E. G. Maksimov. *Use of computers in the physics of the condensed state.* Recent years have been characterized by the increasing penetration of computer science into all branches of human activity. Neither physics as a whole nor the physics of the condensed state have lagged behind in this general computerization process. The particular feature of the current state of computerization in the physics of the condensed state is the transformation of the computer into an equal participant, both in experimental and theoretical research. A new trend in physics has been created or, more precisely, a new branch of physics, i.e., computational physics, with its own methods and techniques for studying nature. In general, these are different from the traditional methods of experimental and theoretical physics. Unfortunately, we are well behind the West in developing this branch of physics. There are at least two reasons for this. The first is objective and is due to the fact that we are lagging behind the West in computer science generally. There is, however, another, subjective, reason, namely, some members of our scientific community have underestimated the importance and possibilities of computational physics.

In a brief, thirty-minute report, we cannot, of course, examine all aspects of the computational physics of the condensed state. We can merely briefly recall the rapid development of molecular dynamics and the Monte Carlo technique, which has led to considerable advances in our understanding of the physics of the liquid state, in calculations of the properties of highly nonideal classical and quantum plasmas, and in calculations of the critical indices in phase transitions. We shall use the example of a relatively narrow problem in the physics of the condensed state, namely, the calculation of the electronic properties of crystals, to demonstrate the development and advances in both theoretical approaches to this question and our computational possibilities.

The single-particle description of the electron system in a crystal has for long been one of the popular models used in solid-state physics. Powerful and effective methods have now been available for a relatively long time[1] for the solution of the Schroedinger equation describing an electron in a periodic field $V(r)$:

$$\left[\frac{p^2}{2m}+V(r)\right]\psi(r)=E\psi(r). \tag{1}$$

Calculations of the electron band structure within the framework of this equation have been performed for a large number of metals, semiconductors, and dielectrics. These calculations reached the peak of their development in the sixties and seventies in connection with the idea of the pseudopotential.[2] However, all these calculations suffered from one important defect: there was no rigorous justification for the corresponding single-particle description of a system of strongly interacting electrons. This meant that there was also no rigorous procedure for calculating the parameters of the potential (or pseudopotential) from "first principles." The parameters of the empirical potential were usually chosen by comparing calculations with experimental data for some particular phenomenon. Once this was done, calculations were performed on other effects as well. The results obtained in this way were in surprisingly good agreement with a whole range of physical properties of crystals.

The density functional method (DFM), developed in recent years since the early paper of Kohn and Hohenberg,[3] has provided a rigorous theoretical basis for both the use of

The second-generation systems also incorporate specialized processors that improve the performance of the computing assembly by a factor of 2–3 for particular classes of problems (Fourier processor, matrix processor) or implement programming languages (ANALITIK interpreter, accounting language processor).

Special attention has been devoted in the second-generation machines to adaptors and multiplexers for computer networks and remote communication between SCS machines and other computers. The manufacture of new peripheral storage devices, input-output systems, and so on, has also begun.

Experience gained with first- and second-generation SCS has shown that their range of application is much greater than was envisaged during the initial development. the single-particle description of electrons in crystals and the derivation of the potential $V(r)$ itself from "first principles." As part of the development of this method, it was shown rigorously that calculations of the ground-state energy and the thermodynamic properties of a system of strongly-interacting electrons could be reduced to the solution of the single-particle problem of an electron in an external self-consistent potential that depends only on the electron-density distribution. The self-consistent potential is defined as follows:

$$V(r) = V_{\rm ion}(r) + l^2 \int \frac{n(r')\,dr'}{|\mathbf{r}-\mathbf{r}'|} + V_{\rm xe}(r); \qquad (2)$$

where $V_{\rm ion}(r)$ is the Coulomb potential of the ion, the second term is the Hartree potential for the electrons, and $V_{\rm xe}(r)$ is the exchange-correlation potential. The precise form of $V_{\rm xe}(r)$ is not known. However, advances made in the study of the homogeneous interacting gas can be used as a basis for formulating different approximate expressions for $V_{\rm xe}(r)$.

By using the potential given by (2) and solving the Schroedinger equation (1), it is possible to calculate the electron energy for different crystal volumes and different crystal structures. Calculations of the bonding energy of the crystal, its elastic moduli, phase diagram, and many other properties can be calculated in this way. Recent calculations[4] show that all these quantities can be calculated without the use of adjustable parameters, simply from the given atomic number to within better than 10%.

Generally speaking, there is no justification for using the single-electron states, obtained within the framework of DFM, to calculate the transport properties of electrons or their dynamic response functions. However, it has been shown (in particular, by our own group) that calculations of the electrical resistance of metals due to scattering by phonons, and of their optical properties using the electron spectrum obtained in DFM, also result in reasonable agreement with experiment.[5,6] Similar calculations for semiconductors and dielectrics have yielded results that turn out to be too far removed from experiment although the ground-state energy, obtained for semiconductors and dielectrics, can be calculated just as well as for metals.

The above brief review of the present state of microscopic calculations of crystal properties clearly shows the necessity for an importance of such studies, and the urgency of further computational as well as theoretical work in this field.

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