc (dashed line). Horizontally is plotted the magnetic field H, given in terms of the flux (Area $\times\, H$) in basic flux units $\phi_0=\hbar c/e^*$ ($e^*=2e$), i.e. ϕ/ϕ_0. Vertically is plotted the area of the sample in units of the the Landau-Ginzburg coherence length, $\xi^2(T)=\xi^2(0)T_c(0)/(T_c(0)-T_c(H))$, i.e. Area$/\xi^2(T)=$ Area$\xi^{-2}(0)(T_c(0)-T_c(H))/T_c(0)$.

For the disc one can choose the gauge in which the radial component of the vector potential vanishes, but a simple gauge choice does not exist for the square. Instead we discretized the Schrödinger equation. Like in lattice gauge theories it is essential that the gauge invariance of the discretized Schrödinger equation is maintained. In condensed matter theory this is known under the name of the Peierls trick in tight binding models, the best way to describe our method, apart from the fact that the lattice points in this case are not related to positions of atoms. The order parameter $\psi(x)$ is associated to a lattice point. The gauge field is associate to a link, running from a point x in the direction k, as $U_k(x) = \exp(iA_k(x)a)$, where a is the lattice spacing. After appropriately rescaling variables, introducing $\hat{H} = \pi\phi/\phi_0$, with $\phi = \text{Area} \times H$ and $\phi_0 = \frac{1}{2}\hbar c/e$, one finds that $\text{Area}/\xi^2(T)$ is given, for a discretization by a $N \times N$ lattice, by the lowest eigenvalue of the positive definite matrix $\pi N^2 D_k^\dagger D_k$, where D_k is the discretized covariant derivative

$$D_k\psi(x) = U_k^\dagger(x)\psi(x+\hat{k}) - \psi(x) \quad , \quad D_k^\dagger\psi(x) = U_k(x-\hat{k})\psi(x-\hat{k}) - \psi(x)$$
$$U_1(x) = \exp(-i\hat{H}x_2/N^2) \quad , \quad U_2(x) = \exp(i\hat{H}x_1/N^2) \quad .$$

Here all x are two dimensional integer vectors (with $\hat{k}$ the unit vector in the k-direction). The boundary conditions are given by $D_k^\dagger\psi(x) = 0$ at $x_k = 1$ and $D_k\psi(x) = 0$ at $x_k = N$. Relatively small lattices and a careful finite size study (we verified that the results scale inversely proportional to the total number of lattice points, N^2) allowed us to get accurate results. The biggest value of N used was 30, for which the Schrödinger operator is converted to a 900×900 matrix, easily diagonalized on the Cray. In figure 4 we give the extrapolated results as compared to those for the disc. Somewhat to our surprise the results of the square could be mapped quite accurately on those of the disc by (separately) scaling the area and the "mass" of the order parameter. These quantities are experimentally hard to measure directly and our result explains why the experiment was successful in comparing with the disc geometry, but that the experimentally observed small deviations most likely have a different source, possibly the influence of the leads.