CHAPTER VII

COMPUTER SIMULATIONS FOR TYPE II SUPERCONDUCTORS

Previous Work

Before the description of our work as shown below, we will first discuss a paper by Doria *et al.*, 1990, which we choose as a prototype attempt. They used the numerical optimization technique called *simulated annealing* (Kirkpatrick *et al.*, 1983) to minimize the Helmholtz free energy directly. Their result agrees very well with an analytic solution of the Ginzburg-Landau theory, the Abrikosov lattice solution. However, the agreement with theory was obtained in a rather artificial manner, by assuming *a priori* that the solution was periodic with unit cell lengths in the ratio $\sqrt{3}/2$: 1(unlike our calculation in chapter V, where the ratio was unconstrained). Therefore, they have forced the solution to lie on an equilateral triangular lattice. Furthermore, they restricted their simulations to values of κ and H_c for which the analytic solution is well known. In fact, it is these two deficiencies in their work which motivated our work on this problem. Our goals were 1) to make no priori assumptions except at the boundary, and 2) to derive numerical solutions for cases for which no analytic solution is available.

There are several differences between the work of Doria *et al.*, 1990 and our work. Firstly, their discretized Helmholtz free energy equation (scaled into dimensionless form) was:

$$\Delta F = \frac{1}{N_x N_y} \sum_{\text{Points}} \left[-|\Psi_i|^2 + 0.5|\Psi_i|^4 \right] + F_{kin} + F_{field} \qquad (7.1)$$

where the average kinetic energy is

$$F_{kin} = \frac{1}{N_x N_y} \left[\sum_{x \text{ bonds}} \frac{1}{a_x^2} \left| \Psi_j - \exp\{-ia_x A_x^{right}\} \Psi_i \right|^2 + \sum_{y \text{ bonds}} \frac{1}{a_y^2} \left| \Psi_j - \exp\{-ia_y A_y^{up}\} \Psi_i \right|^2 \right]$$

(7.2)

and the average field energy is

$$F_{field} = \frac{\kappa^2}{N_x N_y} \sum_{\text{squares}} \left[\frac{1}{a_y} \left(A_x^{down} - A_x^{up} \right) + \frac{1}{a_x} \left(A_y^{right} - A_y^{left} \right) \right]^2 \qquad (7.3)$$

ΔF is the energy difference between the normal and the superconducting states per unit volume, N_X and N_y are the number of lattice points in the x and y directions. They assume that the external magnetic field is in the z direction , so by translational invariance they need to solve for Ψ and **A** as functions only of x and y. On each lattice point the complex order parameter has a value Ψ_i and at each points there are associated 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} and A_y^{down}. Also, at each lattice point they evaluate $\nabla \times \mathbf{A}$ as a sum around a square of nearest -neighbor bonds circulating to the right, up, left, and down.

The gauge transforms that Doria *et al* used were:

$$\Psi_i \rightarrow \Psi_i e^{i\phi_i} \tag{7.4}$$

$$A_x^{ij} \rightarrow A_x^{ij} + (\phi_j - \phi_i)/a_x$$

$$A_y^{ij} \rightarrow A_y^{ij} + (\phi_j - \phi_i)/a_y \tag{7.5}$$

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 **A** between site i and its neighbor j.

It has been shown that the expression (7.1) above for the free energy is invariant under this transformation. In consequence all physical quantities desired are also invariant. In practice they choose $A_X = 0$, so they must choose ϕ so that $\mathbf{A} + \nabla\phi$ is unchanged, since

$$\nabla \times \mathbf{A} = \mathbf{h} \tag{7.6}$$

where **h** is the internal magnetic field. On the other hand, we choose to use the gauge-independent quantity,

$$\mathbf{A} + \nabla\phi = \mathbf{Q} \tag{7.7}$$

where **Q** is the supervelocity and is gauge invariant, and we have that

$$\nabla \times \mathbf{Q} = \mathbf{h} \tag{7.8}$$

We emphasis that we can always use a real order parameter, in which case the phase of the original complex order parameter is always paired with the vector potential **A** in the combination $\mathbf{A} + \nabla\phi$. Our free energy is obviously gauge invariant. This is a much simpler approach than that of Doria *et al.*

Secondly, Doria *et al.* fixed the magnitude of the magnetic induction **B** instead of the external magnetic field **H**, which means they have already assumed that a certain, finite amount of magnetic flux has penetrated through the superconducting sample (since the flux is quantized, this means they keep the number of flux lines constant). Therefore they have forced the solution to have the right amount of flux penetration for the triangular lattice solution - again an artificial assumption. In practice one cannot do that - it is very difficult or impossible to control the internal magnetic field **h** (the magnetic induction $\mathbf{B} = \langle \mathbf{h} \rangle$). Instead of following their idea, we fixed the external magnetic field **H**, which is in practice easier to control than the magnetic induction **B**. This is why we use the Gibbs free energy instead of the Helmholtz free energy. Thirdly, they choose a fixed lattice dimension from the Abrikosov theory, as mentioned before in chapter V. If the magnetic induction **B** and the Ginzburg-Landau parameter κ are known, by this theory the lattice constant can be determined. (their simulations took place when the external magnetic field H was very close to the upper limit H_{c2}, so that the analytic solution is known). Finally, one more assumption which will guarantee that the Abrikosov lattice will surely be found is the periodic boundary condition, which is a strong constraint.

Lattice Equation

We have tried to derive the Abrikosov lattice solution without any *a priori* assumptions except the Ginzburg-Landau free energy. As in the previous chapter for the type I superconductors, we start with the Ginzburg-Landau function in two dimensions for the difference between the Gibbs free energy density for the normal and superconducting states in reduced units

$$G = \frac{1}{V}\int d^3x\Big[- \Psi^2(x,y) + 0.5\Psi^4(x,y) + Q^2(x,y)\Psi^2(x,y) + \big(\nabla\Psi(x,y)\big)^2 + \kappa^2\big(\nabla\times\mathbf{Q}(x,y) - H\big)^2\Big] \qquad (7.9)$$

Discretizing eq. (7.9), we get

$$G = \frac{1}{L_x L_y}\sum_{\substack{\text{Points}\\ij}}\left[- \Psi_{ij}^2 + 0.5\Psi_{ij}^4 + \left(\frac{Q_x^{right} + Q_x^{left}}{2}\right)^2\Psi_{ij}^2 + \left(\frac{Q_y^{up} + Q_y^{down}}{2}\right)^2\Psi_{ij}^2\right]$$

$$+ \sum_{\substack{\text{Vertical}\\ \text{bonds}}}\left[\left(\frac{\Psi^{up} - \Psi^{down}}{\Delta x}\right)^2\right] + \sum_{\substack{\text{Horizontal}\\ \text{bonds}}}\left[\left(\frac{\Psi^{right} - \Psi^{left}}{\Delta y}\right)^2\right]$$

$$+ \sum_{\text{Boxes}}\left[\left\{\left(\frac{Q_y^{right} - Q_y^{left}}{\Delta x}\right) - \left(\frac{Q_x^{up} - Q_x^{down}}{\Delta y}\right)\right\} - H_{ext}\right]^2 \qquad (7.10)$$

where from fig. (7.1) we can see that the order parameter Ψ, which is a real quantity (as we mentioned in the previous section), is defined at points on a grid. Q_x and Q_y are the x and y components of the supervelocity respectively, and are defined on "bonds" between lattice points. The subscripts i and j denote the dummy indices along the x and y axes. L_x and L_y are the dimensions of the superconductor in the x and y directions.

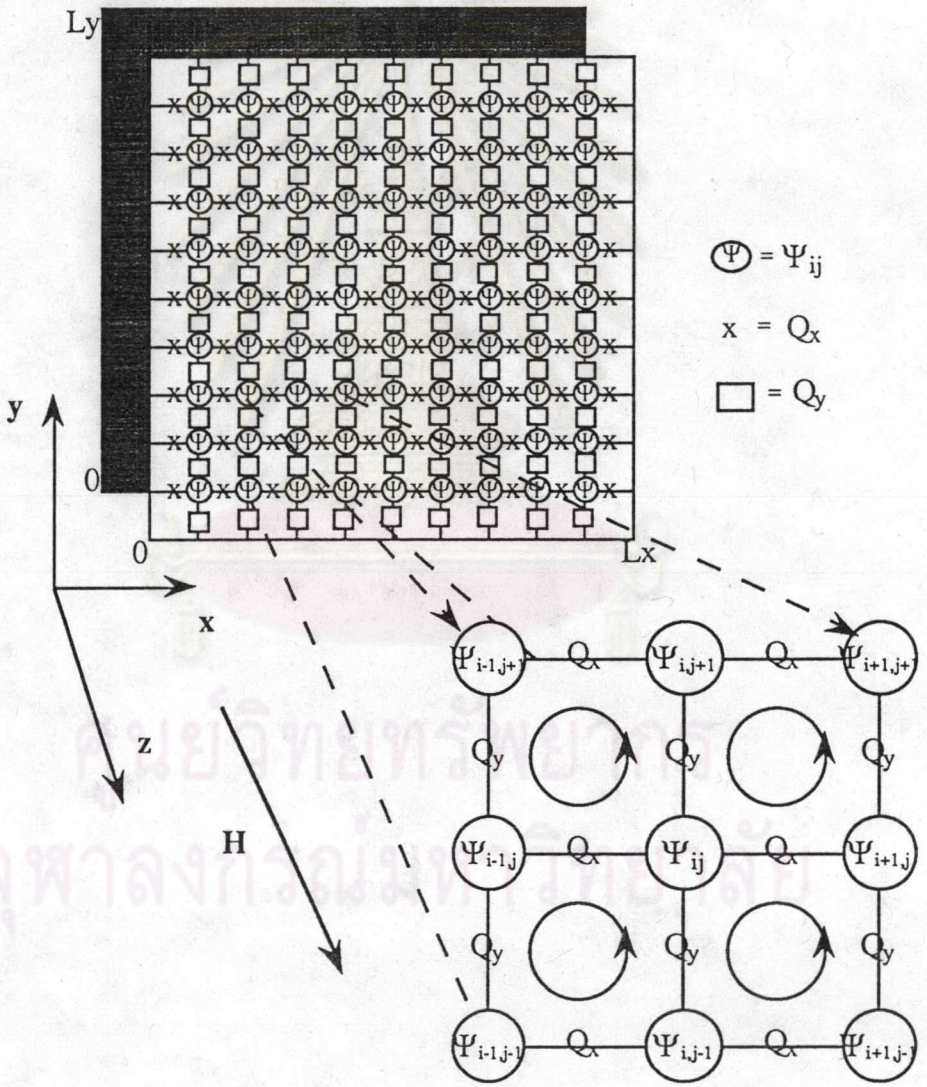

Fig. 7.1 Discretization of a two-dimensional superconducting sample dimension L_x by L_y.

We assumed that the external magnetic field lies in the z direction as shown in fig. (7.1). On each lattice point the order parameter has the value Ψ_{ij}. In each "box" defined with corners on grid points, the x and y components of the supervelocity for the $\nabla\times\mathbf{Q}$ term are Q_x^{up}, Q_x^{down}, Q_y^{left} and Q_y^{right}. We evaluate $\nabla\times\mathbf{Q}$ as a sum around a box of $\mathbf{Q}$ on the surrounding bonds circulating to the right, up, left, and down. As we mentioned earlier, our discretization of the curl is gauge invariant.

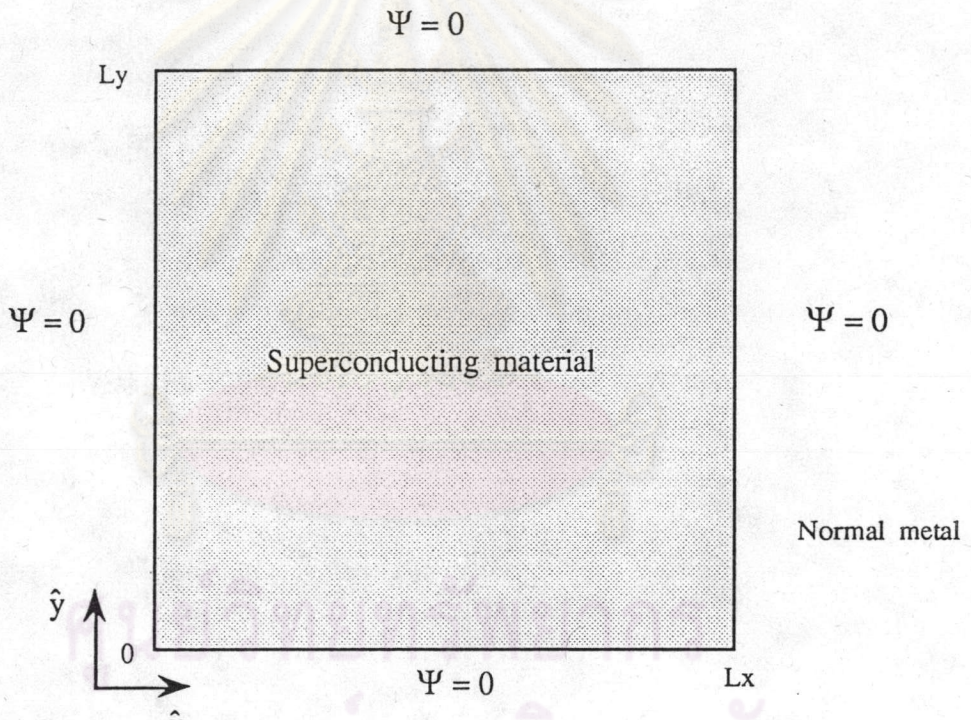

Fig. 7.2 Boundary conditions used to simulate a type II super conductor. The superconducting sample is surrounded by the normal metal. We keep the order parameter equal to zero at the boundary.

However, we separated the $Q^2\Psi^2$ term into two parts $\left(\frac{Q_x^{right} + Q_x^{left}}{2}\right)^2\Psi^2$ and $\left(\frac{Q_y^{up} + Q_y^{down}}{2}\right)^2\Psi^2$, where Q_x^{right}, Q_x^{left}, Q_y^{up}, and Q_y^{down} are the values of the supervelocity with respect to the order parameter Ψ_{ij}, that is, up, down , left and right denote the bonds next to the location of Ψ_{ij} .

Our boundary condition in these simulations is:

$$\Psi(0,y) = \Psi(L_x,y) = \Psi(x,0) = \Psi(x,L_y) = 0 \qquad (7.11)$$

We expect Ψ to be rather small everywhere especially for H close to H_{c2}. In consequence we feel that this boundary condition is the most appropriate. That is, we keep the superconducting sample surrounded by the normal metal as shown in fig 7.2. The supervelocity in the normal metal is unconstrained : it is assumed to be such that $\nabla\times\mathbf{Q} = \mathbf{H}$, so as to make the magnetic free energy term zero in the normal metal, indicating that the magnetic field fully penetrates.

The Simulated Annealing Technique

As we shall see, our problem can be expressed as that of finding the global minimum, or a local minimum which is almost as good as the true global minimum, of a function f(x) of N variables, $x = (x_1,x_2,x_3,...x_N)$. The function f(x) possibly has many extraneous local minima. Conventional optimization methods, such as the *downhill simplex method* (Press *et al.*, 1986), the *conjugate gradient method* (Press *et al.*, 1986), etc., are ineffective here, because they tend to converge to whichever local minimum they first encounter.

Simulated annealing (Kirkpatrick *et al.*, 1983, Press *et al.*, 1986, Press *et al.*, 1991, Silverman and Adler, 1992) is a stochastic, optimization technique for functions of many variables. The principle of the method of simulated annealing is an analogy with thermodynamics, especially with the way that liquids freeze and crystallize, or metals cool and anneal. At high temperatures, the molecules of a liquid move freely with respect to one another. If the liquid is cooled slowly, thermal mobility is gradually lost. The atoms are often able to line themselves up and form a crystal which is the state of minimum energy for this system. The amazing fact is that, for slowly cooled systems, nature is able to find this minimum energy state. In fact, if a liquid metal is cooled quickly or *quenched*, it does not reach that state, but rather ends up in a polycrystalline , amorphous , or glassy state (Ruffolo and Boolchand, 1985) having a somewhat higher energy.

So the essence of the process is slow cooling, allowing ample time for redistribution of the atoms as they lose mobility. This is the technical definition of annealing, and it is essential for ensuring that a low energy state will be achieved.

For a clear understanding, let us compare annealing and quenching as methods for reaching the global minimum of f(x) see fig 7.3.

If we start the system at point A at a high temperature, then a rapid quenching would lead the system directly to the nearest valley or local minimum L with no way to escape to the global minimum G. An annealing algorithm probably would lead, via a path such as ABCDG or perhaps ABLCDG, to the global minimum G (Silverman and Adler, 1992).

The heart of this method is implemented by the Metropolis procedure (Metropolis *et al.*, 1953), for which the source code is listed in appendix B. This algorithm will give a verdict on whether to accept that state or not if the latest free energy is less than the previous one, the algorithm will tell the program to accept that state. If the latest free energy value is higher, there is still a probability to accept that state by the relation

$$p = e^{-(\Delta E)/kT} \tag{7.12}$$

where p is the probability, k is the *Boltzmann constant*, T is a fictitious temperature. This is so called the *Boltzmann probability distribution*. In practice, k is set to 1, so the temperature has units of energy.

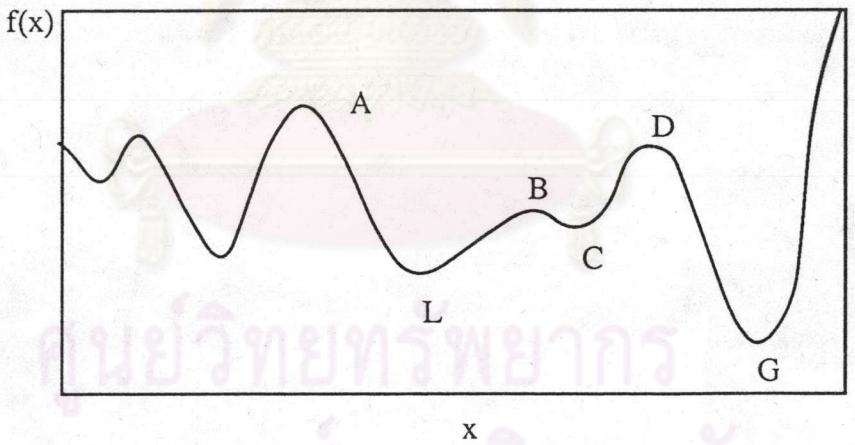

Fig. 7.3 Schematic plot of a function, f(x), that has several local minima and one global minimum (marked by G). The parameter x represents different configurations of moving variables in the system.

We can see that a higher temperature gives us a higher probability to accept the higher state, which means there is an opportunity to skip out of the metastable state to another state. However, when the temperature is very low it is difficult or impossible to jump out of a valley for the duration of the program. Whether the global minimum is attained or not depends on the last valley it was trapped in when the temperature was very low, so it is very important to reduce the temperature of the state slowly. Therefore, in practice it is important to find an appropriate temperature schedule for our program - this is usually determined by experimentation.

Results and Conclusion

Our program was designed to study the behavior of the whole parameter set which comprised the Gibbs free energy function (eq. 7.9), such as the order parameter Ψ at a given external magnetic field **H**, and each value of the Ginzburg-Landau parameter κ, the characteristics of the supervelocity **Q**, and the arrangement of the flux lines (we expect the Abrikosov lattice). So, all of our simulation was done in the regime where we expect the so-called *mixed state*, which is an interesting state. This would be the first step to lead us to an understanding of the dynamics of the flux lines (such as flux line motion, pinning, melting , etc.) in a more complicate system.

In our simulations we found a negative free energy : as we mentioned in the chapter V, this means that a mixed state was found. We chose the dimension of the superconducting sample equal to 10 by 10 in coherence length units, the Ginzburg-Landau parameter $\kappa = 3.0$, the external magnetic field $H = 0.5$ and we chose $N = 9$ (so we have 10 by 10 strips) from fig 7.1. We will see that now we have 261 moving variables in our simulation. While either accepting or rejecting the latest state, the count was kept until it reached ten times the numbers of variables (2610) and the

fictitious temperature was then decreased with a rate equal to 25% (we got this from experiment) from the starting temperature 10.0. The program stops when the temperature has reached the lowest limit 0.0001.

Although we got the mixed state (the free energy density was negative), we have no adequate detail about the order parameter, the supervelocity, and the internal magnetic field because having only 10 by 10 strips in a 10 by 10 sample is very crude. The boundary effect will decrease the observing area to a depth approximately equal to the Ginzburg-Landau parameter κ (remember that $\kappa = \lambda/\xi$) at each side. However from chapter V we have

$$\ell^2 = \frac{2\pi}{Hb_2} \qquad (7.13)$$

where ℓ is the lattice constant and, b_2 for triangular lattice is equal to $\sqrt{3}/2$. We consider two cases

a). When the external magnetic field H is very close to H_{c2} ($H_{c2} = 1$). From eq. (7.13) the lattice constant ℓ for this case is equal to 2.68 (in units of the coherence length, ξ). This case was considered by Doria *et al.*, 1990 (they chose H = 0.96).

b). When the external magnetic field H is less than H_{c2}, the lattice constant ℓ gets bigger. In our first simulation we chose H = 0.5, so we have only a 4 by 4 effective sample size which is insufficient.

Inevitably, we must increase the sample size to at least 20 by 20 and we need 100 by 100 strips (5 strips per unit of length, that is N = 99), so we have 29601 moving variables ! However, the computer time to perform the simulation for the

previous case ; 10 by 10 sample, and only 261 variables, was at least a half an hour on a Nixdorf mini-computer. Many days or weeks for 20 by 20 samples with , 100 by 100 strips would be needed for one simulation. As we mentioned in the previous section, we don't know the temperature schedule before some experiments have been performed and we must try many times for this purpose, so a fast computer system such as a *supercomputer* may be necessary.

We know the free energy of the *Meissner state* is positive for $\kappa > 1/\sqrt{2}$ (fig. 7.4), and equal to zero in the *normal state*. However, for the *Mixed state* there are several possible negative energy levels which are very close together when the external magnetic field H is close to H_{c2} and more separated for lower values of the external magnetic field H ($H < H_{c2}$). This is one of the very important reasons why we consider using the simulated annealing method.

Although, we failed to simulate the type II superconductors by the simulated annealing technique, we have learned more about this method which has nowadays become a popular optimization method for minimizing multiparameter functions.

For practical purposes, simulated annealing has effectively solved the famous traveling salesman problem (Kirkpatrick *et al.*, 1983) of finding the shortest cyclic itinerary for a traveling salesman who must visit each of N cites in turn. The method has also been used successfully for designing complex integrated circuits. Some hundreds of thousands of circuit elements on a silicon substrate can be permuted and assigned to locations that minimize the amount of wire required to connect the transistors on a microchip (Vecchi *et al.*, 1983).

In future we will try to solve this problem again with a bigger computer system.

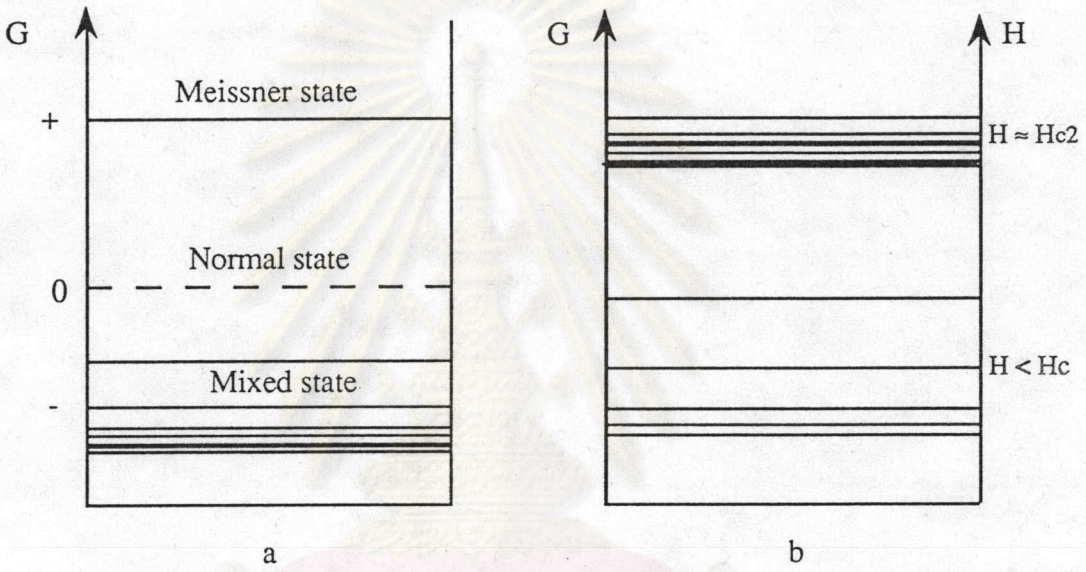

Fig. 7.4 a) Schematic of the free energies of various states of a type II superconductor. The free energy of the Meissner state is positive, that of the normal state is zero, and there are several negative values for mixed states. b) The possible energy levels for mixed states are very close to zero when $H \approx H_{c2}$ and more separated and more negative when $H < H_{c2}$.

CONCLUDING REMARKS

The rapid advances in computer technology have ensured that microcomputers of sufficient power are now available to the general public at modest cost. Modern computers range from the relatively cheap, but powerful, single-user workstations to the extremely fast and expensive supercomputers.

Some problems in statistical mechanics are exactly soluble. By this, we mean that a complete specification of the microscopic properties of a system leads directly, and perhaps easily, to a set of interesting results or macroscopic properties (such as an equation of state $PV = Nk_BT$). There are only a handful of non-trivial, exactly soluble problems in statistical mechanics; the two-dimesional Ising model is a famous example (Baxter, 1982).

Some physical problems, while not being exactly soluble, succumb readily to analysis based on a straightforward approximation scheme. Computers may have an important role to play in such work. A great task is (to begin) constructing an approximate theory in a reasonable way. The more difficult and interesting the problem, the more desirable it becomes to have some exact results available for special cases, both to test existing approximation methods and to point the way towards new approaches. It is also important to be able to do this without necessarily introducing the additional question of how closely a particular model (which may be very idealized) mimics a real physical system, although this may also be a matter of interest.

Computer simulations have a valuable role to play in providing essential results for problems in physics which would otherwise only be soluble by approximate methods. In this sense, compter simulation is a test of theories and, historically,

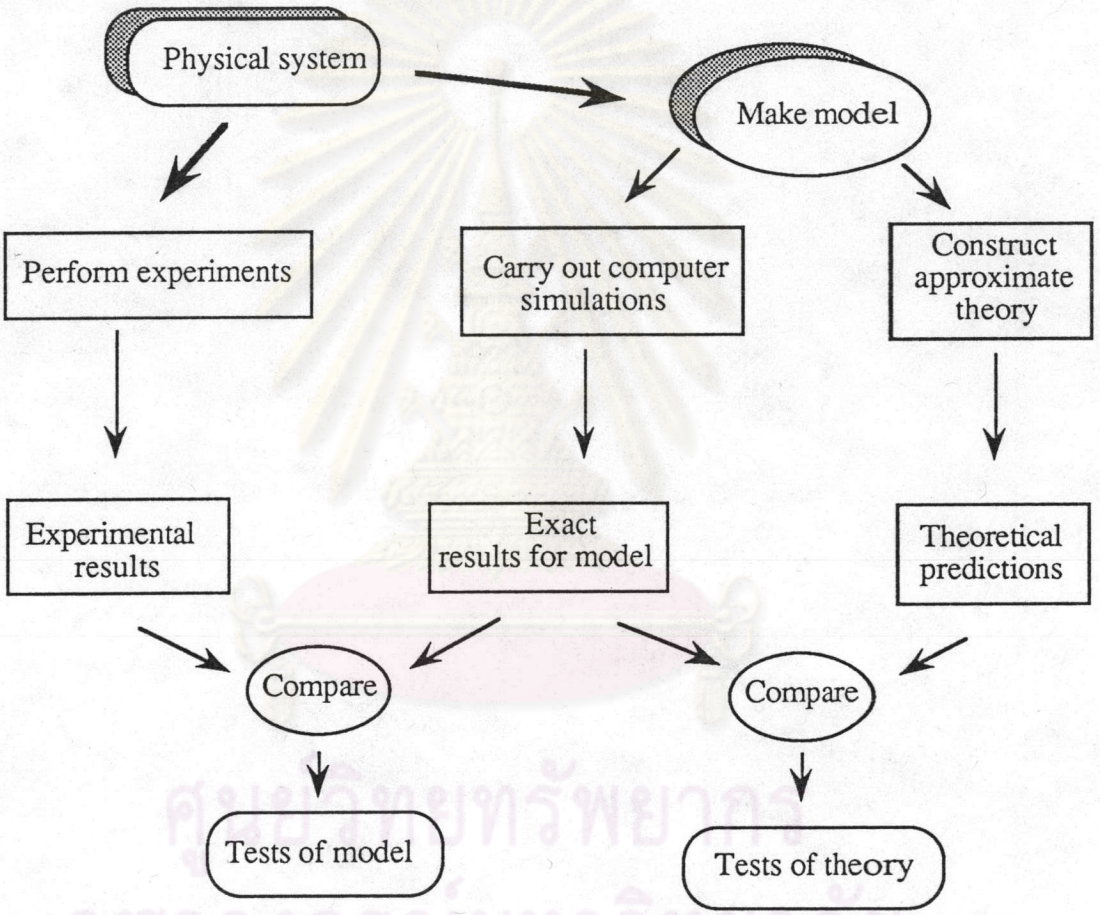

Fig. 1 The connection between experiment, theory, and computer simulation (modified from Allen and Tildesley,1987).

simulations have indeed discriminated between well-founded approaches and ideas that are plausible but, in the event, less successful. The results of computer simulations

may also be compared with those of real experiments (the schematic diagram is shown in fig. 1).

The principle of this thesis according to a fundamental rule of physics is that *physical systems seek their lowest possible free energy state.* An example is directly (numerically) minimizing the Gibbs free energy of a superconducting sample, for a given Ginzburg-Landau parameter κ, size, and external applied magnetic field. At the lowest possible energy state, the behavior of the order parameter Ψ, the supervelocity **Q**, and the internal magnetic field **h** are revealed. As we mentioned in chapter VI, the problem of the type I superconductor (1 dimension) is not so complicated as the type II superconductors (chapter VII). The agreement is excellent except for a very thin sample (there is defect in the Ginzburg-Landau theory, that is that the gradient of the order parameter at the superconductor-normal boundary should be zero). Computer simulations for the type II superconductors are more complicated and difficult. There are several local minima of the energy state levels with a tiny difference. This will cause a lot of great trouble in seeking a proper global minimum.

We hope that this thesis will be useful to students , research workers and to teachers and lecturers who want to use the computer to illustrate the way superconductors behave, on a macroscopic scale, by using the Ginzburg-Landau theory.