PHYSICAL REVIEW B VOLUME 28, NUMBER 9 1 NOVEMBER 1983

Phase structure of a lattice superconductor

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(Received 25 July 1983)

A lattice Ginzburg-Landau model of superconductivity is explored in a Monte Carlo computer simulation (for charge $e^2=5$). The superconducting-normal transition is strongly first order deep in the type-I region and becomes more weakly first order moving in the direction of the type-II region. Beyond a certain point, the data suggest a second-order transition. The data are consistent with the existence of a tricritical point separating these two regimes.

The description of superconductivity has a rich history. The Ginzburg-Landau model (at tree level) predicts second-order behavior; this model has become a prototype for second-order transitions. But later, Halperin, Lubensky, and Ma[1] argued that fluctuations in the electromagnetic field might drive the transition first order. More recently, Dasgupta and Halperin[2] argued that, in the extreme type-II limit, this first-order behavior does not occur; instead, there is a second-order transition of inverted-XY type. This study further explores the phase diagram of the superconductor.

The Ginzburg-Landau model of superconductivity in three dimensions has action

$$S[A,\phi]=\int[|(\partial_\mu - ieA_\mu)\phi|^2+\tfrac{1}{4}F_{\mu\nu}^2+V(\phi)]d^3x \quad ,$$

with partition function

$$Z=\int_A\int_\phi e^{-S[A,\phi]} \quad ,$$

where ϕ is a complex scalar field (Cooper-pair wave function), A_μ is the photon field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, and the potential is $V(\phi)=a|\phi|^2+b|\phi|^4$; e is the charge coupling A_μ to ϕ. The Ginzburg-Landau parameter (ratio of penetration depth to correlation length) is $\kappa=\sqrt{b}/e$; a superconductor with $\kappa<1/\sqrt{2}$ is called type I, and one with $\kappa>1/\sqrt{2}$ is called type II. This study addresses the nature of the transition as κ is varied.

Halperin, Lubensky, and Ma[1] reasoned that for the strongly type-I case ($\kappa\rightarrow 0$), the transition is first order. They obtained an effective action by integrating out the A_μ field (taking $\arg\phi=\text{const}$). A $|\phi|^3$ term with negative coefficient is induced in the potential, indicating a first-order transition. This argument seems plausible in a regime where the correlation length, penetration depth, and e^2 are small.[3] In the strongly type-II case ($\kappa\rightarrow\infty$), a lattice realization of $S[A,\phi]$ (Villain form) duals[2,4,5] into the generalized Villain XY model. The pure XY model exhibits second-order behavior; Dasgupta and Halperin[2] pointed out that if the generalized model does also it suggests that the superconductor has an "inverted-XY" transition in this region. Further, Dasgupta and Halperin did Monte Carlo simulations on the generalized Villain XY model and did find evidence for a second-order, inverted-XY transition at $e^2=5$.

The study attempts to reconcile these two analyses by exploring the phase diagram between these two extremes.[6] Summarizing the results, it is found that for $e^2=5$, the jump in $|\phi|$ across the transition indeed is large in the strongly type-I region, indicating strongly first-order behavior. The jump decreases as b (hence κ) increases and, beyond a certain point, is consistent with zero, suggesting a second-order transition. The approach of the jump to zero is consistent with the existence of an ordinary ϕ^4-ϕ^6 tricritical point separating a line of first-order transitions and a line of second-order transitions.

One realization of $S[A,\phi]$ on the lattice is

$$S_L[A,\rho,\theta]=\sum_x\left[-2\sum_\mu\rho(x)\rho(x+\mu)\cos(\partial_\mu\theta-eA_\mu)+\tfrac{1}{4}F_{\mu\nu}^2+(a+6)\rho^2+b\rho^4\right] \quad ,$$

where $\phi=\rho e^{i\theta}$, ρ (positive real) and θ ($0\leq\theta<2\pi$) are site fields, and A_μ (real) is a link field. The sum on x is over sites, and the sum on μ is over directions of the three-dimensional cubic lattice.[7]

The Metropolis algorithm[8] was used in a Monte Carlo simulation of S_L. At each b value, for various lattice sizes, from 6 to 13 runs at different a values were made. Data were extracted from typically 8000 iterations on a 5^3 lattice, 6000 on a 9^3, and 3000 on a 15^3 (fewer fixed-a runs were usually made in the 15^3 case). In total, approximately 1000 h of Vax CPU (central processing unit) time were used. Once in equilibrium, the expectation value of ρ, $\langle\rho\rangle$, and other data were measured. Error bars were determined by blocking the data in successively larger bins until the errors appeared uncorrelated.

Graphs of $\langle\rho\rangle$ vs a at fixed b are shown. Figure 1(a), for $b=0.25$, shows a clear, strong, first-order transition. This validates the predicted first-order behavior of Halperin, Lubensky, and Ma. Figure 1(b), for $b=0.7$, shows continuous behavior in $\langle\rho\rangle$, indicating the transition is by now probably second order.

To further isolate the critical value of a, a_c, the system was prepared with half the lattice in a representative disordered state and half in an ordered state.[9] Two methods of

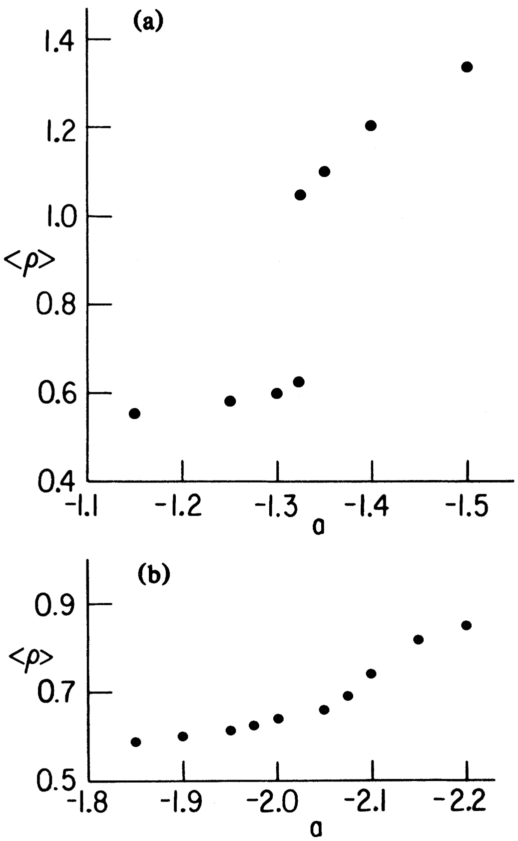

FIG. 1. $\langle\rho\rangle$ vs a for $e^2=5$; (a) $b=0.25$ (first-order regime) on a 9^3 lattice; (b) $b=0.7$ (second-order regime) on a 15^3 lattice. The error bars are within the size of the dots.

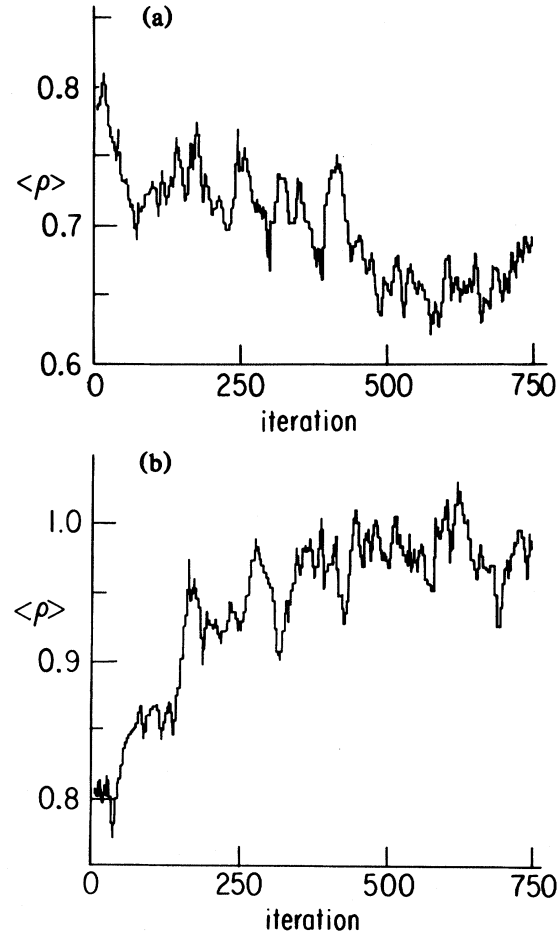

FIG. 2. Disordered-ordered mixed starts for $e^2=5$, $b=0.325$ on a 9^3 lattice; (a) $|a|=1.4775<|a_c|$ equilibrating to disorder; (b) $|a|=1.4975>|a_c|$ equilibrating to order.

setting starting configurations were used: (a) The configuration for the disordered state was ρ's $=\langle\rho\rangle$ determined by other Monte Carlo runs at the given parameter values, A_μ's random (within a range), and θ's random. For the ordered state, ρ's $=\langle\rho\rangle$ from Monte Carlo runs, A_μ's $=0$, and θ's all equal. (b) Equilibrium field configurations were taken from previous Monte Carlo runs for two a values straddling a_c. The system was then allowed to evolve over 500 to 3000 iterations, choosing the preferred state. At a given b, for the various lattice sizes, from 5 to 19 such runs were made. Figures 2(a) and 2(b) display example equilibrations.

A graph of $\Delta\rho$, the jump in $\langle\rho\rangle$ across the transition, versus b, for $e^2=5$, is shown in Fig. 3. Beyond $b\approx0.44$, $\Delta\rho$ is consistent with zero. These results show there is a region of strongly first-order behavior for b sufficiently small. As b increases, $\Delta\rho$ decreases, until it cannot be distinguished from zero, suggesting a regime of second-order behavior. However, a very weakly first-order transition for all large b cannot be ruled out.

There arises the possibility of a tricritical point. A simple renormalization-group argument predicts that near a standard ϕ^4-ϕ^6 tricritical point b_{tc}, $\Delta\rho\propto b_{tc}-b$.[10] Figure 3 shows the decrease of $\Delta\rho$ to be consistent with linearity; the scatter in the points is discussed below. A power-law fit to the last seven 9^3 points gives the exponent of $b_{tc}-b$ as 0.97 ± 0.03 with $b_{tc}=0.44\pm0.01$.[11] Including more or fewer points in the average does not affect b_{tc} substantially.

The $\langle\rho\rangle$ vs a data are straightforward to obtain, and the data are of good quality. The key question is in determining a_c, which gives the point to take the difference of $\langle\rho\rangle$ between the two phases. For the various lattice sizes, the branches of the $\langle\rho\rangle$ vs a curves are nearly identical in their region of overlap; finite-size differences in $\Delta\rho$ are due primarily to differences in a_c.

The two methods of disordered-ordered starts give differences in a sufficient to account for the $\Delta\rho$ variation with lattice size and the scatter of the points from linearity (see the displaced error bar for $b=0.35$ in Fig. 3). These error bars are roughly consistent with the range in a of metastability achievable in runs of several thousand iterations. Kinetic effects at the disordered-ordered interface may be important, and affect, at least in the short run, the vacuum preferred.

On the 9^3 lattice, near the hypothesized tricritical point, there were found modes in $\langle\rho\rangle$ versus time of very long periods (many thousand time steps). For the 15^3 lattice, near b_{tc}, it was impossible to sample over a requisite number of cycles to get a good $\langle\rho\rangle$ value; in the running time available, $\langle\rho\rangle$ seemed to depend on the starting configuration. Therefore it was impossible to get nearer to the

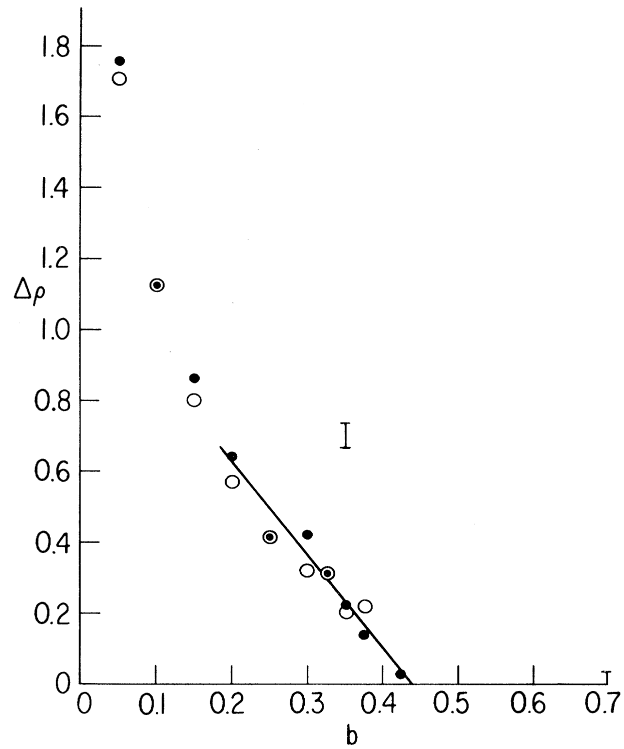

FIG. 3. The jump in $\langle \rho \rangle$ across the transition vs b for $e^2=5$ on 9^3 (closed circles) and 15^3 (open circles) lattices. The displaced sample error bar, for the 15^3 $b=0.35$ point, results from using both methods to determine a_c, as descibed in the text. The point at $b=0.7$ gives an upper bound for $\Delta\rho$ (15^3 lattice). The line results from a power-law fit of the last seven 9^3 points.

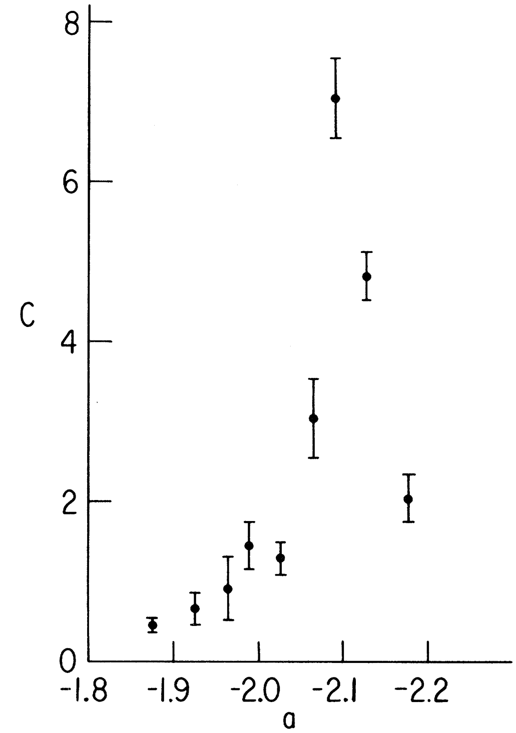

FIG. 4. Specific heat for $e^2=5$, $b=0.7$ on a 15^3 lattice.

tricritical point than indicated in Fig. 3. Because more iterations could be made on the 9^3 lattice near b_{tc}, and because as such these points have greater reliability than the 15^3 ones there, the power-law fit was made to the 9^3 points.

The differences between the 15^3 and 9^3 points are in themselves a measure of error. To distinguish between weakly first-order tunneling between vacuua and long-period cycles, analyses of size dependence must be made. Finite-size effects were hard to control at small $\Delta\rho$. To have convincing evidence of tricriticality, analyses right at b_{tc} are needed.

To further address the hypothesized region of second-order behavior, Fig. 4 shows a specific-heat curve for $b=0.7$ (15^3 lattice) ($C=\Delta S_L/\Delta a$).[12] The singularity is weaker than the δ function spike seen for $b < b_{tc}$. Note the slight rise of the right shoulder on the side of increasing $|a|$ (decreasing temperature). In the $b \rightarrow \infty$ limit, Dasgupta and Halperin found a pronounced shoulder on the opposite (left) side. Figure 4 thus seems to exhibit crossover between tricritical and inverted-XY behaviors. (The behavior in the XY limit at $e^2=5$ has been checked and the shoulder is indeed found to be on the left side—the reversed asymmetry from the pure-XY, $e=0$ case.)

For a real metal with $e^2=2^2(4\pi/137)\approx 0.37$, the phase diagram might also have a tricritical point; however, other possibilities exist. Also, at sufficiently high e^2, the model may always be in the normal state.[2,13]

In conclusion, evidence has been presented showing strongly first-order behavior in a type-I superconductor which becomes weaker moving toward the type-II region. Beyond a certain point, the jump is consistent with zero, suggesting a second-order transition. The data are consistent with a tricritical point separating a line of first-order transitions and a line of second-order transitions, but the possibility always does exist of a vanishingly small first-order transition throughout the whole type-II region.

The first-order jump for a real metal is expected to be small[1] and, so far, hard to detect experimentally. The jump is expected to be larger for certain liquid crystals, where a similar phase structure is expected[14]; this may be the best place to look for a tricritical point.

Note added in proof. There is a heuristic argument concerning the type of tricritical point expected: At the tricritical point, the ρ field is massive, which implies effective short-ranged interactions between vortices in the dual[4,5] XY model. This presumably can be represented as an ordinary XY model with local, but complicated, interactions. It is believed this model has an ordinary $n=2$, ϕ^4-ϕ^6 tricritical point lying in the space of Hamiltonians. (I thank Stephen Shenker for pointing this out.)

ACKNOWLEDGMENTS

I thank Stephen Shenker for proposing this project and for many helpful discussions. This research was supported by the National Science Foundation under Grant No. DMR 82-16892 and by the U.S. Department of Energy under Contract No. DE-AC02-81ER10957.

This work was submitted to the Department of Physics, the University of Chicago, in partial fulfillment of the requirements for the Ph.D. degree.

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[2]C. Dasgupta and B. I. Halperin, Phys. Rev. Lett. 47, 1556 (1981).

[3]Reference 1 also gave an ϵ-expansion argument that the type-II region should flow into the type-I region under renormalization group, and so experience first-order behavior. But, as $\epsilon = 4 - d = 1$, the expansion may have broken down, invalidating this conclusion.

[4]M. Peskin, Ann. Phys. (N.Y.) 113, 122 (1978).

[5]P. R. Thomas and M. Stone, Nucl. Phys. B144, 513 (1978).

[6]Exploration of tricriticality has also been carried out by H. Kleinert, Lett. Nuovo Cimento 35, 405 (1982).

[7]In polar coordinates, $-\log\rho$ is added to S_L due to the measure in the functional integral. Note also that the Q.E.D. is noncompact.

[8]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).

[9]M. Creutz, Phys. Rev. D 20, 1915 (1979).

[10]The marginally irrelevant ϕ^6 operator in three dimensions produces logarithmic corrections; these data suggest that these corrections are not extremely large. Much higher-precision data are necessary to ascertain their amplitude and the detailed shape of the curve; this would be necessary to determine the number of spin dimensions n in an "order parameter"; a guess might be that $n = 2$. See M. J. Stephen, E. Abrahams, and J. P. Straley, Phys. Rev. B 12, 256 (1975); F. J. Wegner and E. K. Riedel, *ibid.* 7, 248 (1973).

[11]For $e^2 = 5$, the critical b separating the two types of superconductors is $\frac{5}{2}$, so that the tricritical point occurs in the nominal type-I region.

[12]The data in Figs. 1(b) and 4 may not be completely equilibrated; however, this would tend to accentuate the size of any jump. While the data may not be precise quantitatively, the curves display general shapes.

[13]For runs made at e^2 different from 5, it was found that for fixed b, as e increases, $|a_c|$ increases.

[14]B. I. Halperin and T. C. Lubensky, Solid State Commun. 14, 997 (1974). I thank John Toner for discussions on this point.