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1957

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Abstract

Full Text

PHYSICS

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ON THE THEORY OF THE PHASE TRANSITION

As was shown in works ([1,2]), it is convenient to develop the theory of superconductivity starting from a model Hamiltonian of the form

$$H = H_0 + H_{int}, \tag{1}$$

$$H_0 = \sum_{k,s}(E(k)-\lambda)a^+_{k,s}a_{k,s}, \qquad H_{int} = -\frac{J}{V}\sum_{(k+k')} a^+_{-k,-1/2}a^+_{k,1/2}a_{k',1/2}a_{-k',-1/2}.$$

The summation in H_{int} is extended over momenta k, k' belonging to the energy shell

$$E_F - \omega < E(k) < E_F + \omega. \tag{2}$$

We shall show that for this Hamiltonian one can construct the thermodynamic potential

$$\Psi = F - \lambda N = -\theta \ln \mathrm{Sp}\, e^{-H/\theta}$$

asymptotically exactly (as $V \to \infty$). Moreover, we shall show that such a calculation is also possible for the more general expression

$$H = \sum_{k,s}(E(k)-\lambda)a^+_{k,s}a_{k,s} - \frac{1}{V}\sum_{(k,k')} J(k,k')a^+_{-k,1/2}a^+_{k,1/2}a_{k',1/2}a_{-k',-1/2}, \tag{3}$$

which contains a real, bounded function $J(k, k')$, practically vanishing outside some finite region of momenta k, k'.

In view of the fact that in the theory of phase transitions there are only very few exactly solvable examples, the development of a method for calculating thermodynamic functions for the Hamiltonian (3) seems expedient to us, especially since applications to the theory of superconductivity are obtained here.

Let us perform our canonical transformation:

$$\alpha_{k,1/2} = u_k \alpha_{k,0} + v_k \alpha^+_{k,1}, \qquad \alpha_{-k,-1/2} = u_k \alpha_{k,1} - v_k \alpha^+_{k,0}$$

with real functions u_k, v_k, connected by the relation

$$u_k^2 + v_k^2 = 1.$$

We obtain

$$H = H^{(0)} + H', \tag{4}$$

$$H^{(0)} = U + \sum_k H_k, \qquad H' = -\frac{1}{V} \sum_{(k,k')} J(k,k') B^+_k B_{k'},$$

where

$$U = \text{const} = 2 \sum_k (E(k) - \lambda) v_k^2 - \frac{1}{V} \sum_{(k,k')} J(k,k') u_k v_k u_{k'} v_{k'},$$

$$\begin{aligned} H_k = {} & \left\{ (E(k) - \lambda)(u_k^2 - v_k^2) + 2u_k v_k \sum_{k'} \frac{J(k,k')}{V} u_{k'} v_{k'} \right\} (\alpha^+_{k0}\alpha_{k0} + \alpha^+_{k1}\alpha_{k1}) \\ & + \left\{ 2(E(k) - \lambda) u_k v_k - (u_k^2 - v_k^2) \sum_{k'} \frac{J(k,k')}{V} u_{k'} v_{k'} \right\} (\alpha^+_{k0}\alpha^+_{k1} + \alpha_{k1}\alpha_{k0}), \end{aligned} \tag{5}$$

$$B_k = u_k v_k (\alpha^+_{k0}\alpha_{k0} + \alpha^+_{k1}\alpha_{k1}) - u_k \alpha_{k1}\alpha_{k0} + v_k^2 \alpha^+_{k0}\alpha^+_{k1}.$$

Let us note that all the operators H_k, B_k, B^+_k commute with one another for different k.

We apply statistical perturbation theory to formula (4). We obtain:

$$\frac{\mathrm{Sp}\, e^{-H/\theta}}{\mathrm{Sp}\, e^{-H^{(0)}/\theta}} = 1 + \sum_{(n>1)} (-1)^n \int_0^{1/\theta} dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n \, \frac{\mathrm{Sp}\{e^{-H^{(0)}/\theta} H'(t_1) \ldots H'(t_n)\}}{\mathrm{Sp}\{e^{-H^{(0)}/\theta}\}},$$

where

$$H'(t) = e^{H^{(0)}t} H' e^{-H^{(0)}t}.$$

This relation may also be represented in the form

$$\ln \operatorname{Sp} e^{-H/\theta} - \ln \operatorname{Sp} e^{-H^{(0)}/\theta} = \ln \left\{ 1 + \sum_{(n>1)} \int_0^{1/\theta} dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n \, \mathfrak{A}_n \right\}, \tag{6}$$

where

$$\mathfrak{A}_n = \frac{1}{V^n} \sum_{\substack{(k_1,\ldots,k_n) \\ (k'_1,\ldots,k'_n)}} J(k_1,k'_1),\ldots,J(k_n,k'_n) \times$$

$$\times \frac{\operatorname{Sp}\{e^{-H^{(0)}/\theta} \widetilde{B}_{k_1}(t_1) B_{k'_1}(t_1) \ldots \widetilde{B}_{k_n}(t_n) B_{k'_n}(t_n)\}}{\operatorname{Sp}\{e^{-H^{(0)}/\theta}\}}, \tag{7}$$

$$B_k(t) = e^{H^{(0)}t} B_k e^{-H^{(0)}t} = e^{H_k t} B_k e^{-H_k t}, \qquad \widetilde{B}_k(t) = e^{H_k t} B_k^+ e^{-H_k t}.$$

We shall show that, if for all k

$$\operatorname{Sp}(e^{-H_k/\theta} B_k) = 0, \tag{8}$$

then each of the $\mathfrak{A}_n$ remains bounded in the course of the limiting transition $V \to \infty$.

Indeed, take in the sum (7) some term for which there is at least one momentum k_q or k'_q not equal to any of the other momenta k_j, k'_j. It is not difficult to see that such a term will be proportional to

$$\operatorname{Sp}\{e^{-H_{k_q}/\theta} \widetilde{B}_{k_q}(t)\} = \operatorname{Sp}\{e^{-H_{k_q}/\theta} B^+_{k_q}\} = 0,$$

or

$$\operatorname{Sp}\{e^{-H_{k'_q}/\theta} B_{k'_q}(t)\} = \operatorname{Sp}\{e^{-H_{k'_q}/\theta} B_{k'_q}\} = 0.$$

Therefore, in the sum (7) it is necessary to take into account only those terms for which, among the momenta $k_1, k'_1, \ldots, k_n, k'_n$, there are no more than n distinct ones. But they lead to a quantity of order V^n, which is compensated by the factor $1/V^n$. Consequently, $\mathfrak{A}_n$ remains finite as $V \to \infty$. On the other hand, both terms on the left-hand side of (6) must be proportional to V for $V \to \infty$. Neglecting, on this basis, terms of finite order, we may replace $\ln \mathrm{Sp}\, e^{-H/\theta}$ by $\ln \mathrm{Sp}\, e^{-H(0)/\theta}$ and obtain for the thermodynamic potential under consideration an expression of the form

$$\Psi = U - \theta \sum_k \ln \mathrm{Sp}\, e^{-H_k/\theta}. \tag{9}$$

Thus, in order to solve the problem posed, we must determine u_k, v_k from condition (8) and then use formula (9).

Technically, it is convenient to carry out this program by diagonalizing the form H with the aid of the canonical transformation

$$\alpha_{k0} = \lambda_k \beta_{k0} - \mu_k \beta_{k1}^+, \qquad \alpha_{k1} = \lambda_k \beta_{k1} + \mu_k \beta_{k0}^+ \tag{10}$$

with real coefficients related by

$$\lambda_k^2 + \mu_k^2 = 1.$$

We determine these coefficients from the condition that the nondiagonal part of the operator H_k, which proves to be proportional to

$$\beta_{k1}\beta_{k0} + \beta_{k0}^+\beta_{k1}^+,$$

vanish.

Substituting then (10) into expression (5) for B_k, we expand equation (8). In this way we find that

$$u_k v_k = \frac{C(k)}{2\Omega(k)} \frac{1 - e^{-\Omega(k)/\theta}}{1 + e^{-\Omega(k)/\theta}},$$

$$C(k) = \frac{1}{V} \sum_{k'} J(k,k') u_{k'} v_{k'}, \qquad \Omega(k) = \sqrt{(E(k) - \lambda)^2 + C^2(k)}. \tag{11}$$

Hence we obtain the equation for determining $C(k)$:

$$C(k) = \frac{1}{2V} \sum_{k'} J(k,k')\ \mathrm{th}\, \frac{\Omega(k')}{2\theta} \frac{C(k')}{\Omega(k')}. \tag{12}$$

It is interesting to note that this equation, especially if it is written in the form

$$2\Omega(k)u_k v_k = \frac{\operatorname{th}\dfrac{\Omega(k)}{2\theta}}{V} \sum_{k'} J(k,k')u_{k'}v_{k'},$$

has a certain analogy with the two-body problem equation written in the momentum representation.

Let us note that equation (12) always has the trivial solution $C(k)=0$.

Expanding relation (9), we obtain

$$\Psi = \sum_k \left\{ E(k) - \lambda + \frac{C^2(k)}{2\Omega(k)} \operatorname{th}\frac{\Omega(k)}{2\theta} - \Omega(k) - 2\theta \ln\left(1 + e^{-\Omega(k)/\theta}\right) \right\}. \qquad (13)$$

We shall regard this expression as a function $\Psi(\ldots C^2(k)\ldots)$.

Then

$$\frac{\partial\Psi}{\partial C^2(k)} = C^2(k)\frac{\partial\Omega(k)}{\partial C^2(k)}\left\{\frac{\partial}{\partial\Omega(k)}\frac{1}{2\Omega(k)}\operatorname{th}\frac{\Omega(k)}{2\theta}\right\} = -\frac{C^2(k)}{4\theta^3} f\left(\frac{\Omega(k)}{\theta}\right),$$

where

$$f(x) = \frac{\operatorname{sh} x - x}{2x^3 \operatorname{ch}^2 \frac{x}{2}} > 0.$$

Therefore, for $C^2 \neq 0$, the quantity Ψ always has a smaller value than for the trivial solution.

Thus, the phase transition will occur at the temperature at which equation (12) acquires a nontrivial solution.

Passing to Bardeen' s model, in which J and C do not depend on k, we obtain for C the equation:*

$$1 = \rho \int_0^\omega \frac{\operatorname{th}\dfrac{\sqrt{\xi^2+C^2}}{2\theta}}{\sqrt{\xi^2+C^2}}\, d\xi, \qquad (14)$$

where

$$\rho = \frac{J}{2\pi^2}\left(\frac{k^2}{\partial E/\partial k}\right)_{k=k_F}.$$

We note that for $\theta = 0$, equation (13) gives for the gap the expression obtained in (1^2).

It is not difficult to see that equation (14) has solutions only for $\theta < \theta_0$, where θ_0 is determined from equation (13) at $C = 0$

$$1 = \rho \int_0^\omega \frac{\operatorname{th} \dfrac{\xi}{2\theta_0}}{\xi}\, d\xi, \tag{15}$$

whence

$$\theta_0 = 1.13\, \omega e^{-1/\rho}. \tag{16}$$

Equation (14) determines C as a function of θ. At $\theta = 0$ we have $C(0) = 2\omega e^{-1/\rho}$ (^{2}).

Near the point $\theta = \theta_0$ the gap C tends to zero and has the form

$$C^2 = 9.39\, \theta_0(\theta_0 - \theta). \tag{17}$$

From equation (13), taking (17) into account, we see that at the point $\theta = \theta_0$ the entropy is continuous, while the heat capacity $\mathfrak{S}$ has a finite jump equal to

$$\frac{\Delta \mathfrak{S}}{\mathfrak{S}_0} = 1.43, \tag{18}$$

where $\mathfrak{S}_0$ is the heat capacity of the ideal Fermi gas at $\theta = \theta_0$. Consequently, at the point $\theta = \theta_0$ we have a second-order phase transition.

Received
13 XI 1957

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[3] J. Bardeen, L. N. Cooper, J. R. Schrieffer, Preprint, University of Illinois, Techn. Rep., No. 9, June, 17 (1957).

* The thermodynamic formulas in the simplest case $J =$ const were also obtained by Bardeen, Cooper, and Schrieffer (^{3}), proceeding from other ideas, with the aid of an approximate variational method.

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