Solving the Ginzburg-Landau equations by simulated annealing

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We propose and demonstrate the power of a novel approach to the solution of the Ginzburg-Landau equation based on minimizing the free-energy functional with the numerical technique of simulated annealing instead of minimizing it analytically and then solving the resulting nonlinear partial differential equations. We present calculations of the magnetization versus magnetic field that agree well with the predictions of Abrikosov and others for a homogeneous, isotropic type-II superconductor near H_{c1} and H_{c2}. We also summarize the extension of the method to the calculation of the properties of an inhomogeneous, anisotropic superconductor.

I. INTRODUCTION

The Ginzburg-Landau equation provides an important and useful starting point for studying the basic phenomenology of superconductivity. In this note we present a novel approach to the solution of this equation that is as simple to implement for an anisotropic, inhomogeneous superconductor as it is for an isotropic, homogeneous one. The approach is based on the use of a global optimization technique, called simulated annealing,[1] to directly minimize the Helmholtz free energy instead of minimizing it analytically and then solving the resulting nonlinear, partial differential equation.

There appears to be few numerical attempts to solve the Ginzburg-Landau equations. Those commonly referenced are by Abrikosov,[2] Kleiner *et al.*,[3] and Brandt.[4] In these works an approximate solution to the equations is assumed, the free energy is then made stationary with respect to the parameters in the approximations, and the resulting equations for stationary values of the parameters are solved. This procedure leads to surprisingly precise results and has established that the minimum solution is a triangular lattice of vortices. It also has been useful in studying the behavior of the magnetization as a function of the external field near the upper and lower critical values, but because of the assumptions in the choice of the assumed solution, the approach appears limited in application to homogeneous superconductors.

The approach presented here, compared to these other works, is inefficient if used to study homogeneous superconductors; however, because of the ease with which it can be applied to inhomogeneous superconductors, it appears to offer an attractive opportunity to study the phenomenology of such materials, particularly because of the simplicity with which a variety of inhomogeneities, anisotropies, and unconventional order parameters can be modeled. There appears to be no prior numerical studies of the effects of inhomogeneities on the vortex lattice and the magnetization curve with which this work can be compared.

Simulated annealing is a stochastic, optimization technique for multivariant functions. It mimics the metallurgical annealing process by introducing a fictitious temperature, and it cycles and lowers this temperature to move the variables, or "atoms," from their values when the function is in a "high-energy state" at elevated temperatures into their values when it is its lowest-energy or "crystalline" state at low temperatures. The values of the variables are moved by the Metropolis Monte Carlo algorithm, and since in this algorithm movements that raise the energy are probable, the technique allows "thermal fluctuations" to move the variables from a metastable state towards the minimum state as the temperature is lowered. The specific simulated annealing algorithm we use is that of Corana *et al.*[5]

The function we minimize is the lattice gauge form of the Landau expansion for the free energy of a superconductor in the presence of a magnetic field. The variables we "move" are the values of the order parameter and vector potential associated with each site. This lattice formulation is similar to that used by Ebner and Stroud[6] to study phase coupling in granular and amorphous superconductors. By basing their simulation on the partition function

$$Z=\exp(-F/kT)\ ,$$

these authors focused on properties derived from thermal fluctuations when the vector potential was constrained to be that of the external field. Although our program can easily be adapted to study these same thermal properties simultaneously with the minimization, what we obtain most directly with this program is information about the magnetic properties of the system. It is interesting to note that Ebner and Stroud observed that disorder frus-

trates local gauge invariance, while Kirkpatrick *et al.*[1] remarked that simulated annealing should work best when frustration exists.

In this paper we illustrate the use of the simulated annealing technique in the solution of the Ginzburg-Landau equation by applying it to a homogeneous superconductor. Since much is known about the solution in this case, we can obtain useful ideas about the possible effectiveness of the approach when inhomogeneities are present. In the next section we describe our lattice gauge equations, and in Sec. III, we present results of calculations for the vortex lattice, magnetization curve, and the upper and lower critical fields of a simple isotropic, homogeneous superconductor. In the last section we conclude with remarks on more complicated modeling possibilities and on the application of the annealing method to other optimization problems.

II. LATTICE EQUATIONS

We start with the Ginzburg-Landau functional for the difference ΔF between the free energies per unit volume of the normal and superconducting states

$$\Delta F=\frac{1}{V}\int d^3x\left[\alpha|\Delta(\mathbf{x})|^2+\tfrac{1}{2}\beta|\Delta(\mathbf{x})|^4+\frac{1}{2m}\left|\left(\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}\right)\Delta(\mathbf{x})\right|^2+\frac{1}{8\pi}[\nabla\times\mathbf{A}(\mathbf{x})]^2\right]. \tag{1}$$

The variation of ΔF with respect to the fields $\Delta(\mathbf{x})$ and $\mathbf{A}(\mathbf{x})$ leads to the Ginzburg-Landau equation and the equation for the supercurrent. We will not need these equations in the following and refer the reader to standard textbooks[7] for notation and details. Obviously, the absolute minimum of the free energy (1) is the field-free state, $\nabla\times\mathbf{A}=0$, which is not of interest here. In order to describe a superconductor in the presence of an external field, one has to abandon the unrestricted minimization of (1) and impose constraints on the fields Δ and $\mathbf{A}$. We use the constraint of fixing the average magnetic field $\mathbf{B}$. The constrained minimum of ΔF is now a function of $\mathbf{B}$, and standard thermodynamic arguments yield the external field as the derivative of ΔF with respect to $\mathbf{B}$,

$$\mathbf{H}=4\pi\frac{\partial\Delta F}{\partial\mathbf{B}}. \tag{2}$$

The vector notation in (2) is unconventional but self-explanatory.

In the following we implement the average magnetic field by imposing what will be called "periodic boundary conditions." In a perfect, infinite, type-II superconductor these boundary conditions fix the lattice parameters of the vortex lattice and lead to Abrikosov's vortex state.[2] On the other hand, we can also use this boundary condition for nonperfect, nonperiodic superconductors with, for example, normal-metal inclusions, grain boundaries, inhomogeneities in the chemical composition, or other defects. In this case, the unit cell of our periodic lattice must be interpreted as an artificial supercell, chosen large enough such that the defect superstructure has no significant physical consequences.

Before discretizing (1), we put it into dimensionless form by scaling energies by $\alpha^2/4\pi\beta$ and lengths by the coherence length $\xi=(-\hbar^2/2m\alpha)^{1/2}$. Then, with the use of forward difference approximations for the derivatives, the dimensionless free-energy functional per unit volume becomes

$$\Delta F=\frac{1}{N_xN_y}\sum_{\text{points}}(|\Delta_i|^2+\tfrac{1}{2}|\Delta_i|^4)+F_{\text{kin}}+F_{\text{field}}, \tag{3}$$

where the average kinetic energy is

$$F_{\text{kin}}=\frac{1}{N_xN_y}\left[\sum_{x\text{ bonds}}\frac{1}{a_x^2}|\Delta_j-\exp(i\alpha_x A_x^{\text{right}})\Delta_i|^2+\sum_{y\text{ bonds}}\frac{1}{a_y^2}|\Delta_j-\exp(ia_y A_y^{\text{up}})\Delta_i|^2\right] \tag{4}$$

and the average field energy is

$$F_{\text{field}}=\frac{\kappa^2}{N_xN_y}\sum_{\text{squares}}\left[\frac{1}{a_y}(A_x^{\text{down}}-A_x^{\text{up}})+\frac{1}{a_x}(A_y^{\text{right}}-A_y^{\text{left}})\right]^2 \tag{5}$$

with

$$\kappa=\frac{mc}{2e\hbar}\sqrt{\beta/2\pi},$$

and N_x and N_y are the number of lattice points in the x and y directions. We assume that the external magnetic field is in the z direction, so by translational invariance we need to solve for Δ and $\mathbf{A}$ as functions only of x and y. On each lattice point the complex order parameter has the value Δ_i and with each point we associate horizontal and vertical bonds. The lattice constants along these bonds are a_x and a_y, and between nearest-neighbor sites the x and y components of the vector potential are A_x^{right}, A_x^{left}, A_y^{up}, etc. Also at each lattice point, we evaluate the $\nabla\times\mathbf{A}$ as a sum around a square of nearest-neighbor bonds circulating to the right, up, left, and down. It is easy to show that this discretization of the curl is gauge invariant; accordingly, so are ΔF and other physical quantities such as the magnetic field and the current. At lattice site i, the gauge transformations are

$$\Delta_i\to\Delta_i e^{i\phi_i},$$
$$A_x^{ij}\to A_x^{ij}+(\phi_j-\phi_i)/a_x,$$
$$A_y^{ij}\to A_y^{ij}+(\phi_j-\phi_i)/a_y,$$

where ϕ_i is the phase of the order parameter at site i, and A^{ij} is the x or y component of the vector potential between site i and its neighbor j.

Since our minimum is constrained to produce a given value of $\mathbf{B}$, we find ΔF as a function of $\mathbf{B}$ and could use (2) to find $\mathbf{H}$. In practice we fix the magnitude $\mathbf{B}$ by specifying the number of vortices $n=\Phi/2\pi$ in our unit cell. Here $\Phi=BL_xL_y/\kappa$ where L_x and L_y are the sizes of

our unit cell in the x and y directions. Instead of the error susceptible process of numerical differentiation, we compute $\mathbf{H}$ from the discretized form of the virial relation[8]

$$\mathbf{H}\cdot\mathbf{B}=4\pi(F_{\text{kin}}+2F_{\text{field}}) . \tag{6}$$

In practice, we chose a gauge such that $A_x=0$. For the purposes of the simulated annealing process, this means we can regard $\Delta F=f(\mathbf{X})$ where $\mathbf{X}$ is of length $3N$ with N being the number of lattice sites at each of which there are three degrees of freedom, the real and imaginary parts of Δ and the y component of $\mathbf{A}$. In this gauge the periodic boundary conditions are

$$\Delta(L_x,y)=\Delta(0,y)e^{iy\Phi/L_y} ,$$

$$\Delta(x,L_y)=\Delta(x,0) ,$$

$$A_y(L_x,y)=A_y(0,y)+\Phi/L_y ,$$

$$A_y(x,L_y)=A_y(x,0) .$$

With the imposition of periodic boundary conditions, quantities such as the magnetic field and current are periodic.

III. RESULTS

The simulations require the specification of two classes of parameters. One class consists of n, κ, N_x, N_y, a_x, and a_y. These parameters control the discretization and the physics of the problem. For the results reported here, except near H_{c1}, we chose $n=2$ and $a_y=\sqrt{3}a_x$. This choice defines a unit cell commensurate with a triangular lattice of vortices. By varying a_x, N_x, and N_y, we varied the external magnetic field. When near H_{c1}, we took $n=1$ and $a_x=a_y=0.7945$, so by increasing N_x and N_y from 20 to 50, we are able to let the magnetic-field approach its lower critical value.

The second class of parameters control the annealing process. These parameters include the starting temperature, the number of Monte Carlo steps at each temperature, the fraction by which the temperature is reduced at each annealing step, the maximum number of annealing steps, and the allowable error for the result. Of these the error criterion is the most important. After each Monte Carlo step, we record the lowest value of the free energy obtained until then. When the absolute value of the relative difference between this value and the values of the free energy at the end of three consecutive temperature reduction steps were within 10^{-4} of each other, the simulation was stopped. The other parameters only seemed to control how fast this point was reached. We made no attempt to optimize their choice, and used 0.1 for the initial temperature, 250 for the number of Monte Carlo sweeps, 0.5 and 0.75 for the reduction parameter, and 40 for the maximum number of reductions.

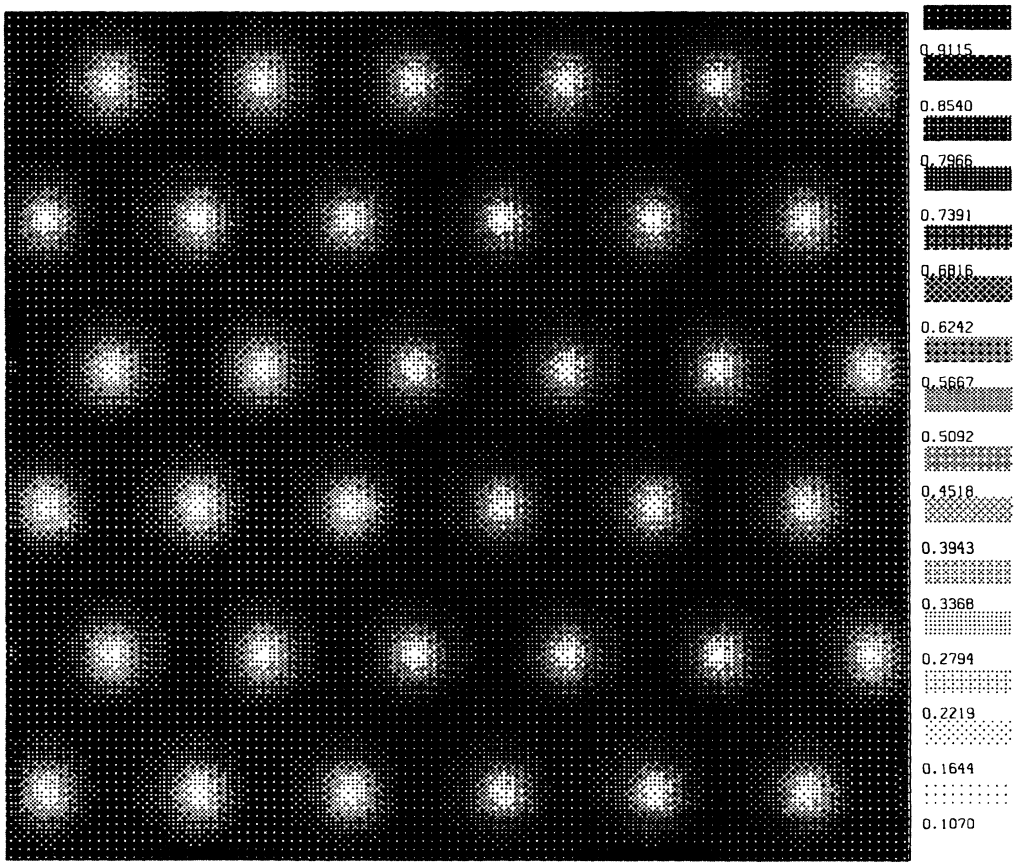

FIG. 1. A half-tone plot of the magnitude of the order parameter for $\kappa=5$ and $H=0.96$. The solution in the rectangular unit cell with two vortices and $a_y=\sqrt{3}a_x=0.4$ was replicated six times in the x direction and three times in the y direction.

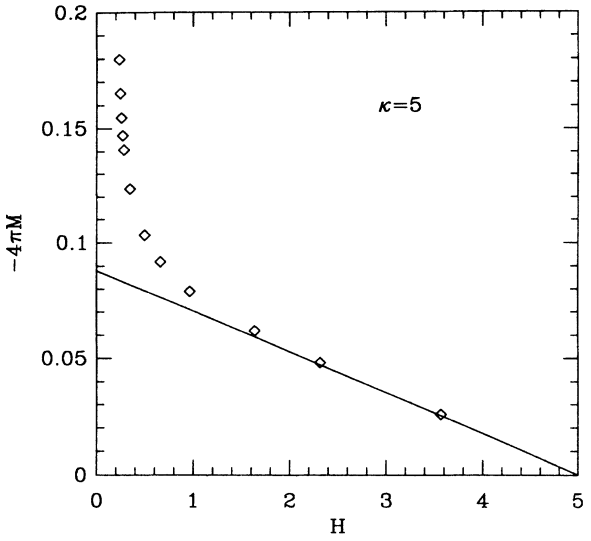

FIG. 2. The magnetization vs external magnetic-field curve for $\kappa=5$. The solid line is Abrikosov's prediction for very large κ.

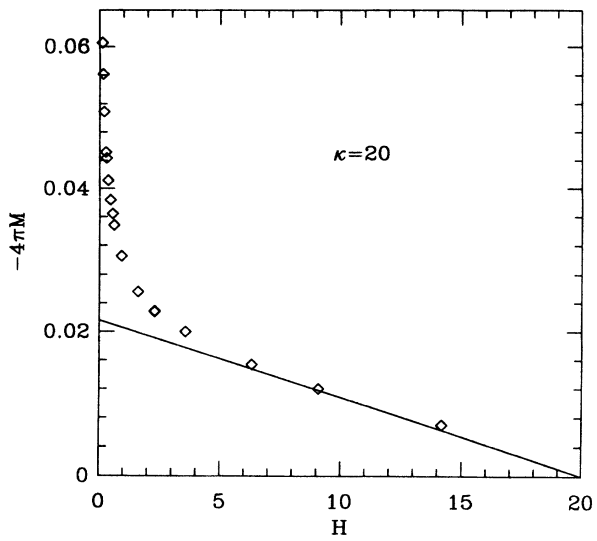

FIG. 4. The magnetization vs external magnetic-field curve for $\kappa=5$. The solid line is Abrikosov's prediction for very large κ.

To start the annealing process, we also have to specify initial values of the order parameter and vector potential. The final result was found to be exceptionally independent of this choice. For consistency we decided always to start the system in the normal state. The particular simulated annealing algorithm used also had the feature of an adaptive adjustment of the allowable Monte Carlo step size for each variable in the problem. Here we used exactly the procedure discussed by Corana *et al.*[5]

When we chose $a_y=\sqrt{3}a_x$ and $n=4$ and 8, we found by tiling space with our unit cell, the vortices, which developed in the cell, generally formed a lattice with a sixfold coordination. A triangular lattice was often formed, but since the precision to which we computed was within a small multiple of the known free-energy difference between a triangular and square lattice, it is not surprising that a distorted structure or one with interstitials and vacancies would also occur. If we choose a stopping criterion of 10^{-3} instead of 10^{-4}, we would find fourfold coordination about as often as we would find sixfold coordination.

In Fig. 1 we show a half-tone plot of the magnitude of the order parameter for $\kappa=5$ and $a_y=\sqrt{3}a_x$ obtained by putting two vortices in our unit cell and then forming a

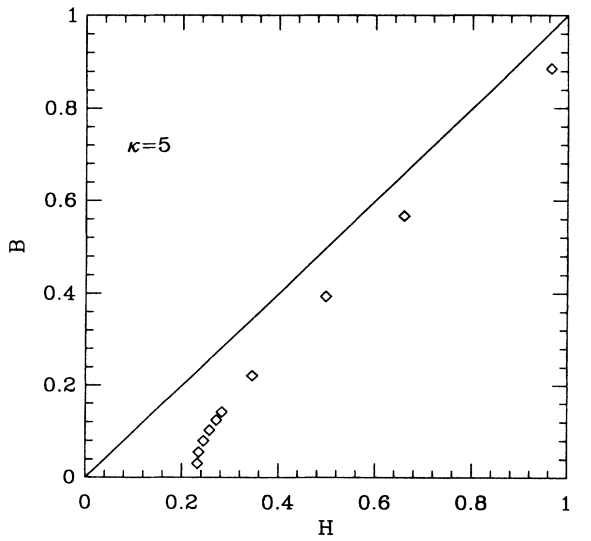

FIG. 3. The magnetic induction vs the external magnetic field for $\kappa=5$ near H_{c1}. The exact value of H_{c1} is 0.233; the large κ asymptotic prediction is 0.211.

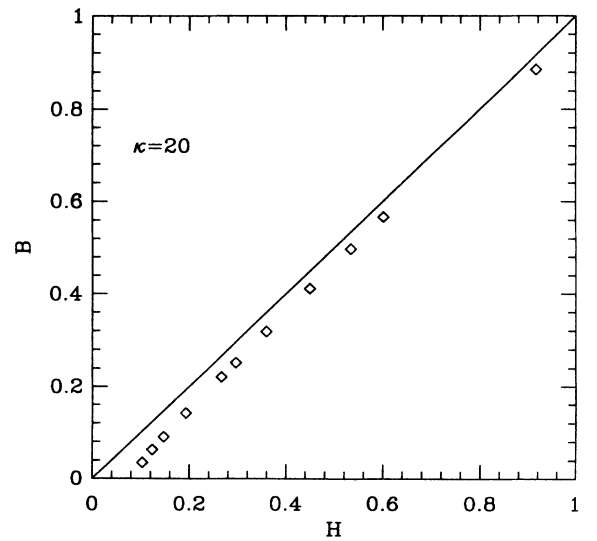

FIG. 5. The magnetic induction vs the external magnetic field for $\kappa=5$ near H_{c1}. The exact value of H_{c1} is 0.088; the large κ asymptotic prediction is 0.087.

6×3 rectangle with the cell. One clearly sees a triangular lattice. Therefore, even when our numerical grid is rectangular, we can produce the correct structure for the vortex lattice, if proper care is taken.

Our main interest was in the M versus H curve and not in the vortex lattice. In Fig. 2 we show this curve for $\kappa=5$. We note that simulation data appear to extrapolate to a value of $H_{c2}\approx\kappa$. With H_{c2} taken to be κ, the solid line is Abrikosov's[2,3,9] prediction

$$4\pi M=\frac{H-H_{c2}}{1.1596(2\kappa^2-1)}$$

of how the magnetization curve should vary near H_{c2}. It is also interesting to note the degree to which the data follow this curve to values of H approach H_{c1}. This behavior was also noted by Brandt.[4] To see more easily how the results vary near H_{c1}, we plot the B versus H curve in Fig. 3. The last data points that are converging onto the H axis have the value of 0.232, which is very close to the exact answer, 0.233.[10] We remark that the exact value is about 10% higher than that predicted by large κ expression[11] of Abrikosov's equations,

$$H_{c1}=\frac{1}{2\kappa}(\ln\kappa+0.497)\ .$$

By increasing n, N_x, and N_y, while decreasing a_x, we were able to approach H_{c2} closer than shown in Fig. 2; however, both near H_{c1} and H_{c2} the value of B is small and it is difficult to obtain accurate results.

Results for similar calculations for $\kappa=20$ are shown in Figs. 4 and 5. For the M versus H curve, Fig. 4, the agreement with the $H_{c2}\approx\kappa$ and Abrikosov's asymptotic result is as satisfactory as it was for $\kappa=5$. In Fig. 5, we see, however, that we are just beginning to predict H_{c1}. The calculation is difficult because the size of the field, whose exact value is 0.088, is becoming quite small.

IV. FINAL COMMENTS

We described and demonstrated the utility of a novel approach to the solution of the Ginzburg-Landau equation based on minimizing the free-energy functional by the numerical technique of simulated annealing instead of minimizing it analytically and then by solving the resulting nonlinear partial differential equations. We presented calculations of the magnetization versus magnetic field that agreed well with the predictions of Abrikosov and others for a homogeneous, isotropic type-II superconductor near H_{c1} and H_{c2}. The larger the value of κ, however, the more difficult it became to predict H_{c1}.

Our principal intent was to determine if the optimization approach would work. We believe we have demonstrated that it does. Our longer term objective is to study the properties of disordered and anisotropic superconductors. An attractive feature of our approach is the ease in which it can be applied to models of such materials. To introduce disorder, we simply have to make the α, β, and m in (1) position dependent, and to introduce anisotropy, make the mass a tensor μ. Equation (1) becomes

$$\Delta F=\frac{1}{V}\int d^3x\left[\alpha(\mathbf{x})|\Delta(\mathbf{x})|^2+\tfrac{1}{2}\beta(\mathbf{x})|\Delta(\mathbf{x})|^4 -\frac{1}{2}\sum_{kl}[\mu^{-1}(\mathbf{x})]_{kl}\left[\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}(\mathbf{x})\Delta(\mathbf{x})\right]_k\left[\frac{\hbar}{i}\nabla+\frac{2e}{c}\mathbf{A}(\mathbf{x})\Delta(\mathbf{x})\right]_l+\frac{1}{8\pi}[\nabla\times\mathbf{A}(\mathbf{x})]^2\right]\ . \tag{7}$$

Clearly, discretizing this expression is as easy as discretizing (1). What is different about the disordered case is that the dimensionless form of (7) does not depend as (3) on a single parameter κ. Since α in (1) equals $a(T-T_c)$ where T is the temperature and T_c is the critical temperature, this means we have at least two additional input parameters for the calculation that affect the physics, but the manner in which we apply simulated annealing to the problem is basically unchanged from the way we applied it to (1). What we do have to change slightly is the way in which we place (7) in dimensionless form, the strategy we suggest is to scale the energies and the lengths by an $\alpha_0^2/4\pi\beta_0$ and ξ_0 of some homogeneous isotropic (or anisotropic) superconducting material. A simple choice is an effective material whose superconducting state is the same as the disordered material. The T_{c0} of this material is straightforwardly found from an eigenvalue problem.[12] Extensive calculations of simple models of disordered superconductors are currently underway and the results will be reported elsewhere.[12] Being studied are not only the effects of disorder on the magnetization curve but also ways to estimate the relation between the disorder and pinning forces.[12]

Although the computation time to perform the simulations is relatively modest (a few minutes to at worst a few tens of minutes on a Cray XMP computer, simulated annealing, as most Monte Carlo calculations, is difficult to speed up on a vector computer, making large grids with complicated disorder structures potentially expensive to perform. The method has many parallel elements and ultimately may be best suited for certain types of parallel computers. Extensions of the basic method, supplementing it with steepest descent or other information,[13] exist and are being studied. Additionally, modern nonlinear, partial differential equation methods, tuned to today's supercomputers, appear attractive and may offer distinct advantages over the current approach, but to date they appear to have difficulty in obtaining good solutions without a good guess to the solution.[14]

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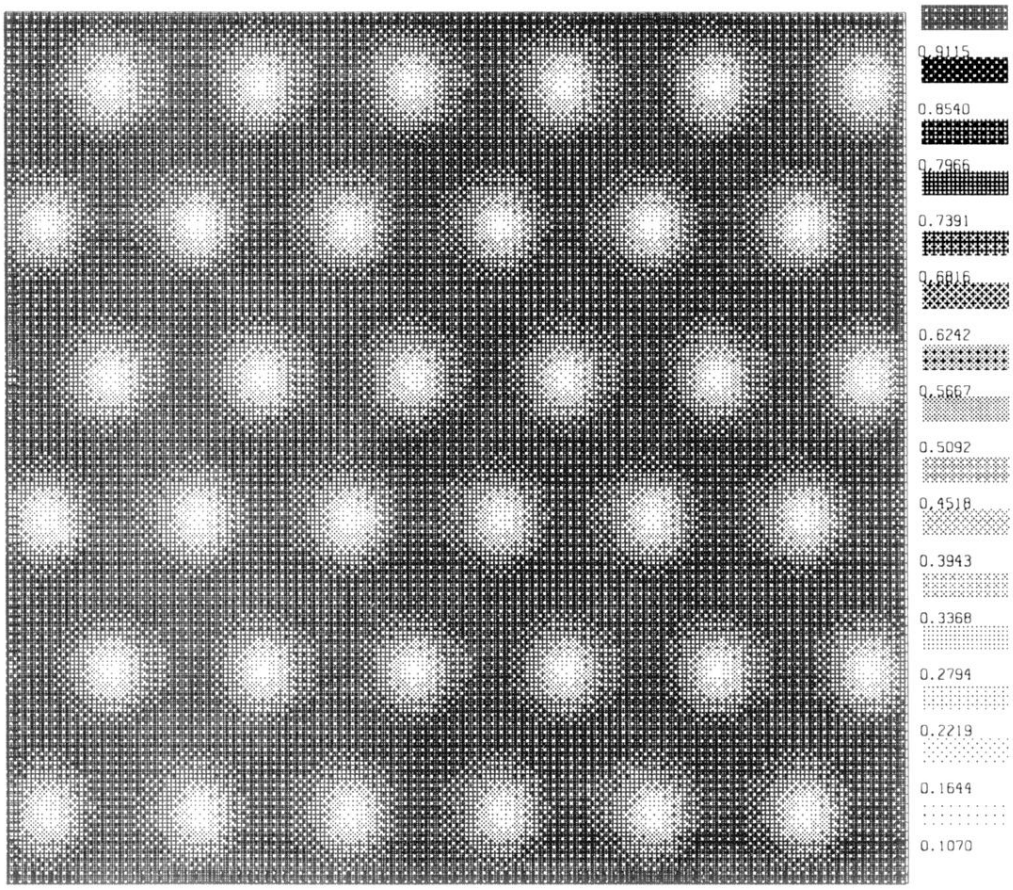

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