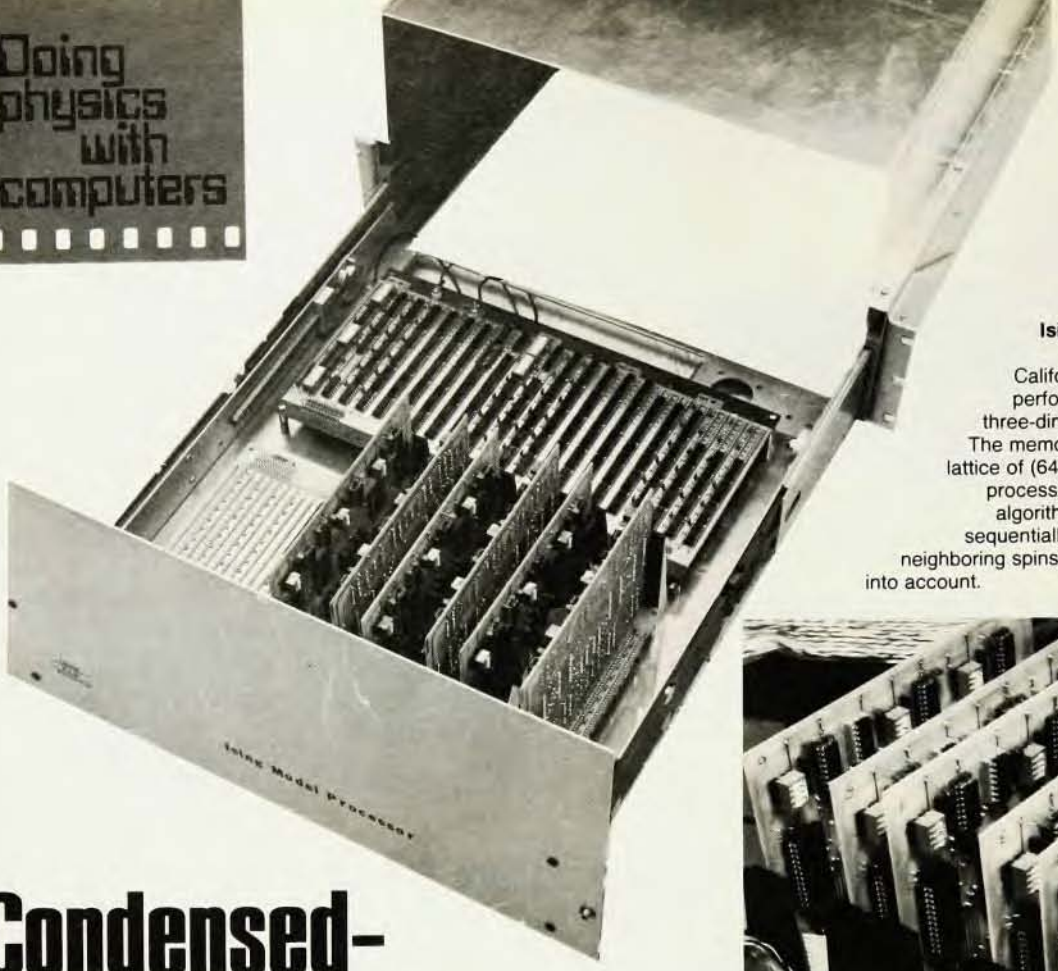
Doing physics with computers



Ising-model processor at the University of California at Santa Barbara performs simulations of the three-dimensional Ising model. The memory can hold data for a lattice of $(64)^3$ spins, and a special processor uses a Monte Carlo algorithm to update the spins sequentially, taking the values of neighboring spins and the temperatures into account. Figure 1

Condensed-matter physics

Experimenters use computers to control experiments and to gather and analyze data; theorists use them for detailed predictions based on realistic models and for studies on systems not realizable in practice.

Jorge E. Hirsch and Douglas J. Scalapino

Computers are playing an integral role in both experimental and theoretical condensed-matter physics: In laboratories they are being used to control experiments as well as to gather and analyze data; in theoretical studies they provide the means for making detailed predictions for realistic models, for exploring systems that cannot be realized in the laboratory, such as four-dimensional systems undergoing phase transitions or materials under extreme conditions of pressure or temperature, and for complicated symbolic manipulations. Often computers provide an essential link between experiment and theory, allowing experimentalists to test critically theoretical predictions and allowing theorists to make predictions for realistic models.

Because computers allow both experimentalists and theorists to explore physical systems in a manner not previously possible, there is an increasing need for a clear understanding of the physics to sort out what is relevant from the mass of irrelevant information that can easily be generated. Here the computer itself can be a valuable tool. Experimentalists can analyze and display their data in many ways, developing a feeling for the problem. Theorists can simulate model systems to see if they exhibit the essential qualitative features of the real system and can test the limits of various analytic approximations, sometimes using special-purpose machines such as that shown in figure 1.

Beyond this, the computer gives the experimentalist an extended working day, gathering data around the clock. By changing the software one can redesign an experiment and quickly explore a new idea. The theorist can study realistic models and compare them with experiment. One can also explore the system under extreme conditions of temperature, density or pressure, for example, which cannot be achieved in the laboratory. One can also study model systems in unphysical limits of dimensionality or coupling strength to gain insight into their basic structure.

In the following we will illustrate some of the ways computers are being used in condensed-matter physics and

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will conclude with some comments about the future.

Experimental work

Condensed-matter experimentalists are using computers in a variety of ways: to control experiments, to gather data and to analyze data.

Experiment control. Computers, for example, now perform the complex timing, ramping and trimming operations necessary to run synchrotron storage rings for the production of uv or x-rays, they control linear accelerators, used to produce pulsed beams of neutrons by spallation reactions, and they drive free-electron lasers. In x-ray diffraction experiments, computer-controlled stepping motors reproducibly set the configuration of a triple axis spectrometer to a given scattering configuration; the computer then controls the collection of data and automatically steps the motors to the next programmed scattering angle. While large-scale systems have operated under this kind of computer control for some time, it has spread during the past five years to all levels of condensed-matter experimental work. For example, in one laboratory a hundred measurements of the electrical resistance and thermopower of an organic conductor at each of fifty preselected temperatures are carried out overnight. In a parallel experiment, the relative changes in the optical spectrum of a polymer are measured by a computer-controlled spectrophotometer while the sample is being electrochemically doped to various prescribed levels; the results are recorded, stored on disc, and displayed on a monitor. Both of these experiments were run by the same computer and various analog-to-digital converters, all mounted on a portable rack, which was moved from one experimental setup to the other; only the software and some of the connections were changed in the move.

Because the experimenter can change a measurement by changing software, computer control allows one to run experiments that simply could not be satisfactorily carried out by hand. One example of this is work on fluid flow, where the large numbers of states the system can take on at some Reynolds numbers makes the state of the system depend upon the details of how a particular flow rate was reached. Computer control of a given time sequence of Reynolds numbers provides the means for reproducibly reaching a given final state repeatedly.

Data collection. The large capacity of computers for gathering and analyzing data is also making important changes in the types of measurements that can be made. A measurement at a given temperature, such as the transport-property measurement mentioned previously, can be repeated 100 or 1000 times to obtain good statistics; while such measurements could in principle be done by hand 100 times at each temperature, a human operator would require strong motivation to undertake such a project. Just because something can be done with computer control does not necessarily make it worthwhile. If, however, there is some reason to suspect from previous rougher measurements or theoretical suggestions that the system is undergoing a phase change in a certain temperature region, one can simply program a careful scan through this region, taking sufficient data to resolve what is happening.

In infrared Fourier-transform spectroscopy, interferograms containing as many as 5×10^5 data points are generated in a few seconds. Switching back and forth between a reference sample to obtain a difference spectrum allows one to remove source or detector drifts while building up hundreds of spectra, which can then be averaged. Naturally, the computer can also contain various calibration data to normalize the final transmission or reflectivity output.

One example[1] of the elegant representation of data that computers can provide is shown in figure 2, which is a correlated plot of bromide-ion concentrations in the course of a complex chemical reaction called the Belousov–Zhabotinskii reaction. The reaction takes place in a stirred vessel, with reactants flowing in at a constant rate and products and reactants flowing out at the same rate. The reaction can exhibit a variety of different kinds of behavior because of the nonlinearity of the coupled reactions. The concentrations can settle down to a steady state, they can oscillate in a regular fashion or they can vary chaotically. In this experiment a computer recorded data for 16 384 time points and computed power spectra of the bromide-ion concentration as well as the phase portrait shown in figure 2, where bromide-ion concentration at times t_i, is plotted against the concentration at $t_i + T$, a fixed time later. An analysis of this phase portrait showed that the nonperiodic regimes correspond to deterministic chaos and not to stochastic noise arising from fluctuations in the environment. Work is now in progress using sets of 32 000 data points to determine how rapidly initially neighboring points separate in time, and thus to describe the sensitivity to initial conditions characteristic of the chaotic regime.

Data analysis. The example of the computation of the power spectra and phase portraits for the Belusov–Zhabotinskii reaction shows the use of computers for data analysis. The analysis is often done by the same computer that controls the experiment, providing an online capability that is very useful in determining what is to be done next and in helping one develop an intuitive feeling for the measurement. In other cases, the data are sent to a large mainframe for analysis. For example, x-ray crystallographic problems may involve nonlinear least-squares adjustments of a few hundred structural parameters on data from several thousand reflections. In the case of experiments involving inelastic neutron scattering, quantitative interpretation of the data generally requires convoluting trial cross sections with the known instrumental resolutions to obtain the dynamic structure factor $S(q,\omega)$; such four-dimensional numerical integrations are relatively time-consuming and account for the bulk of the computer use for inelastic-scattering studies.

The nonlinear least-squares fitting procedure, mentioned in connection with x-ray crystallography, can be used in many contexts to make detailed comparisons of data and theory and to find the significance of any differences. Such comparisons are one kind of example of calculations in which computers are an invaluable aid in comparing theory with experimental results.

Electronic structure

Computers play a central role in calculations of the electronic structure of real materials. In these calculations one assumes a given location for the nuclei and then develops an effective one-electron description for the electrons. A key feature of recent calculations is the achievement of self-consistent solutions such that the potential used in the effective one-electron Hamiltonian is consistent with the ground state computed by diagonalizing it. The interaction between electrons and ions can be treated in various ways. One approach is to compute the eigenvalues of all valence and core electrons; another is to simulate the interaction between the valence electrons and the ion cores by a pseudopotential and compute only the states of valence electrons. (See "The pseudopotential panacea" by Marvin Cohen, PHYSICS TODAY, July 1979, page 40.) Originally the Fourier transform of the pseudopotential was constructed by fitting optical or photoemission data, but recently theorists have found procedures for extracting pseudopotentials from *ab initio* atomic calculations. The effects of electron–electron interactions is expressed as a functional of the electron density. Although the exact form of the density functional is not known, various local-density functionals have yielded excellent results for a variety of ground-state properties.

Mingtang Yin and Cohen have used[2] the *ab initio* pseudopotential approach

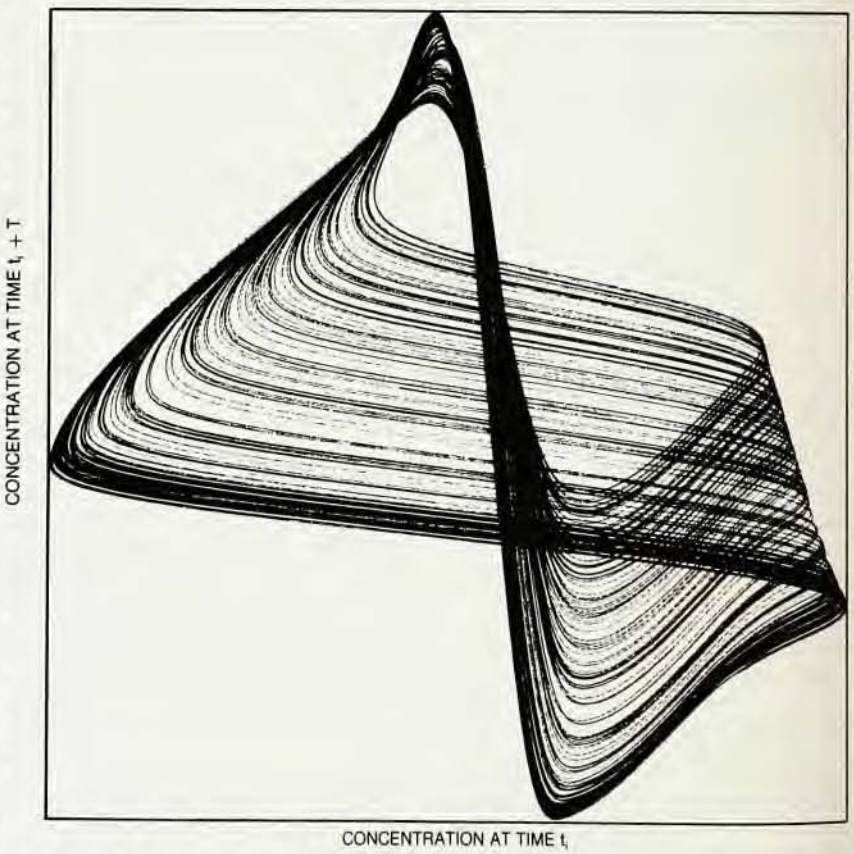
to calculate the cohesive energy, lattice spacings and bulk modulus of Si, Ge and C; the table on page 51 compares their results with experimental values. In these calculations the basic input was the crystal structure and the atomic number to generate the pseudopotentials. Similar calculations have been carried out for most of the III–V semiconductors. By starting with a specific lattice, one can also study the crystal structure as a function of volume (see the article by Michael Schlüter and Lu Jeu Sham, PHYSICS TODAY, February 1982, page 36). In such a calculation for silicon, Yin and Cohen found that the diamond structure has the lowest energy at low pressures (large volumes per atom) while at smaller volumes (high pressure) the white tin structure has a lower energy than any other of six studied structures; these results agree with experiment. Several other groups have also used this approach and calculated phonon energies and higher order elastic constants by comparing total energies for the distorted and undistorted crystal structure. These calculations are usually in good agreement with experiment.

In an extensive set of calculations, Victor Moruzzi, J. F. Janak and Arthur Williams[3] at the IBM Watson lab used a local-density functional along with a calculational scheme called the Korringa–Kohn–Rostoker method to calculate properties of the first 50 elemental metals in the ground state, including the cohesive energy, the equilibrium lattice constants and the elastic bulk modulus. The agreement with experiment was generally within 10% or better. In similar first-principles studies on magnetic properties of metals, Moruzzi, Janak and Williams found that only Co, Ni and Fe should show a magnetic moment, in agreement with experiment.

These calculations for bulk properties of crystalline solids make use of the lattice periodicity to reduce the problem to the behavior of an electron in one unit cell. One constructs a Hamiltonian matrix for the unit cell, using a suitable set of basis functions such as plane waves, localized Gaussian orbitals or, in some cases, numerical radial functions plus plane waves. One then diagonalizes this Hamiltonian, and from the resulting ground-state wavefunction one can determine the charge density, and from the charge density one obtains the screening potential by solving Poisson's equation. Finally, this screened potential is added to the original ion potential and the exchange-correlation term from the local density functional to obtain a new effective one-electron potential. Then the entire procedure is iterated until the results converge.

The calculations for silicon used 100 plane-wave basis states per atom in the unit cell; thus for the diamond lattice with two silicon atoms per unit cell this leads to the construction and diagonalization of a 200×200 matrix while the hexagonal diamond lattice, with four atoms per unit cell, has a correspondingly larger matrix. The calculation of the screening charge is carried out in k-space with a fast Fourier transform routine. In iterating the ground state charge density and potential to self-consistency, one must take care to damp out the instabilities that can easily occur due to the long-range Coulomb forces. For example, to produce the results for silicon shown in the table, Yin and Cohen performed five iterations to reach self-consistency; the calculations required several minutes on a CDC7600. The calculations of the silicon structure required about three hours of running time.

Catalysis and the properties of d-band metallic surfaces and interfaces are currently of great interest. To compute local chemical properties, theorists have used linear combinations of Gaussian orbitals, chosen to approximate atomic wave functions with additional local functions for flexibility, as basis functions for both valence and core electrons. One uses roughly as many basis functions per atom as there are electrons per atom. To make use of the simplification allowed by periodic structures, one often considers a large slab of identical unit cells so that the dimension of the Hamiltonian matrix is given by the number of atoms per unit cell times the number of basis functions per atom. John R. Smith, J. G. Gay and Francis J. Arlinghaus at General Motors have recently reported[4] results for a nine-layer copper slab, oriented to have a (100) face. The calculations involved a basis containing several hundred linearly independent functions, and about 60 iterations were necessary to achieve self-consistency; a typical calculation took approximately an hour on an IBM 3033. (At a surface, the "sloshing" of electrons which occurs under iteration must be carefully controlled to obtain self-consistency.) This calculation demonstrated that over a third of the electrons in the surface layer are in surface states, and that these states primarily have d-type symmetry. Figure 3 shows the surface-state charge distribution for the higher-lying surface states. Photoemission difference spectra between a clean Cu(100) surface and surfaces with fractional mono-



Phase portrait of bromide-ion concentrations in a Belousov-Zhabotinskii reaction corresponds to a pair of measurements of the concentration separated by a time T of 53 sec. The system ultimately occupies points throughout the "strange attractor" shown here. Figure 2

layers of N, O and S reveal surface states and support this picture. One can use such a comparison between theory and experiment to determine atomic surface geometries quantitatively. Similar studies have been undertaken for many other metal and semiconductor surfaces.

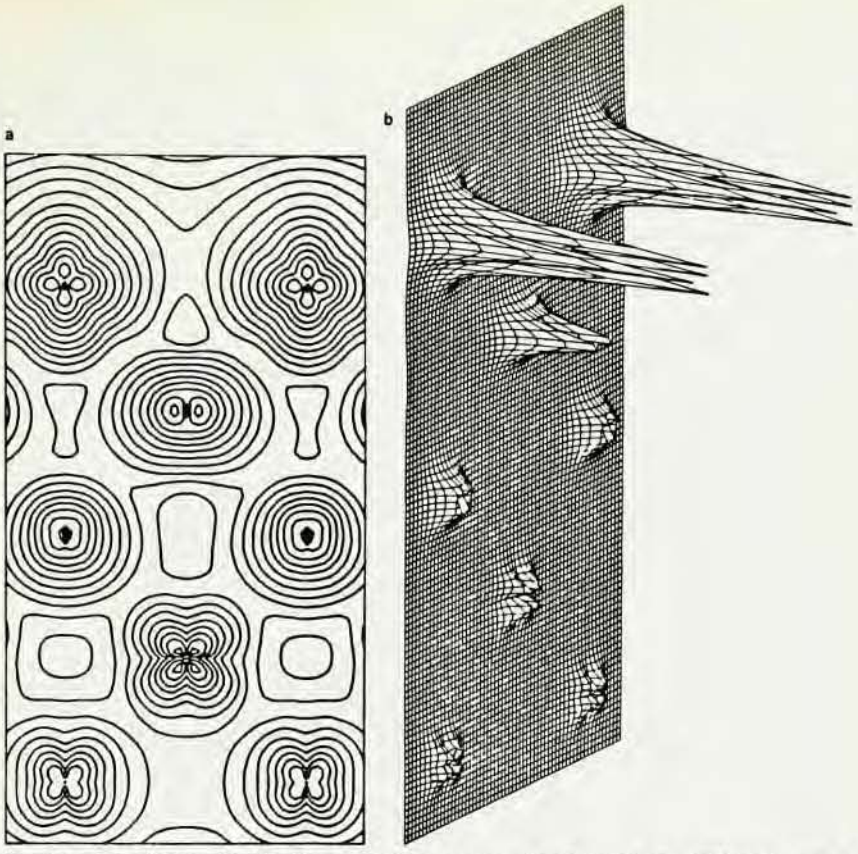
Further reductions in the symmetry increases the computational problem. Thus the study of individual chemisorbed molecules and atoms or various local bulk defects requires a significantly larger computational effort, typically a factor of ten more than the surface problem. It is here that new, more powerful machines as well as further improvements on algorithms will be needed. One must, of course, also look for further conceptual simplifications of the physics, which, as in the past, remain the key for continued progress.

Statistical mechanics

It is surely in statistical mechanics that the largest number of computer hours have been spent using numerical simulation techniques such as molecular dynamics methods or Monte Carlo techniques.

In molecular-dynamics simulations, one follows the time evolution of a system by numerically integrating the classical equations of motion governing the behavior of the particles. The time average of a property of a system in equilibrium is an approximation to the thermodynamic ensemble average of that property. In a typical calculation, say on liquid argon, the time step corresponds to a time of the order of 10^{-14} sec, and the integration extends over several thousand time steps. This is a short time period in macroscopic terms, but long enough for many collisions to occur, yielding the data required to calculate thermodynamic properties and correlation functions. This method also allows one to study dynamic properties as well as nonequilibrium behavior.

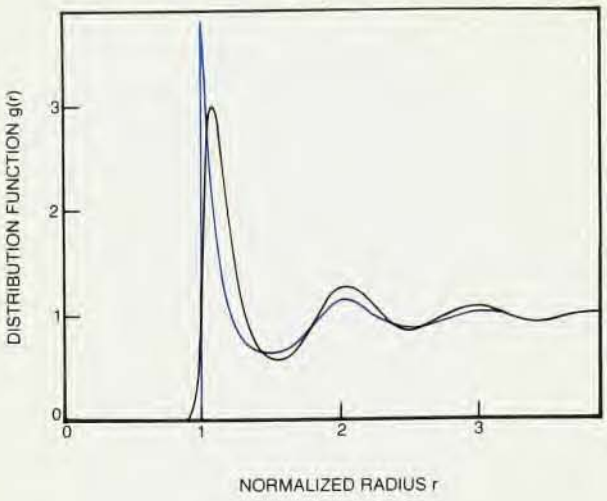
The Monte Carlo method is used in statistical mechanics to compute the multi-dimensional integrals over phase space which arise in performing ensemble averages in statistical mechanics. A brute-force numerical integration over all configurations is clearly impossible. However, to obtain a meaningful estimate it is sufficient to sum over a limited number of configurations, provided they are distributed in the same way as the full ensemble. This approach, known as "importance sampling," makes Monte Carlo simulations of many-particle systems possible. The first algorithm for carrying out such calculations was developed[5] by Nicholas Metropolis, A. Rosenbluth, Marshall Rosenbluth, A. H. Teller and Edward Teller. Their algorithm generates a sequence of configurations whose distribution tends toward an equilibrium ensemble as follows: From a given configuration, a new configuration is selected at random by changing one or more degrees of freedom, and the change in energy ΔE of the system is evaluated; the new configuration is kept if $e^{-\Delta E/kT}$ is greater than a random number r, uniformly distributed between 0 and 1.



Surface-state charge density for a nine-layer copper slab aligned in the (100) direction: **a** charge contours, with successive contours increasing by a factor of 2; **b** the corresponding amplitudes. The surface of the slab is at the top of the figure. Only those states with energies above -6.5 eV are included. (From reference 4.) Figure 3

The importance of numerical simulations in statistical physics resides in the fact that they provide a nonperturbative approach to the solution of model systems. Applied to complex systems, they can provide a useful bridge between analytic theories and experiments on real systems. Often, in comparing theory with experiment, it is difficult to identify whether disagreements are due to the approximations used in solving the theory or to basic inadequacies of the model Hamiltonian being studied. Using simulations, one can examine whether a particular model contains the essential qualitative features of the real system. Furthermore, by comparing numerical simulations with theory, one can check the validity of various approximations made in the theory. There are, of course, limitations on numerical simulation methods: an important one is the size of the system being studied. Because of limitations on both memory and computer time, one can typically consider systems of only 10^3 to 10^6 degrees of freedom, which are far from the size of real thermodynamic systems. This can be a severe limitation in systems that undergo phase transitions. Fortunately, various sophisticated techniques have been developed to allow extrapolation to infinite systems of results for finite systems. Another limitation can be slow convergence in systems that have long-lived metastable states. Despite these limitations, numerical simulation methods together with high-speed computers represent a very important tool for the advance of our understanding of physics in classical statistical mechanics problems.

There is a vast literature[7] of applications of molecular-dynamics simulations and Monte Carlo methods in classical statistical mechanics, and we can only select examples here which illustrate some of the points mentioned. One example in which the nonperturbative nature of molecular dynamic simulations provided essential information for developing a theoretical framework has been in the study of classical liquids. Here simulations of a simple model, the "hard sphere" or "billiard ball" fluid, made clear the close similarity in structure between this simple model and a Lennard–Jones fluid, as figure 4 illus-



Radial distribution function $g(r)$ for a hard-sphere fluid (colored curve) compared with that for a Lennard–Jones fluid (black curve). (From reference 6.) Figure 4

trates. This in turn led to the development of quantitatively successful theories[6] in which the attractive forces between molecules were treated as perturbations on the hard-sphere model. Before this development, no satisfactory starting point for a perturbation theory of liquids was known, because of the absence of simplifying features such as the low densities of gases or the regular periodic structure of solids.

For complex systems, simulations provide contact between theoretical models and experimental measurements. Figure 5 shows results of a Monte Carlo study[8] of the magnetic-ordering temperature of $Eu_xSr_{1-x}S$. To model this system, Karl Binder and his colleagues used a classical Heisenberg spin model, with a nearest-neighbor ferromagnetic exchange coupling and a next-nearest-neighbor antiferromagnetic exchange coupling of half the strength. The nonmagnetic Sr atoms were represented by dilution sites. The basic question was whether this model could explain the disappearance of ferromagnetic order at europium concentrations x less than 0.5, while the ferromagnetic bonds still "percolate" for x greater than about 0.2. The simulation results showed that the model does indeed account for the observed boundary of the ferromagnetic phase. No analytical methods exist for reliably calculating such phase boundaries.

As noted previously, in calculations of the critical behavior near a phase transition, the finite nature of the lattice must be taken into account. One useful approach is finite-size scaling: From simulations on lattices of varying sizes one extracts critical indices from the *size dependence* of various quantitites. Another powerful approach is the Monte Carlo renormalization-group method, which Robert Swendensen has recently developed:[7] One groups the degrees of freedom of a finite system into blocks and looks, using Monte Carlo techniques, at the correlations between effective degrees of freedom representative of each block; by comparing these correlations with those of the bare degrees of freedom, one is able to obtain accurate results for the critical exponents of an infinite system. This work illustrates how the combination of theoretical and numerical methods can give rise to powerful new techniques. Currently, a detailed study of a three-dimensional Ising model using the Monte Carlo Renormalization Group is being carried out in Edinburgh using DAP, a distributed array processor, built by combining 2^{12} individual microprocessors.

Besides numerical simulations, there are many other areas in statistical mechanics where the computer plays an essential role. One set of examples in which on-line interactive computing and convenient graphics have played an important role is the application of various real-space renormalization groups to the problem of adsorbed monolayers; a wide variety of beautiful work[10] has led to the computation of phase properties of realistic models. Another area of great current interest[11] is the behavior of mathematical mappings $x \rightarrow x'$, in which the variables x are discrete and the relation is nonlinear. These maps exhibit a rich variety of features such as bifurcations and chaotic behavior, and are thought to describe the essential physics of the transition from ordered to chaotic behavior in a variety of real systems. (See the article by Joseph Ford, PHYSICS TODAY, April, page 40.) By iterating these maps on the computer, one gains qualitative and quantitative insight into these features which are an important complement to theoretical analysis.

Quantum many-body systems

There are a number of ways in which the computer has become an essential tool in the theoretical study of quantum many-body systems. One approach is the exact numerical diagonalization of the Hamiltonian of a system with few degrees of freedom. By studying small systems of varying size, and using finite-size scaling, one can seek to extrapolate the results to the infinite-volume limit. As an example, the numerical results[12] obtained by Jill Bonner and Michael Fisher for finite Heisenberg–Ising chains are often used to interpret experimental results on magnetic properties of quasi-one-dimensional compounds. Typically, a 16-site spin-$\frac{1}{2}$ system can be easily diagonalized with present-day computer capabilities. However, because the computer time for such a diagonalization increases exponentially with the number of degrees of freedom, this approach is limited to low-dimensional systems with few degrees of freedom per site.

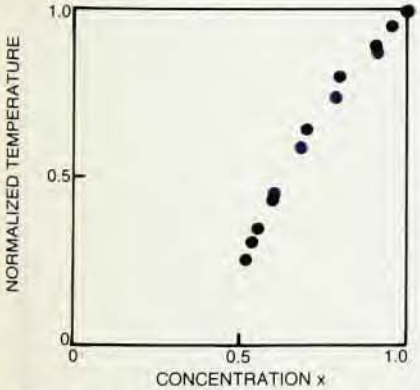
A second, very fruitful approach, is the numerical implementation of renormalization-group ideas, including degrees of freedom sequentially in the diagonalization of the Hamiltonian and discarding unimportant states at each step to keep the calculation within a manageable size. Kenneth Wilson's calculation[13] for the Kondo problem, where this method was first introduced, used 1000 basis states. The Kondo model, which describes the interaction of a magnetic impurity immersed in a nonmagnetic host, had defied an exact solution for many years. Wilson's solution, although approximate, was thought to be very accurate, and this was confirmed by the spectacular agreement between it and the recent exact solution[14] of the problem by Natan Andrei and John Lowenstein. Wilson's method has since been used to study a more general model for impurities in metals, the Anderson model, and for studies of disordered magnetic and electronic systems.

Finally, various stochastic methods are being used to study interacting many-body quantum systems. In a method introduced[15] by William McMillan in 1965, one uses a trial wave function of a simple form (usually including only two-body correlations) to construct a variational estimate of the ground-state energy and uses Monte Carlo methods to evaluate the multidimensional integrals. More recently, Robert M. Panoff and colleagues at Washington University, New York University and Cornell used this technique to predict[15] that spin-aligned deuterium is a self-bound liquid at zero

temperature and pressure.

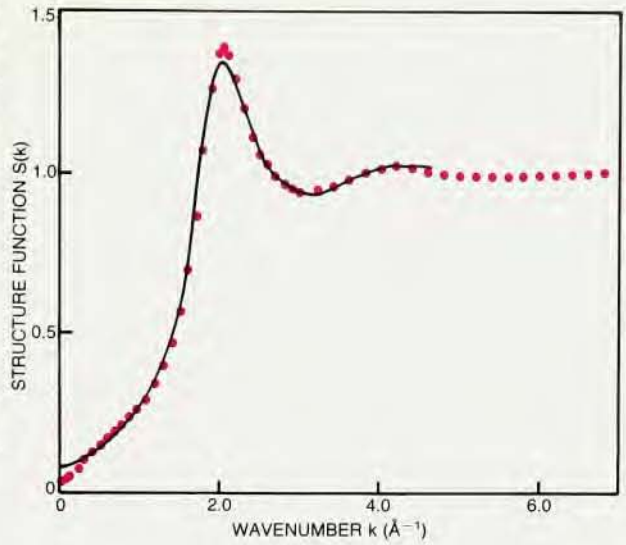
More elaborate Monte Carlo methods attempt to integrate numerically the Schrödinger equation. Malvin Kalos has developed[16] a procedure in which the successive convolutions of an initial state with Green's function projects out the ground-state component and eigenvalue of the initial state. The calculations are performed with a random-sampling algorithm guided by a suitable variational wave function. Essentially, the method evaluates stochastically the deviations of the exact solution from the variational trial function. Kalos and his colleagues have used[16] this method to simulate a model of 64 atoms of helium-4 interacting via a realistic potential; their results for the liquid structure factor are compared with neutron-scattering data in figure 6. Similar calculations for the equations of state for both liquid and crystalline He^4 yield excellent agreement with measured values.

The application of this method to fermion systems is difficult because the projection technique tends to drive the system towards a Bose ground state. An approximation that avoids this problem is to fix the nodal surface of the many-body wave function to be that of the trial state. Using this "fixed-node approximation," David Ceperly and Berni Alder have calculated[17] the equation of state of hydrogen shown in figure 7; their calculation started with only electrons, protons and Coulomb forces. Extensions of this scheme, in which the system is allowed to evolve freely from either the fixed-node or the variational solution, give "transient" estimates for fermion properties. For example, such a calculation[18] for the binding energy per atom of liquid helium-3 gives 2.2 kelvin, in quite good agreement with the experimental value of 2.5 K.



Magnetic-ordering temperature as a function of europium content of $Eu_xSr_{1-x}S$. The graph plots theoretical (color) and experimental values of T_c. The Monte Carlo calculations show that the Heisenberg model can account for the disappearance of magnetic order at all temperatures for x less than about $\frac{1}{2}$. (Reference 8.) Figure 5

Structure function $S(k)$ for liquid helium 4. The solid curve is the result of a Monte Carlo simulation for 64 atoms at the equilibrium density (reference 16). The circles are the smoothed values for $S(k)$ measured with neutron diffraction, at saturated vapor pressure and 1.0 K, by V. F. Sears, E. C. Svensson, A. D. B. Woods and P. Martel, Atomic Energy of Canada, Limited (Report No. AECL-6779). Figure 6



Recently both condensed-matter and high-energy theorists have used various path-integral formulations to map d-dimensional quantum-mechanical problems on a lattice onto $d+1$-dimensional classical problems. These formulations are directly applicable to finite temperatures. For one dimension we have developed[19] a formalism that allows for a direct simulation of systems with fermion and boson fields by following the fermion world lines. The resulting Monte Carlo algorithm is as fast as algorithms for classical systems in two dimensions. For more than one dimension all path-integral formulations known to date for systems with fermions involve performing a trace over configurations of quantities that change sign frequently. The resulting cancellations make a direct evaluation of the trace by Monte Carlo methods impossible. To avoid this problem, theorists have proposed various techniques based on analytically integrating out the fermion degrees of freedom at the outset. They are much more time consuming than corresponding Monte Carlo calculations on classical systems, because they involve computing the determinant or the inverse of a large matrix at each step of the updating procedure. Julius Kuti has recently suggested[20] a promising approach to this problem, based on random-walk methods to perform the stochastic inversion of a matrix.

The active investigation of quantum fields illustrates the fact that numerical simulation techniques, rather than being a fixed set of rules that are simply applied to larger problems as more powerful computers are developed, are themselves constantly evolving.

We conclude this section by discussing some recent work on one-dimensional quantum systems related to the study of various quasi-one-dimensional materials such as organic charge-transfer salts and conjugated polymer chains. We have recently to investigated[21] the instabilities of a one-dimensional electron gas as a function of the Coulomb interaction and band filling. As an example, figure 8 shows the wavevector-dependent polarizability for a quarter-filled "Hubbard model" in which the electrons interact with an on-site repulsive interaction. These calculations were done on chains of 20 sites, and typical runs involving 30 000 sweeps of the lattice took around an hour on a Vax 11/780. For the noninteracting case, the polarizability exhibits a peak at a wavevector twice the Fermi wavevector, p_F. In quasi-one-dimensional materials, this can give rise to a Peierls instability in which the lattice develops a distortion at twice the Fermi wavevector for temperatures below a critical value. As figure 8 shows, the instability at $2p_F$ is suppressed when the repulsive Coulomb potential is increased, and a new instability appears at $4p_F$. A systematic study of these instabilities as a function of interaction strength, temperature and band filling provides information about the underlying interactions in quasi-one-dimensional organic charge-transfer compounds; such compounds show temperature-dependent diffuse x-ray scattering peaks at $2p_F$ and $4p_F$. A related study[22] of the stability of the Peierls-distorted ground state with respect to quantum fluctuations of the phonon field found that in a quarter-filled band system with strong repulsive on-site interactions, quantum fluctuations give rise to a metallic ground state; this contradicts the results of mean-field theory, which predict a semiconducting Peierls-distorted ground state.

Various other stochastic methods exist or are currently being developed for the study of quantum many-body

systems. Together with an increase in the available computing power, it appears that many previously intractable problems will become amenable to detailed study in the near future.

Prospects

As we have tried to illustrate in this article, computers have become widely and deeply embedded in the fabric of condensed-matter physics as individual experimentalists and theorists have found ways to use them effectively to provide solutions and insight into physics problems.

In looking towards the near future, it is useful to understand what condensed-matter physicists want now. From conversations with our colleagues, we have learned that many condensed-matter experimentalists have access to machines that have the computational power to support their laboratory needs. Only one experimentalist we visited with spoke of the need for fundamentally more powerful computers. (He was carrying out a numerical simulation of a spinodal phase separation to compare with his experimental light-scattering data.) Even the experimentalists active in x-ray crystallography find the present mainframes adequate. Naturally this may change when the new synchrotron sources begin to produce time-resolved data on less symmetric structures, such as those involved in surface catalysis or biological materials.

Condensed-matter experimentalists noted that they were benefiting from the steady improvement in the speed and accuracy of electronics used as interfaces between computers and their equipment, such as analog-to-digital converters. For example, a 12-bit A/D converter gives a measurement precision of one part in 4096, while a 16-bit converter can measure to a part in 65 000. Condensed-matter experimenters would welcome further standardization, such as the present IEEE-bus requirements, so that instruments manufactured by all manufacturers are computer-compatible with each other. They would also like systems to have a common language or to accept readily programs written on another system. Like theorists, they look forward to the future possibility of having the power of a "supermini" in desk-top or small rack-mounted machines, with no air conditioning or special operator required. They are also interested in improved graphics and hard-copy units.

Structural properties of crystals

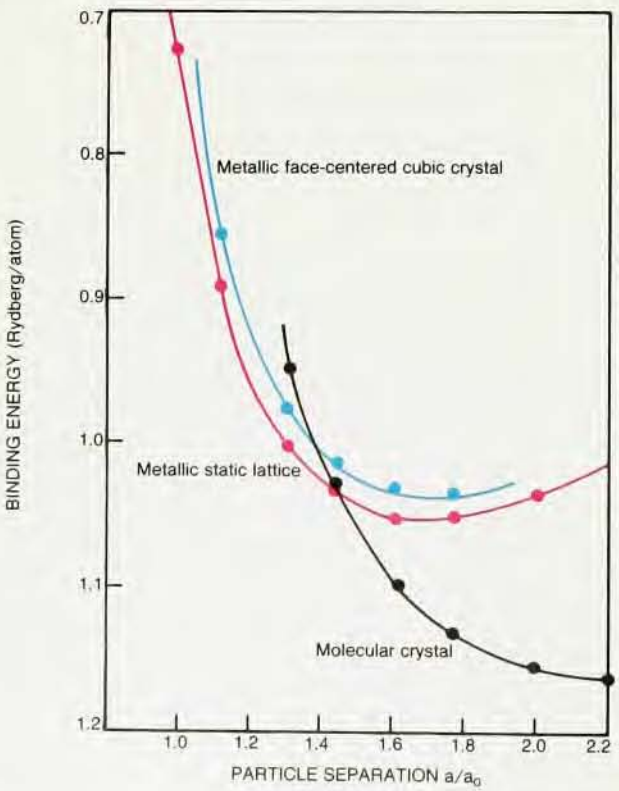
	Lattice constant (Å)	Cohesive energy (eV)	Bulk modulus (Mbar)
Silicon			
Calculated	5.45	4.84	0.98
Experimental	5.43	4.63	0.99
Germanium			
Calculated	5.66	4.26	0.73
Experimental	5.65	3.85	0.77
Carbon			
Calculated	3.60	8.10	4.33
Experimental	3.57	7.35	4.43

With the rapid changes in computer technology, there is a real need for more funding to modernize laboratory equipment. Theorists are also experiencing, some for the first time, a growing need for capital-equipment funding. Five years ago, most theorists used their computing funds to purchase time at large central facilities rather than equipment, because they wanted the computing power of a mainframe. Although for some the purchase of time on a central computer remains the most suitable way of satisfying their computational needs, in recent years computers smaller than mainframes that can be dedicated to a few users have become popular acquisitions. Theoretical groups are joining together to purchase their own superminis and array processors. For a number of problems, easy access and rapid turnaround times are critical in creating the proper environment for working out solutions. Some physicists are using individual work stations, which allow just this type of on-line response for medium-sized jobs and can send larger jobs over networks directly to superminis or mainframes. Theorists also are interested in better graphics and hard-copy units. However, the major desire of a number of theorists still remains that of more raw computing power and memory.

There are various ways in which increased computing power will be obtained. First, as a consequence of continued miniaturization, increases in gate switching speeds will lead to a steady increase in computer power from the fastest, hundred million floating-point operations per second (100 megaflop) machines of today to the gigaflop machines of the near future, such as the Cray-2. There is great interest in policy arrangements that could provide physicists remote access to such supercomputers.

As a further consequence of miniaturization, the price of superminis will continue to decrease while their performance increases. Furthermore, we expect that the size and air-conditioning requirements of computers will decrease enough so that desk-top megaflop machines will soon appear in individual laboratories and offices. Some array processors coupled to a supermini can provide the power of a 10-megaflop or even a 100-megaflop machine. Moreover, such machines can, like the present superminis, run on one problem for a week, if necessary.

Finally, one can also increase the computing power that can be brought to bear on a given theoretical problem, with special-purpose hardwired proces-



Ground-state energy of hydrogen atoms as a function of particle separation a, normalized to a_0, the Bohr radius. The black points are the results of a fixed-node Monte Carlo simulation of a molecular crystal; the curve agrees with experiment at pressures below 500 kbar (a/a_0 greater than 1.75). The light colored curve is the result for an atomic fcc crystal, and the dark color indicates the results for a static atomic lattice. The calculations indicate that the transition from metal to molecular solid occurs at a density corresponding to a value of a/a_0 of 1.35. (From reference 17.) Figure 7

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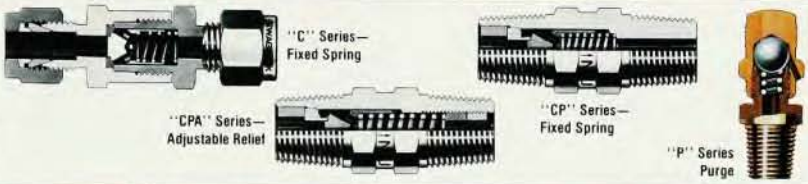

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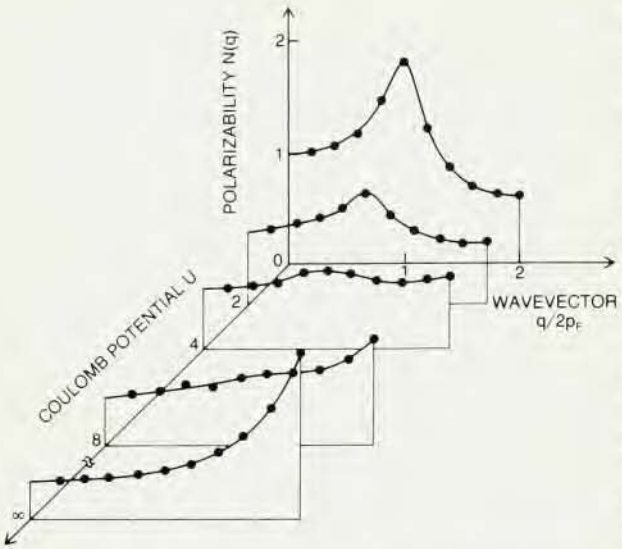

Electron polarizability for a one-dimensional chain of 20 sites (a one-quarter filled "Hubbard model"). The graphs show the polarizability N as a function of wavevector q, normalized to twice the Fermi momentum p_F, at various values of the Coulomb interaction, U, measured in units of the electron-transfer interaction $U = 4$ thus corresponds to an interaction strength equal to the bandwidth). The temperature T in units of the bandwidth is 0.034. (From reference 21.) Figure 8

sors. Hardwired special-purpose experimental equipment, such as the Malvern Correlator which produces an autocorrelation function of its input, is already in fairly widespread use. One example of a special-purpose processor for theory is a machine built five years ago by CHI Systems for the UCLA plasma group. Here a modified array processor coupled to a multiport memory follows the trajectories of 10^6 particles, updating their positions, velocities and the electromagnetic field produced by the combined effects of the particles themselves and an external field. Its performance equaled that of, for example, the CDC7600 at a fraction of the cost. More recently, a processor was constructed at Delft to study molecular dynamics with short-range interactions; for this problem, it offered the performance of a Cray-1. A special-purpose processor has been built at Santa Barbara that performs a Monte Carlo simulation of the three-dimensional Ising model.[23] The present memory can hold the data for a $64 \times 64 \times 64$ lattice, and additional memory is being installed to go to a lattice with $(128)^3$ points. The parts and labor for the processor, which is shown in figure 1, cost approximately $20 000. In the processor the 3-dimensional lattice of spin variables is laid out in memory as a one-dimensional shift register; to update the spin at one point, the values of the spins at the six real-space neighboring sites are hardwired into an updating box, which generates the new spin according to a "heat-bath" algorithm that takes the neighboring values and the temperature into account. After one clock cycle, the lattice is shifted by one site, and the process is repeated. The processor is pipelined, and its speed of 40 nsec per clock cycle is set by the access time of a small lookup table memory. It can update 25×10^6 spins per second. For comparison, a carefully coded FORTRAN program running on a CDC7600 updates fewer than 10^6 spins per second and a Cray-1 is capable of updating approximately 2×10^6 spins per second. In one 24-hour period of operation, the 3-D Ising processor is capable of performing computations that would take a few years to run on a Vax 11/780. It has run essentially continuously for the past four months, collecting data to determine T_c and the critical exponents of the 3-D Ising model. A value for T_c of 0.22166 ± 0.00001, in close agreement with the high-temperature series result has been found, and a finite-size scaling analysis of the data gives critical indices in agreement with hyperscaling, that is, with the simplest way in which the free-energy density can scale with temperature.

Naturally, we expect significant advances in algorithms in the future. With the continued development of parallel machines, algorithms must be specifically optimized for parallel rather than sequential computation. This seems to be relatively unexplored territory, and it may offer important advances in the future. Furthermore, computing, like all mathematics, is easily transferred across boundaries between areas of physics. Thus, for example, there are the overlapping interests of both high-energy and condensed-matter physicists in Monte Carlo algorithms, Langevin algorithms, and the stochastic inversion of large matrices. Significant progress will continue to come from the combination of theoretical ideas and numerical techniques, as exemplified by electronic structure calculations, the Monte Carlo Renormalization Group method and the use of variational information in Monte Carlo calculations.

The style of condensed-matter physics has changed and will continue to change with future developments in computers and in our ability to make use of them.

* * *

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