VORTEX LINE FLUCTUATIONS AND PHASE TRANSITIONS IN TYPE II SUPERCONDUCTORS

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Abstract. The helicity modulus is defined as a criterion for superconducting order in a fluctuating type-II superconductor. Numerical simulations of a lattice London superconductor in an external magnetic field are carried out, and evidence is found that superconducting order parallel to the applied magnetic field persists above the vortex lattice melting, into the vortex line liquid.

1. Introduction

A key feature of the high temperature superconductors, as opposed to conventional superconductors, is the strong effect of thermal fluctuations on macroscopic behavior and the phase diagram [1]. Once one includes these thermal fluctuations, it becomes necessary to have a criterion for the existence of superconducting order, that is expressed in terms of a well specified correlation function. Here we discuss one approach to this problem, in terms of the helicity modulus [2], which is the linear response coefficient giving the supercurrent induced by a perturbation in the applied magnetic field. We will define the helicity modulus in the context of a London model of interacting vortex lines, and show that the mixed state of a type-II superconductor exhibits a total Meissner effect with regard to the perturbation that induces supercurrents parallel to the applied field. We carry out numerical simulations on a lattice London model in an applied magnetic field, and find that this parallel superconductivity persists into the vortex line liquid state, for the parameters we have studied [3].

2. Model

2.1. HAMILTONIAN

We will assume here a London approximation in which the amplitude of the superconducting wavefunction is constant outside of vortex cores, and only the phase angle $\theta(\mathbf{r})$ varies. Aside from additive constants, the Ginzburg-Landau free energy functional for phase angle configurations is then determined solely by the kinetic energy of flowing supercurrents, and the magnetic field energy. Taking for simplicity isotropic couplings, and using the Gibbs ensemble, we have the Hamiltonian,

$$\mathcal{H}[\theta, \mathbf{A}^{\rm ind}] = \tfrac{1}{2}J\int d^3r\left[|\nabla\theta - \mathbf{A}^{\rm ind} - \mathbf{A}^{\rm ext}|^2 + \lambda^2|\nabla\times\mathbf{A}^{\rm ind}|^2\right] \quad , \tag{1}$$

where $\mathbf{A}^{\rm ext}$ and $\mathbf{A}^{\rm ind}$ are the vector potentials of the applied and induced magnetic fields. If $\mathbf{A} = \mathbf{A}^{\rm ind} + \mathbf{A}^{\rm ext}$, then $\nabla\times\mathbf{A} = 2\pi\mathbf{b}$ gives the total internal magnetic field, with $\mathbf{b} = \mathbf{B}/\phi_0$ the density of flux quanta, and $\nabla\times\mathbf{A}^{\rm ext} = 2\pi\mathbf{h}$ gives the applied magnetic field, with $\mathbf{h} = \mathbf{H}/\phi_0$. The bare magnetic penetration length is λ, and the coupling is $J = \phi_0^2/(16\pi^3\lambda^2)$.

We now transform Eq.(1) to the vortex degrees of freedom. The vortex line density $\mathbf{n}(\mathbf{r})$ is determined from the circulation of the supercurrent $\mathbf{j}(\mathbf{r})$,

$$\nabla\times\mathbf{j} \equiv \nabla\times J(\nabla\theta - \mathbf{A}) = 2\pi J(\mathbf{n} - \mathbf{b}) \quad . \tag{2}$$

Taking Fourier transforms, one can solve Eq.(2) for $\mathbf{j}_q$, giving,

$$\mathbf{j}_q = 2\pi i J\left[\mathbf{q}\chi_q + \frac{\mathbf{q}\times(\mathbf{n}_q - \mathbf{b}_q)}{q^2}\right] \quad , \tag{3}$$

where the curl-free part of $\mathbf{j}$ is given by an arbitrary scalar potential χ. Using Eq.(3) to rewrite $\mathcal{H}$ of Eq.(1) in terms of $\mathbf{n}$, $\mathbf{b}$, and $\mathbf{h}$, and completing the square in $\mathbf{b}_q$ yields,

$$\begin{aligned}\mathcal{H} \quad = \quad & \frac{4\pi^2 J}{2V}\sum_q\left[\frac{(\mathbf{n}_q - \mathbf{h}_q)\cdot(\mathbf{n}_{-q} - \mathbf{h}_{-q})}{\lambda^{-2} + q^2}\right. \\ & \left. + (q^{-2} + \lambda^2)\delta\mathbf{b}_q\cdot\delta\mathbf{b}_{-q} + q^2\chi_q\chi_{-q}\right] \quad . \end{aligned} \tag{4}$$

The first term gives the familiar London interaction between vortex lines. The second term is the energy of magnetic field fluctuations $\delta\mathbf{b}_q$ away from the value $\mathbf{b}_q^0 \equiv (\mathbf{n}_q + \lambda^2 q^2\mathbf{h}_q)/(1 + \lambda^2 q^2)$ which minimizes $\mathcal{H}$ for a given configuration of $\mathbf{n}_q$ and $\mathbf{h}_q$. The last term is the energy of smooth "spin wave" distortions of $\theta(\mathbf{r})$ about a given vortex configuration. To compute thermodynamic quantities, one has to average over all smooth χ_q, all divergenceless $\delta\mathbf{b}_q$, and all singular vortex line configurations $\mathbf{n}_q$, for a fixed external $\mathbf{h}_q$. V is the volume of the system.

2.2. HELICITY MODULUS

Consider now a small perturbation about a uniform applied field $h_0\hat{\mathbf{z}}$, $\mathbf{A}^{\rm ext} = 2\pi h_0 x\hat{\mathbf{y}} + \delta\mathbf{A}^{\rm ext}$. The helicity modulus tensor $\Upsilon_{\mu\nu}(\mathbf{q})$ is defined as the linear response coefficient between the induced supercurrent and the perturbation $\delta\mathbf{A}^{\rm ext}$,

$$\langle j_{q\mu}\rangle = -\Upsilon_{\mu\nu}(\mathbf{q})\delta A^{\rm ext}_{q\nu} \ . \tag{5}$$

From Eq.(1) we find that,

$$\Upsilon_{\mu\nu}(\mathbf{q}) = V \left.\frac{\partial^2\mathcal{F}}{\partial A^{\rm ext}_{q\nu}\partial A^{\rm ext}_{-q\mu}}\right|_0 = J\left[\delta_{\mu\nu} - \frac{1}{VTJ}\langle j_{q\mu} j_{-q\nu}\rangle_0\right] \ , \tag{6}$$

where $\mathcal{F} = -T\ln\left\{\int {\rm e}^{-\mathcal{H}/T}\right\}$ is the total free energy, and the subscript "0" indicates the ensemble in which $\delta\mathbf{A}^{\rm ext} = 0$. For a pure system, the off diagonal parts of $\Upsilon_{\mu\nu}$ should vanish, and since a longitudinal $\mathbf{A}^{\rm ext}$ can be removed with a gauge transformation, we restrict ourselves to the diagonal transverse case, $\Upsilon_\mu(q\hat{\nu}) \equiv \Upsilon_{\mu\mu}(q\hat{\nu})$ where $\hat{\mu} \perp \hat{\nu}$. Henceforth we will take μ, ν, σ to be any cyclic permutation of x, y, z. To express Υ_μ in terms of vortex correlations, one can either substitute for $j_{q\mu}$ from Eq.(3) into Eq.(6) and evaluate the averages over $\delta\mathbf{b}$ and χ, or, noting that $2\pi h_{q\sigma} = -iqA^{\rm ext}_\mu(q\hat{\nu})$, we can explicitly use the form of Eq.(4) for $\mathcal{H}$, when taking derivatives, to get,

$$\Upsilon_\mu(q\hat{\nu}) = \frac{Jq^2}{\lambda^{-2}+q^2}\left[1 - \frac{4\pi^2 J}{VT}\frac{\langle n_\sigma(q\hat{\nu})n_\sigma(-q\hat{\nu})\rangle_0}{\lambda^{-2}+q^2}\right] \ . \tag{7}$$

The helicity modulus contains within it information about the screening of magnetic fields. To see this, we can combine the definition of Eq.(5) with Ampère's law, $\langle\mathbf{j}_q\rangle = -J\lambda^2\langle\mathbf{q}\times(\mathbf{q}\times\delta\mathbf{A}^{\rm ind}_q)\rangle$, to get for the total average magnetic field inside the superconductor produced by the pertubation,

$$\langle\delta A_{q\mu}\rangle = \delta A^{\rm ext}_{q\mu} + \langle\delta A^{\rm ind}_{q\mu}\rangle = \left[1 - \frac{\Upsilon_\mu(\mathbf{q})}{J\lambda^2 q^2}\right]\delta A^{\rm ext}_{q\mu} \ . \tag{8}$$

If we now assume that there are no vortices in the system, as in the mean field treatment of the Meissner state, then the helicity modulus has the simple form $\Upsilon_\mu(q\hat{\nu}) = Jq^2/(\lambda^{-2}+q^2)$, which combined with Eq.(8) gives, $\langle\delta A_{q\mu}\rangle = q^2\delta A^{\rm ext}_{q\mu}/(\lambda^{-2}+q^2)$. Taking $q\to 0$, we see that the total internal field $\langle\delta A_{q\mu}\rangle \sim q^2 \to 0$ vanishes, i.e. the external perturbation is completely screened out, and this screening takes place on the length scale λ. If we now include vortex fluctuations, either in a fluctuating Meissner state, or in the mixed state, the vortex correlation that appears in Eq.(7) is non zero, and for small q may be expanded as,

$$\langle n_\sigma(q\hat{\nu}) n_\sigma(-q\hat{\nu})\rangle_0 = n_0 + n_1 q^2 + n_2 q^4 + \ldots \tag{9}$$

One can then rewrite Υ_μ for small q in the form

$$\Upsilon_\mu(q\hat{\nu}) = \frac{\gamma_\mu J q^2}{\lambda^{-2} + \alpha_\mu^2 q^2} \ , \tag{10}$$

where,

$$\gamma_\mu = 1 - \frac{4\pi^2 J\lambda^2}{VT} n_0 \ , \quad \text{and} \quad \alpha_\mu^2 = 1 - \frac{4\pi^2 J\lambda^2}{VT}\frac{n_0 - n_1\lambda^2}{\gamma_\mu} \ . \tag{11}$$

Using Eq.(10) in Eq.(8) then gives,

$$\langle \delta A_{q\mu}\rangle = \left[(1-\gamma_\mu) + \frac{\gamma_\mu q^2}{q^2 + (\alpha_\mu\lambda)^{-2}}\right]\delta A_{q\mu}^{\mathrm{ext}} \ . \tag{12}$$

We thus see the physical meaning of the parameters γ_μ and α_μ: $1-\gamma_\mu$ is the fraction of the external perturbation that penetrates the system, and $\alpha_\mu\lambda$ is the length scale on which the remainder is screened out. We therefore have for the magnetic susceptibility and *renormalized* penetration length,

$$(1-\gamma_\mu) = \left.\frac{dB_\sigma(q\hat{\nu})}{dH_\sigma(q\hat{\nu})}\right|_0 \ , \quad \text{and} \quad \lambda_{\mu\mathrm{R}} = \alpha_\mu\lambda \ . \tag{13}$$

When $\gamma_\mu = 1$, or equivalently by Eq.(11) when $n_0 = 0$, we have a complete Meissner screening of the pertubation. Such a Meissner effect will be our criterion for superconducting order. For the Meissner state, the criterion $n_0 = 0$ has a simple physical interpretation: there are no infinite vortex loops. If the superconducting to normal transition is second order, we would expect that $\lambda_{\mu\mathrm{R}}$ diverges as T_c is approached from below, with $n_s \sim 1/\lambda_{\mu\mathrm{R}}^2$ the density of superconducting electrons. In the normal state above T_c, γ_μ and $\lambda_{\mu\mathrm{R}}$ are small and finite, reflecting the correlations associated with ordinary fluctuation diamagnetism.

For the mixed state, with external field $h_0\hat{\mathbf{z}}$, there are three types of perturbations to consider. These are illustrated schematically in Fig. 1, and will be referred to as the tilt, compression, and shear perturbations. For a vortex line lattice in a continuum, the vortex correlations of Eq.(9) can be evaluated using the elastic medium approximation. In particular one finds [2],

$$\langle n_y(q_x\hat{\mathbf{x}} + q_z\hat{\mathbf{z}}) n_y(-q_x\hat{\mathbf{x}} - q_z\hat{\mathbf{z}})\rangle = \frac{q_z^2 b_0^2 VT}{c_{66}q_x^2 + c_{44}q_z^2} \ , \tag{14}$$

Figure 1. Three types of perturbing magnetic fields for the mixed state.

where b_0 is the average internal magnetic field induced by h_0, and c_{66} and c_{44} are the shear and tilt moduli respectively. The tilt perturbation is determined by Eq.(14) taking the limit $q_x \to 0$. One finds a finite $n_0 = b_0^2 VT/c_{44}$, which from Eq.(11) yields a $\gamma_y < 1$. One can show [2] that the result is consistent with the prediction of Eq.(13), $\gamma_y = 1 - dB_\perp/dH_\perp \ll 1$. Similarly, the compression perturbation yields [2] $\gamma_x = 1 - dB_z/dH_z < 0$. These results correspond to the finite magnetic susceptibilities expected for the mixed state. The shear perturbation, however, is determined by taking the limit $q_z \to 0$ in Eq.(14). One finds that, provided $c_{66} \neq 0$, the correlation vanishes and hence $n_0 = 0$, or $\gamma_z = 1$, describing a total Meissner screening of shear perturbations [4]. The criterion $\gamma_z = 1$ will thus be our criterion for superconducting order in the mixed state. We note that the induced currents for this case flow parallel to the applied magnetic field $h_0\hat{\mathbf{z}}$.

3. Simulations

To carry out Monte Carlo simulations of a fluctuating vortex line system, we follow the pioneering work of Carneiro and co-workers [5]. The Hamiltonian (1) is discretized to a cubic grid of points, with grid spacing a in all directions. Using the Villain function for the discretized kinetic energy term, and making standard duality transformations, one finds that virtually all of the continuum expressions of the previous section, and in particular Eqs.(4) and (7-13) remain unchanged, provided one substitutes for the magnitude

Figure 2. Fits to Eq.(16) to extract parameters γ_z and $\lambda_{z\mathrm{R}}$

of the wavevector its discrete lattice version,

$$q^2 \to Q^2 \equiv 6 - 2\cos(q_x a) - 2\cos(q_y a) - 2\cos(q_z a) \ . \tag{15}$$

Henceforth, all lengths are measured in units of a, and temperatures in units of J.

To simulate, we use the Helmoltz ensemble with a fixed density of vortex lines $b_0 = 1/15$. Excitations are created by adding elementary closed vortex loops of unit area, placed at random positions with random orientations. These are accepted or rejected according to the usual Metropolis algorithm. An elementary vortex loop that coincides on one side with a field induced vortex line corresponds to a transverse fluctuation of that line. We use a value of $\lambda = 5$, slightly bigger than the average spacing between vortex lines, $a_{\mathrm{v}} = \sqrt{15}$, and system sizes $L_\perp = 30$, $L_z = 15, 30$. We use 5000 MC passes through the lattice to equilibrate, and 16000 passes to compute averages, at each temperature.

Measuring the helicity moduli $\Upsilon_\mu(q\hat{\nu})$ for the three types of perturbations, we determine the parameters γ_μ and $\lambda_{\mu\mathrm{R}}$ as follows. From Eq.(10) we have,

$$\frac{J\lambda^2 Q^2}{\Upsilon_\mu(q\hat{\nu})} = \gamma_\mu^{-1}\left(1 + \lambda_{\mu\mathrm{R}}^2 Q^2\right) \ . \tag{16}$$

Thus fitting $J\lambda^2 Q^2/\Upsilon_\mu$ vs. Q^2 to a straight line determines γ_μ from the $Q^2 = 0$ intercept, and $\lambda_{\mu R}$ from the slope. We show an example of such fits for Υ_z in Fig. 2, for $L_z = 30$, and various values of T. The straight lines represent fits to the 8 smallest allowed values of Q^2, given by $q_z = 2\pi m/L_\perp$, $m = 1, \ldots, 8$. In Fig. 3 we show the resulting values for γ_μ and $\lambda_{\mu\mathrm{R}}$ for all three cases, for both system sizes $L_z = 15$ and 30. We find that these values are for the most part insensitive to the number of q data points used

Figure 3. *a)* γ_μ and *b)* $(\lambda_{\mu\mathrm{R}}/\lambda)^2$ as obtained from fits as in Fig. 2, for the shear, tilt, and compression perturbations. Solid symbols are for $L_z = 30$, and open symbols for $L_z = 15$.

in the fit to Eq.(16) (we varied $m_{\max}$ from 5 to 8), as well to the inclusion of a Q^4 term in the fitting function.

Considering first the tilt and compression cases, we see in Fig. 3*a* that γ_y and γ_x both decrease from unity to small values at $T_{\mathrm{m}} \simeq 1.2$. Our discussion following Eq.(14) led us to expect a small and positive γ_y, and a small and negative γ_x, even in the vortex lattice state. This would be true for a vortex lattice in a *continuum*. However the discretizing grid that has been introduced in our simulations breaks translational invariance, and thus behaves like an effective periodic pinning potential for the vortex lines. This serves to create an energy gap to the long wavelength elastic fluctuations of the lattice and so, at low temperatures, the vortex lines are strongly pinned and unable to adjust so as to allow additional magnetic flux to penetrate. This yields values $\gamma_{x,y} = 1$ characteristic of a total Meissner effect. As T increases, the pinning weakens and $\gamma_{x,y}$ decreases. When the vortex lines unpin we recover behavior characteristic of the continuum. As a vortex line lattice in 3D has long range translational order, we expect, for a large enough system size, that a vortex line lattice will always be commensurably pinned to a periodic potential, for all temperatures up to its melting T_{m}. Above T_{m} long range order is lost, and lines can unpin. By independent calculation of the in-plane vortex-vortex density correlation function, we have confirmed that the T_{m} indicated in Fig. 3, does indeed coincide with the vortex line lattice melting. Looking at Fig. 3*b*, we see that for the tilt case, $\lambda_{y\mathrm{R}} \sim \gamma_y$ decreases smoothly through the depinning/melting transition, while for the compression case, $\lambda_{x\mathrm{R}}$ increases sharply just below T_{m}.

Turning now to the shear case, we see our main result. Fig. 3 shows that $\gamma_z = 1$, corresponding to a total Meissner effect, for temperatures up to $T_{\mathrm{c}} \simeq 1.8$, well above melting. As L_{z} increases, the width of this transition sharpens, and T_c decreases slightly. λ_{zR} increases to a relatively small peak at T_c. The region $T_m < T < T_c$ thus corresponds to a vortex line liquid which remains superconducting parallel to the applied magnetic field. Similar results have previously been reported by one of us [6] for a related model in which $\lambda \to \infty$.

4. Discussion

One possible explanation for such a superconducting vortex line liquid has been given by Nelson [7], in terms of an analogy between vortex lines and imaginary time world lines of two dimensional bosons. In this analogy, T_c correspond to the normal to superfluid transition of the 2D bosons. According to Nelson however, one expects that T_m and T_c will merge as L_z increases. Feigel'man and co-workers [8] have argued that for large λ, the resulting long range interactions between the analog 2D bosons could lead to $T_c > T_m$, even for the limit $L_z \to \infty$. An alternative theory has recently been proposed by Tešanović [9], in which a $T_c > T_m$ is due to the unbinding of thermally excited closed vortex line loops, as is the case for the zero magnetic field transition. In our simulations, we have seen that T_c did have a very slight decrease as L_z was doubled. However this decrease remained small compared to the separation between T_m and T_c. It thus remains to be determined how T_c will behave as L_z is further increased [10]. If T_c and T_m do indeed merge in the $L_z \to \infty$ limit, it still remains an important question to determine the length scale on which this happens.

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References

1. D. S. Fisher, M. P. A. Fisher, and D. A. Huse, Phys. Rev. B **43**, 130 (1991).
2. T. Chen and S. Teitel, Phys. Rev. Lett. **72**, 2085 (1994).
3. T. Chen and S. Teitel, Phys. Rev. Lett. **74**, 2792 (1995).
4. This shear Meissner effect can be lost, even in the vortex line lattice, if lattice defects proliferate. See, E. Frey, D. R. Nelson, and D. S. Fisher, Phys. Rev. B **49**, 9723 (1994).
5. R. Cavalcanti, G. Carneiro, and A. Gartner, Europhys. Lett. **17**, 449 (1992); G. Carneiro, R. Cavalcanti, and A. Gartner, Phys. Rev. B **47**, 5263 (11993); G.Carneiro, Phys. Rev. Lett. **75**, 521 (1995); G. Carneiro, Phys. Rev. B **53**, 11837 (1996).
6. Y.-H. Li and S. Teitel, Phys. Rev. B **47**, 359 (1993) and *ibid.* **49**, 4136 (1994).
7. D. R. Nelson and H. S. Seung, Phys. Rev. B **39**, 9153 (1989).
8. M. V. Feigel'man, Physica A **168**, 319 (1990); M. V. Feigel'man, V. B. Geshkenbein and V. M. Vinokur, JETP Lett. **52**, 546 (1990); M. V. Feigel'man, V. B. Geshkenbein, L. B. Ioffe, and A. I. Larkin, Phys. Rev. B **48**, 16641(1993).
9. Z. Tešanović, Phys. Rev. B **51**, 16204 (1995).
10. See comment, T. Chen and S. Teitel, Phys. Rev. Lett. **76**, 714 (1996), and reply by Carneiro, for a discussion of conflicting results in this model.