ture, determined by[12]

$$T_K = 0.85D(\rho|J|)^{1/2}e^{1/\rho J}[1+O(\rho J)]. \quad (8)$$

Once V is determined the specific heat can be evaluated.

The motivation for solving the VG model is provided by a consideration of computational cost, the energy accuracy required for a specific-heat calculation being considerably higher than that for the susceptibility. While the specific-heat curve for the spinless VG model requires the diagonalization of a maximum matrix size of 80 × 80, an estimated size of 300× 300 would be needed to ensure the same accuracy in a Kondo calculation. Relative to the Kondo Hamiltonian, a calculation utilizing the VG Hamiltonian amounts to a hundredfold reduction in computing time.

This research was supported in part by the National Science Foundation under Grant No. DMR-80-20429, and in part by the University of São Paulo and the Conselho Nacional de Desenvolvimento Científico e Tecnológico (Brazil).

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[6]Many-body effects resulting from the response of the conduction electrons to the sudden change in the scattering potential reduce further the transition rate and make it temperature dependent, $\Gamma^* \sim \Gamma(T/D)^\alpha$, where $\alpha = 4\delta_G/\pi - (2\delta_G/\pi)^2$.

[7]Thus defined, the operators Q_i and Q_c change sign under the particle-hole transformation $b \to b^\dagger$, $c_k \to -c_{-k}^\dagger$, under which (1) is invariant.

[8]We define $\mu_Q = g\mu_B/\sqrt{2}$ to make the charge susceptibility for the VG model map onto the magnetic suseptibility for the Kondo model. Note that in Ref. 3, where $\mu_Q \equiv 1$, the VG susceptibility maps onto the Kondo susceptibility multiplied by $2/(g\mu_B)^2$.

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Phase Transition in a Lattice Model of Superconductivity

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(Received 18 September 1981)

Monte Carlo data and duality arguments, applied to a lattice model, are presented which indicate that a three-dimensional type-II superconductor should have a transition asymptotically equivalent to that of a superfluid with reversed temperature axis, and not a first-order transition. Results may apply to the nematic–smectic-A transition.

PACS numbers: 74.40.+k, 64.70.-p

Several years ago, Halperin, Lubensky, and Ma[1] argued that the phase transition in superconductors and the nematic to smectic-A (NA) transition in liquid crystals should be weakly first order in character. Although the size of the first-order transition in superconductors was found to be too small to be detected experimentally, the size was estimated[2] to be well within the accessible range for liquid crystals. Experimentally, however, the NA transition often appears to be second order.[3] Recently, Helfrich and Müller[4] have shown that the high-temperature expansion of the XY model represents, upon reversal of the temperature axis, the statistical mechanics of a system of sterically interacting directed loops. This system of loops, therefore, exhibits a phase transition with XY exponents, but distinguished by the fact that the temperature asymmetry of the specific heat and other singular quantities is *inverted* relative to the XY transition. Since the vortex loops in a superconductor interact via a potential which falls off exponentially with distance, Helfrich and Müller speculated that the three-dimensional (3D) superconductor may exhibit the same critical behavior as the loop model. Helfrich[5] and Nelson and Toner[6] have also investigated a dislocation loop mechanism for the NA transition in three dimensions. There, however, the situation is complicated by the possibility of anisotropic scaling,[5-7] which may invalidate the superconductor analogy.

With a view towards providing a better understanding of this situation, we have studied a three-dimensional lattice superconductor model (LSM). This model is defined by the partition function

$$Z_s(\beta,e)=\int_{-\pi}^{\pi}(d\theta_i/2\pi)\int_{-\infty}^{\infty}d[A_{i\mu}]\sum_{[n_{i\mu}]=-\infty}^{\infty}\exp[-\tfrac{1}{2}\beta\sum_{i=1}^{N}\sum_{\mu=1}^{3}(\Delta_\mu\theta_i-2\pi n_{i\mu}-eA_{i\mu})^2-\tfrac{1}{2}\sum_i|\vec{\Delta}\times\vec{A}_i|^2], \tag{1}$$

where θ_i is an angular (phase) variable at site i of a simple-cubic lattice, $\vec{\Delta}$ represents a lattice derivative, and the integer-valued variables $[n_{i\mu}]$ and the real variables $[A_{i\mu}]$ are defined on the directed links between adjacent sites. In Eq. (1), β is the inverse temperature and e is the electric charge which couples the phase variable θ and the vector potential $\vec{A}$. This model is of the Villain type where the exponential of a cosine has been replaced by a periodic Gaussian function. We have found strong evidence which indicates that for $0<e^2<e_c^2\simeq 13$, this model undergoes an *inverted* XY transition. Our study thus confirms the suggestion of Helfrich and Müller and predicts a new type of phase transition for type-II superconductors and possibly for smectic-A liquid crystals in three dimensions. For a type-I superconductor where the magnetic penetration depth is shorter than the coherence length and parallel vortices attract each other, a first-order transition is expected before the asymptotic critical region can be reached,[1] and so our lattice model is not applicable. The present study may also be a step towards understanding several other systems of interest (e.g., 3D crystals and 4D compact quantum electrodynamics) for which the topological excitations are loops.

Our conclusions about the nature of the phase transition in the LSM are derived from two sources. First, we show that exact duality transformations on this model strongly suggest a phase transition of the type described above. Then we show that the results of a Monte Carlo simulation of the thermodynamics of this model are consistent with this description. Duality maps for the LSM have been studied by several authors.[8,9] Here, we propose a new interpretation of the results. First, let us consider the case $e=0$, i.e., the Villain model. By using the Poisson resummation formula and doing the θ integration, the partition function can be written as[8]

$$Z_V(\beta)\propto(2\pi\beta)^{-3N/2}\sum_{[m_{i\mu}]}{}'\exp(-\tfrac{1}{2}\beta^{-1}\sum_{i\mu}m_{i\mu}^2), \tag{2}$$

where $\sum'$ means that the link variables $m_{i\mu}$ have zero divergence at each lattice site. Note that the right-hand side of Eq. (2) can be interpreted as the partition function at temperature $T^{\text{loop}}=2\beta$ of a collection of directed loops with energy per unit length equal to unity, and a repulsive contact interaction between two loop elements. By going to the dual lattice, it can be shown[8] that $Z_V(\beta)\propto Z_{V'}(\beta,0)$, where

$$Z_{V'}(\beta,K)=\sum_{[l_{i\mu}]}{}'\exp[-2\pi^2\beta\sum_{ij\mu}l_{i\mu}G(|\vec{r}_i-\vec{r}_j|)l_{j\mu}-K\sum_{i\mu}l_{i\mu}^2]. \tag{3}$$

In Eq. (3), $G(r)$ is a lattice Green's function which behaves like $1/4\pi r$ for large r. The partition function of Eq. (3) which describes a set of interacting vortex loops defines a *generalized Villain model* when the "chemical potential" K is different from zero. It is generally assumed that the Villain model is in the same universality class as the XY model. Thus, the phase transition should be XY-like for $K=0$ and $\beta=\beta_{cV}$, the inverse transition temperature of the Villain model. It is clear from Eqs. (2) and (3) that the point $(0,1/2\beta_{cV})$ in the β-K plane should then correspond to an *inverted* XY transition. The phase transition at the point $(\beta_{cV},0)$ should be stable with respect to turning on a small K because this changes only the short-distance part of the interaction $G(|\vec{r}_i-\vec{r}_j|)$, whereas the long-range part of the interaction is expected to determine the nature of the transition. The phase transition at the point $(0,1/2\beta_{cV})$ should, on the other hand, be unstable with respect to introducing a small β because this corresponds to turning on a long-range interaction. Thus, it is reasonable to expect a phase diagram of the form shown in Fig. 1(a).

With use of the same transformations as above, the partition function (1) of the LSM can be written as[9]

$$Z_s(\beta,e) \propto (2\pi\beta)^{-3N/2} Z_{V'}(e^2/4\pi^2, 1/2\beta). \qquad (4)$$

The proposed phase diagram [Fig. 1(a)] for the generalized Villain model then implies that the phase diagram of the LSM in the $(T=1/\beta, e^2)$ plane should look like Fig. 1(b). For $e^2 > e_c^2 = 4\pi^2\beta_{cV}$, there is no phase transition.[9] For $0 < e^2 < e_c^2$, the transition is of the *inverted XY* type. This phase diagram is consistent with the renormalization-group result[1] that the ordinary XY fixed point is unstable with respect to e^2 for $d \leq 4$. However, another possibility, consistent with the renormalization-group and duality arguments, is that part or all of the phase-transition lines in Figs. 1(a) and 1(b) are first order.[10]

In order to clarify the situation, we have carried out a Monte Carlo simulation of the thermodynamics of these models. The behavior at $e=0$ was studied by simulating the model of loops described by the partition function of Eq. (2). For $e \neq 0$, we found it most convenient to simulate a model which is dual to the LSM. This model has the partition function

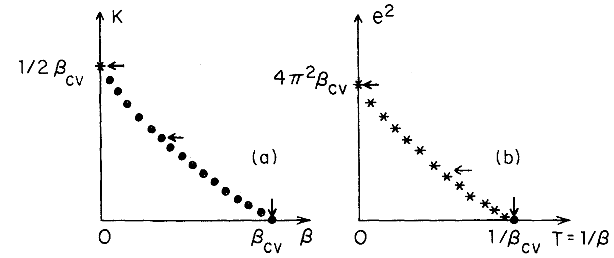

FIG. 1. Proposed phase diagram for (a) the generalized Villain model and (b) the lattice superconductor. The dots and asterisks, respectively, represent normal and inverted XY transitions. The arrows indicate the points where the simulations were done.

$$Z_{s'}(\beta',e) = \sum_{[n_{i\mu}]} \int (d\theta_i/2\pi) \exp[-\tfrac{1}{2}\beta' \sum_i |\vec{\Delta}\times\vec{n}_i|^2 - (e^2/8\pi^2)\sum_{i\mu}(\Delta_\mu\theta_i - 2\pi n_{i\mu})^2]. \qquad (5)$$

It is easy to show[9] that

$$Z_s(\beta,e) \propto (2\pi\beta)^{-3N/2} Z_{s'}(1/\beta, e). \qquad (6)$$

For computational convenience, the continuous variable θ in Eq. (5) was replaced by a discrete variable z_n with $n=100$. The standard Metropolis method was used in the simulations. Typically, 5000–10 000 time steps per site were used to measure the internal energy and the specific heat. The corresponding quantities for the LSM were then calculated by using Eq. (6).

Our first project was to check that the Villain model [or equivalently, the loop model of Eq. (2)] exhibits a continuous transition with XY exponents. In Fig. 2, we have shown the results for the specific heat of the loop model (calculated numerically differentiating the internal energy) for samples with linear dimension $L=5$, 8, and 10 with periodic boundary conditions. The dashed curve shows the specific heat of the $L=10$ Villain model calculated from the data by using Eq. (2). The specific-heat exponent α of the 3D XY model is known to be very close to zero. For a system with $\alpha=0$, one expects[11] the following behavior for the specific heat for $T\to T_c$:

$$C = -A \ln|t| - \tfrac{1}{2}DA\,\mathrm{sgn}\,t + B, \qquad (7)$$

where $t=(T-T_c)/T_c$, and $D\approx 4$ from measurements at the He λ point.[11] From plots of C against $\ln|(T^{\text{loop}} - T^*)/T^*|$, where T^* is the temperature at the specific-heat peak, we find that the data are consistent with Eq. (7) with $A=1.3\pm0.2$ and $D\simeq -1.6$. Because of the inversion of the temperature in going from the Villain model to the loop model, the sign of the asymmetry D is reversed. Although the calculated value of $|D|$ is much less than 4, the results indicate that $|D|$ increases with L. The size dependence of the position and the height of the specific-heat peak is consistent with finite-size scaling[12] with $\alpha\simeq 0$. An extrapolation to $L\to\infty$ gives $T_c^{\text{loop}}=0.66 \pm 0.01$, which implies that $\beta_{cV}=0.33\pm0.005$. This is consistent with the inequality, $\beta_{cV}\geq 0.322$, derived by Myerson.[13]

Our result for β_{cV} implies that for $e^2 > e_c^2 \simeq 13$, the LSM has no phase transition. For e^2 close to zero, the situation is complicated by crossover effects. For this reason, we chose to simulate the LSM with an intermediate value of $e^2=5$, indicated by the arrows in Fig. 1. Figure 3 shows the results for the specific heat for $L=3$, 5, 10, and 15. The data do not show any indication of a first-order transition. We did not find any hysteresis in the internal energy. If we assume that the partition function of a finite system with a first-order phase transition is given by

$$Z(T) \sim \exp(-Nf_1/T) + \exp(-Nf_2/T), \qquad (8)$$

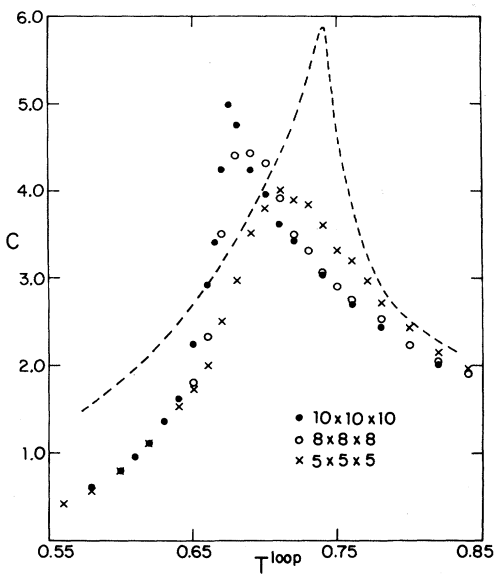

FIG. 2. Specific heat of the loop model. The dashed line shows the specific heat of the Villian model ($L=10$) at temperatures $4T^{loop}$.

where f_1 and f_2 are the free energies per site of the two bulk phases, then it follows that the height of the specific-heat peak is $C_m=\text{const}+N(\Delta S)^2/4$, where ΔS is the jump in the entropy. We find that it is impossible to draw a straight line through all the four data points in a plot of C_m vs $N=L^3$. From the maximum slope of a straight line drawn through the data points for $L=5$, 10, and 15 we estimate that if this transition is first order, it must have $\Delta S \lesssim 0.03$. Since all the parameters in our model are of order unity, there is no reason to expect such a small first-order transition.

As shown in the inset of Fig. 3, C_m is approximately proportional to $\ln L$, which indicates a continuous transition with $\alpha \simeq 0$. We find that plots of C vs $\ln|(T-T^*)/T^*|$ are approximately linear for $T<T^*$, but show considerable curvature for $T>T^*$. However, we have obtained reasonable fits to the data close to T^* with a simple finite-size scaling function of the form

$$C=-\frac{A}{2}\ln[(t+a\tau)^2+b^2\tau^2]-\frac{DA}{\pi}\tan^{-1}\frac{t+a\tau}{b\tau}+B, \quad (9)$$

with $\tau=L^{-3/2}$, which reduces to Eq. (7) for $L\to\infty$. Fits with $A=0.3$, $T_c=1.62$, $a=0$, $b=0.52$, $D=-2.68$, and $B=1.3$ are shown by the solid lines in Fig. 3. Fits to other finite-size scaling forms give somewhat higher values for A, but similar values for D. Because of the uncertainties in-

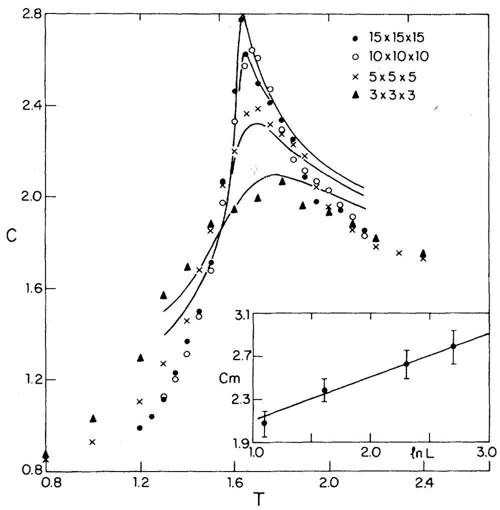

FIG. 3. Specific heat of the lattice superconductor for $e^2=5$. The inset shows the height of the specific-heat peak vs $\ln L$. The solid lines are fits by Eq. (9).

volved in estimating the background and corrections to scaling, these numbers should not be taken very seriously. However, it is clear from Fig. 3 that the specific heat for $T=T^*+\Delta T$ is higher than that for $T=T^*-\Delta T$, which is the reverse of what one expects for the XY model. A comparison with the dashed curve of Fig. 2 clearly shows this inversion. Since the asymmetry increases with L, it is not an effect of the background. Also, the qualitative behavior of the specific-heat peak of the LSM at $e^2=5$ (Fig. 3) is very similar to that of the loop model (Fig. 2) which represents the large-e^2 limit of the LSM and which showed the inverted XY form as expected. Thus, the evidence indicates an inverted XY transition for the LSM at $e^2=5$. Since the simulation was done for only one intermediate value of e^2, we cannot rule out a first-order transition for e^2 close to zero. However, such a first-order transition would presumably be very weak, and therefore hard to detect numerically.

The authors are very grateful to D. R. Nelson, J. Toner, and S. Doniach for stimulating discussions, and to S. Kirkpatrick for his hospitality at the IBM Thomas J. Watson Research Center, where part of the computation was done. This work was supported by the National Science Foundation through the Harvard University Materials Research Laboratory and Grant No. DMR 77-10210.

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Abundance Enhancements in Cosmic Rays Produced by Collisionless Shocks

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It is shown that shocks preferentially accelerate partially ionized heavy elements over protons. Within the framework of a previously published model of injection, the spectra of different ion species are calculated from thermal to ultrarelativistic energies. For typical astrophysical parameters, the predicted enhancement is in qualitative agreement with observations for a 10^6-K preshock plasma; ions with $Z > 10$ are enhanced by about an order of magnitude or so. The continuing increase with energy of the heavy-element abundances into the air-shower regime is discussed.

PACS numbers: 94.40.Lx, 94.40.Cn, 94.40.Ht, 94.40.Pa

The observed composition of cosmic rays is an important constraint on theories of their origin. It indicates, given the composition of the thermal plasma, the relative probability that any given type of ion species meets the criterion for becoming a cosmic ray. Heavy elements, $Z > 10$, appear to be enhanced by about one order of magnitude relative to protons at ~1 GeV/nucleon, and similar enhancements are seen in solar cosmic rays at about 10 MeV/nucleon.[1] The enhancement of heavy elements in the galactic cosmic rays increases with energy, and recent air-shower studies[2] suggest that at *total* energy of about 10^{15} eV, cosmic rays may be mostly iron. This represents an additional enhancement of one to two orders of magnitude above that at 1 GeV.

Recently, a model for cosmic-ray production was proposed[3] in which energetic particles are drawn directly from a thermal pool. In the model, all particles flowing into the shock are compressed and accelerated to some extent, as required by definition of a shock, but a very few receive a far larger share of energy than most, which makes them cosmic rays. The fact that thermal particles as well as superthermal ones are included in the theoretical description of the acceleration makes it possible, in principle, to calculate the composition of cosmic rays relative to the thermal plasma.

In practice, the calculation is very difficult; however, the enhancements can be calculated with analytic approximation at some sacrifice of accuracy. The purpose of this Letter is to show qualitatively why heavy elements are accelerated more effectively than protons, and to calculate the enhancement with use of an analytic approximation.

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