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Abstract

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ON THE THEORY OF THE CRYSTAL

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The difficulties associated with estimating the approximations obtained in the theoretical study of statistical systems of interacting particles by modern methods lead to the necessity of using, for the study of such systems, models that admit exact solutions. Analysis of these solutions makes it possible to indicate both ways of overcoming the above-mentioned difficulties and the very possibilities for studying real systems by modern methods.

Especially valuable are models which, while admitting exact solutions, reflect the principal bonds and the main interactions. Thus, the modern theory of superconductivity proceeds from a model Hamiltonian in which the interactions of pairs of electrons with opposite momenta and spins are taken into account as the basic ones; as was shown in works (1), the use of this Hamiltonian makes it possible to find an asymptotically exact solution of the problem as $V \to \infty$, $N/V = \text{const}$ (V is the volume of the system, N is the number of particles).

In the present work we wish, from the same standpoint, to approach the study of the properties of a crystal, taking as a model a Hamiltonian that contains interactions corresponding to the main property of the crystal—its periodic structure.

1. As is known, the Hamiltonian of a dynamical system of N identical particles in a volume V, in the representation of second quantization, has the form

$$H = \sum_k T(k)\, a_k^+ a_k + \frac{1}{2V} \sum_{k,k',q} \lambda(q)\, a_{k+q}^+ a_k a_{k'}^+ a_{k'+q}, \tag{1}$$

where k is the momentum; $T(k) = k^2/2m$; a_k and a_k^+ are the particle annihilation and creation operators; $\lambda(q)$ is the Fourier component of the potential energy of interaction.

In (1) there enter terms with the quantities $\sum_k a_{k+q}^+ a_k = \rho_q$, which are the Fourier component of the quantum density; therefore (1) may be written in the form

$$H = \sum_k T(k)\, a_k^+ a_k + \frac{1}{2V} \sum_q \lambda(q)\, \rho_q \rho_{-q}. \tag{2}$$

The vector q assumes quasi-continuous values. However, taking into account that in a crystal each particle is most often located in the region of its lattice site*, we shall take for the crystal, as the model Hamiltonian (1)

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* In accordance with this property, in the Hamiltonian (1) as the operators a_k and a_k^+ we shall take the creation and annihilation operators of spinless Fermi particles, so that, without introducing into consideration repulsive forces between particles, one does not allow the concentration of particles near any one position.

with discrete q corresponding to the periods of the reciprocal lattice of the crystal with basis vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$:

$$\mathbf{q} = 2\pi(m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3), \tag{3}$$

where m_1, m_2, m_3 are integers ($|m| \ll \text{const}$).

Thus, we shall start from the model Hamiltonian

$$H = \sum_k T(k) a_k^+ a_k + \frac{1}{2}\sum_{k,q} \lambda(q)\left(\beta_q a_k^+ a_{k+q} + a_{k+q}^+ a_k \beta_q^+\right) - \frac{V}{2}\sum_p \lambda(q)\beta_q\beta_q^+, \tag{4}$$

in which q assumes the discrete values (3), and where

$$\beta_q = \frac{1}{V}\rho_q = \frac{1}{V}\sum_k a_{k+q}^+ a_k,$$

moreover, as is not hard to verify,

$$a_k\beta_q - \beta_q a_k = \frac{1}{V} a_{k-q}. \tag{5}$$

The main interest in considering such a Hamiltonian consists in the fact that, as we shall show, for it one can obtain an asymptotically exact solution.

Indeed, the equation of motion for the operator $a_k(t)$ with the Hamiltonian (4), taking (5) into account, will be

$$i\frac{da_k}{dt} = T(k)a_k + \frac{1}{2}\sum_q \lambda(q)\left(\beta_q a_{k+q} + \beta_{-q} a_{k-q}\right) + \frac{1}{2V}\sum_q \lambda(q) a_k. \tag{6}$$

From (5) it follows that

$$\left|[a_k, \beta_q]\right| \ll \frac{1}{V} \tag{7}$$

and similarly

$$\left|[a_k^+, \beta_q]\right| \ll \frac{1}{V},$$

whence it is seen that as $V \to \infty$ the operator β_q commutes with all the operators a_k and a_k^+, i.e. loses its quantum properties and behaves as a C-number:

$$\beta_q \to \bar{\beta}_p = \langle \beta_q \rangle_H \quad \text{as } V \to \infty, \tag{8}$$

where $\langle \beta_q \rangle$ denotes the mean value of the quantity β_q over the ensemble with Hamiltonian H.

In this limiting case ($V \to \infty$), equation (6) will have the form

$$i\frac{da_k}{dt} = T(k)a_k + \frac{1}{2}\sum_q \lambda(q)\left(\bar{\beta}_q a_{k+q} + \bar{\beta}_{-q} a_{k-q}\right), \tag{9}$$

which is analogous to the equation of motion for the operator $a_k(t)$ with the Hamiltonian H_0:

$$H_0 = \sum_k T(k)a_k^+ a_k + \frac{1}{2}\sum_{k,q} \lambda(q)\left(C_q a_k^+ a_{k+q} + C_q^* a_{k+q}^+ a_k\right) - \frac{V}{2}\sum_q \lambda(q) C_{qC} q^*, \tag{10}$$

where $C_q = \frac{1}{V}\langle \rho_q \rangle$, and $\langle \cdots \rangle = \langle \cdots \rangle_0$ is the mean value of the corresponding quantity over the ensemble with Hamiltonian H_0.

Comparing (4) with (10), we see that as $V \to \infty$, when $\beta_q \to \bar{\beta}_q$, the Hamiltonian (4) takes the form (10).

The asymptotic equivalence of the Hamiltonians (4) and (10) can be proved mathematically more consistently by the method of Green' s functions; the consideration just given makes it possible only to draw the intuitive conclusion that the asymptotic behavior (as $V \to \infty$) of the model system with Hamiltonian (4) is determined, up to terms of order $1/V$, by the Hamiltonian H_0.

The thermodynamic potential of the model statistical system with Hamiltonian H is asymptotically exactly equal to

$$Z = -\theta \ln \operatorname{Sp} e^{-H_0/\theta}. \tag{11}$$

Therefore, in studying such a system we shall henceforth start from the Hamiltonian H_0, which we shall call approximating.

2. As is seen from (10), the Hamiltonian H_0 is a quadratic form with respect to the operators a_k and a_k^+; therefore it can be diagonalized by means of the linear canonical transformation[2]

$$a_k = \sum_{\nu} \varphi_{k\nu} a_{\nu}, \tag{12}$$

in which the orthonormal functions $\varphi_{k\nu}$ are determined from the secular equations corresponding to the Hamiltonian (10),

$$T(k)\varphi_{k\nu} + \frac{1}{2}\sum_{q} \lambda(q) \left(C_q \varphi_{k+q,\nu} + C_{-q}\varphi_{k-q,\nu}\right) = E(\nu)\varphi_{k\nu}. \tag{13}$$

As a result we have

$$H_0 = \sum_{\nu} E(\nu) a_{\nu}^{+} a_{\nu}. \tag{14}$$

From (13) we obtain the equation of motion of a particle in a self-consistent periodic field with potential $V(x)$:

$$T\left(\frac{\partial}{\partial x}\right)\varphi_{\nu}(x) + V(x)\varphi_{\nu}(x) = E(\nu)\varphi_{\nu}(x), \tag{15}$$

where

$$V(x) = \frac{1}{2}\sum_{q} \lambda(q)\left(C_q e^{-iqx} + C_{-q} e^{iqx}\right). \tag{16}$$

Thus, the study of the properties of the crystal is reduced to the analysis of equation (15) and of its solution:

$$\varphi_{\nu}(x) = e^{(\nu x)} u_{\nu}(x), \tag{17}$$

where the function $u_{\nu}(x)$ is periodic in the lattice rhythm.

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CITED LITERATURE

[1] N. N. Bogolyubov, D. N. Zubarev, Yu. A. Tserkovnikov, *DAN*, **117**, 788 (1957); *ZhETF*, **39**, 120 (1960). [2] N. N. Bogolyubov, *DAN*, **119**, 244 (1958).

Note: Figure translations are in progress. See original paper for figures.