DOUBLING OF THE PERIOD IN A ONE-DIMENSIONAL SYSTEM OF FERMI PARTICLES

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The model of a one-dimensional Fermi system with a point interaction that depends on the node number is considered. It is shown that such a model corresponds to introduction of deformation. This is followed by an investigation for stability against periodic deformations. The true ground state has a double period.

1. More than 30 years ago, Peierls[1] called attention to the instability of a one-dimensional metal with a half-filled band (one electron per atom). This instability was attributed by Peierls to the fact that when the ion displacement is such that the energy bands at the Fermi level are broken, i.e., when the period of the one-dimensional lattice is doubled, a gain takes place in the energy of the electron system. In the language of modern diagram technique, Peierls' proof is equivalent to summation, in the vertex part, of a sequence of "ladder" diagrams. However, as was first shown by Bychkov, Gor'kov, and Dzyaloshinskiĭ[2], the "ladder" approximation is insufficient to determine the vertex part in a one-dimensional Fermi system. The analysis of the situation made in[2] in the logarithmic approximation has shown that in the case of effective attraction there occurs, simultaneously with doubling of the period, also a Cooper "pairing." The general conclusion by Hohenberg[3] that there is no anomalous pairing in one-dimensional systems requires that the corrections that follow the logarithmic ones break the Cooper "pairing." However, this conclusion does not hole for the pairing responsible for the doubling of the period $\langle a_p^+ a_{p\pm 2p_0} \rangle$, where p_0 is the Fermi momentum, since it is not anomalous.

We investigate in the present paper the stability of the exact solution of the model problem of interacting Fermi particles[4] against a small periodic distortion of the one-dimensional lattice. To this end, we generalize in Sec. 2 the results of[4] to the case when the interaction force depends on the number of the node. This investigation is carried out in Sec. 3, where the energy difference between the ground state of the deformed and undeformed lattices is calculated. In Sec. 4 we compare our results with the results of the usual analysis in the Hartree-Fock approximation.

2. Let us consider the model problem of a one-dimensional system of interacting fermions with the following Hamiltonian:

$$\hat{H} = -\sum_{\langle ij\rangle\sigma} T_{ij} c_{i\sigma}^+ c_{j\sigma} + U\sum_i c_{i\uparrow}^+ c_{i\uparrow} c_{i\downarrow}^+ c_{i\downarrow}, \tag{1}$$

Here $\langle ij \rangle$ denotes the sum over the nearest neighbors; $c_{i\sigma}^+$ is the operator for the production of an electron at the node i with spin σ; U is the interaction of the electrons in one node. Unlike[4], T_{ij} introduces, as it were, "quenched phonons"—a deformation;

$$T_{ij} = \gamma(1+\alpha\cos qi)(1+\alpha\cos qj).$$

We carry out the canonical transformation

$$c_{i\sigma}^+ = \frac{1}{\gamma 1+\alpha\cos qi} a_{i\sigma}^+.$$

We consider the case $\alpha \ll 1$ and then

$$c_{i\sigma}^+ = a_{i\sigma}^+\left(1-\frac{|\alpha|}{2}\cos qi\right).$$

Now the Hamiltonian (1) is written in the form

$$\hat{H} = -\sum_{\langle ij\rangle\sigma} a_{i\sigma}^+ a_{j\sigma} + 2\sum_i V_i a_{i\downarrow}^+ a_{i\downarrow} a_{i\uparrow}^+ a_{i\uparrow}.$$

Changing over first from the node representation to the k representation, and then to the ordinary coordinate representation, we obtain

$$\hat{H} = -\sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + 2\sum_{i<j} V_j\delta(x_i - x_j). \tag{2}$$

Here N is the number of particles, and V_j is defined by

$$V_j = {}^1/_2 U[1-|\alpha|\cos qj], \tag{3}$$

where $\alpha \ll 1$ is the distortion amplitude; q is the distortion period. We emphasize once more that the Hamiltonian (2) corresponds in the node representation to a deformed lattice (we consider nodes of two types—displaced and not displaced).

There exist N! elementary independent solutions of the equation $\hat{H}\psi = E\psi$, each connected with the same set of different complex numbers $k_1, k_2, \ldots, k_N$. These solutions are superpositions of waves of the type

$$\exp[i(k_{p_1}x_1 + k_{p_2}x_2 + \ldots + k_{p_N}x_N)],$$

where k_{p_i} is one of the $k_1, k_2, \ldots, k_N$. We separate the spin variables from the coordinate variables in the usual manner:

$$\psi = \sum_T \varphi_T(x_1, x_2, \ldots, x_N)\chi_T(S_1, S_2, \ldots, S_N).$$

In this formula the summation is over different Young patterns with two columns of length

$$\nu = {}^1/_2 N + S, \quad \nabla = {}^1/_2 N - S.$$

Now the problem reduces to finding the solutions of the equation

$$\sum_{j=1}^N \frac{\partial^2\varphi}{\partial x_j^2} = E\varphi \tag{4}$$

for each "sector" from the ordered values

$$x_{\sigma 1} < x_{\sigma 2} < \ldots < x_{\sigma N}$$

and "joining together" the solutions in the neighboring sectors. Besides continuity of the function, these "joining" conditions also impose one more condition on its derivatives:

$$\left(\frac{\partial}{\partial x_\alpha}-\frac{\partial}{\partial x_\beta}\right)\varphi|_{x_\alpha=x_\beta}\equiv 2V_\alpha\varphi|_{x_\alpha=x_\beta}. \tag{5}$$

Unlike in[4], in our case the discontinuity of the derivative depends on the number of the node.

We shall seek the solution of Eq. (4) in the form

$$\varphi=\sum_P A\{P\}\exp\left\{i\sum_{j=1}^{N}k_{p_j}x_j\right\}, \tag{6}$$

where the sum is taken over all the permutations. It is further necessary to introduce periodic boundary conditions. In analogy with[4], we define

$$2\left(\frac{k_j}{V_j}-\frac{q_a}{V_a}\right)=\operatorname{ctg}\frac{1}{2}\theta_{ja}. \tag{7}$$

then the periodic boundary condition is written in the form

$$Lk_j=2\pi n_j+\sum_{a=1}^{\bar\nu}\theta_{ja}, \tag{8}$$

where $1\le j\le N$; $1\le a\le\bar\nu$; n_j are integers. The condition (5), on the other hand, can be written in the form

$$\prod_{j=1}^{N}\frac{k_j/V_j-q_a/V_a+i/2}{k_j/V_j-q_a/V_a-i/2}=\prod_{\substack{b=1\\ b\ne a}}^{\bar\nu}\frac{q_b/V_b-q_a/V_a+i}{q_b/V_b-q_a/V_a-i}. \tag{9}$$

If we introduce the notation

$$\frac{q_a}{V_a}-\frac{q_b}{V_b}=\operatorname{ctg}\frac{1}{2}\psi_{ab}, \tag{10}$$

then condition (9) takes the form

$$\sum_{j=1}^{N}\theta_{ja}-\sum_{b=1}^{\bar\nu}\psi_{ba}=0. \tag{11}$$

Equations (7), (8), (10), and (11) are the ones we seek. The obtained equations can be written more compactly:

$$\begin{aligned}Lk_\lambda&=2\pi\lambda+2\sum_{-p\le b\le p}\operatorname{arc\,tg}2\left(\frac{k_\lambda}{V_\lambda}-\frac{q_b}{V_b}\right),\\ Lq_a&=2\pi a+\frac{1}{2}\sum_b\psi_{ba}-\sum_\lambda\operatorname{arc\,tg}2\left(\frac{k_\lambda}{V_\lambda}-\frac{q_a}{V_a}\right),\end{aligned} \tag{12}$$

where a assumes integer values from $-p$ to p; $\bar\nu=2p+1$; λ assumes half-integer values between $-(S-\frac{1}{2})$ and $(S-\frac{1}{2})$. The energy of the ground state is specified in analogy with[4] by the following formula:

$$E=\sum_j k_j^2+2\sum_a q_a^2-\frac{1}{2\bar\nu}\left[\sum_{a=1}^{\bar\nu}|V_a|\right]^2. \tag{13}$$

3. Thus, in order to determine the energy of the ground state, it is necessary first to calculate the values of k_λ and q_a from (12). In the case of an arbitrary interaction force, this is far from a simple problem. However, for $V_a\gg 1$, as can be readily seen from (12), we have

$$k_\lambda=2\pi\lambda/L,\qquad q_a=\pi a/L$$

and the ground-state energy is

$$E=\left(\frac{2\pi}{L}\right)^2\left\{\sum_{a=1}^{p}a^2+2\sum_{\lambda=1/2}^{s-1/2}\lambda^2\right\}-\frac{1}{2\bar\nu}\left[\sum_{-p}^{p}|V_a|\right]^2.$$

To check on the stability, however, we do not need the ground-state energy, but only the difference between these energies for the deformed and undeformed crystals. When $V_a\gg 1$ we have

$$\Delta E=\bar\nu\frac{U^2}{2}-\frac{1}{2\bar\nu}\left[\sum_{-p}^{p}|V_a|\right]^2. \tag{14}$$

Since $|V_a|^2=U^2(1-4|\alpha|\cos qa)$, we get

$$\Delta E=2|\alpha|^2U^2\left[\sum_{-p}^{p}\cos qa\right]^2\bar\nu^{-1},$$

or, using simple summation,

$$\Delta E=2|\alpha|^2U^2\left\{2\frac{\cos{}^1/_2pq\sin{}^1/_2(p+1)q}{\sin{}^1/_2q}-1\right\}^2\bar\nu^{-1}. \tag{15}$$

The dependence of ΔE on q is shown schematically in the figure. We see from it that the lattice is unstable against distortions with a "wave vector" $q=\pi/p$. The part of the curve following $q=2\pi/p$ is not realized, since it corresponds to a distortion with a period smaller than the interatomic one. In the usual units, π/p corresponds to the wave vectors

$$Q=p\frac{N}{L}q=4\frac{\pi p}{L}. \tag{16}$$

Going over to the thermodynamic limit $N\to\infty$ and $L\to\infty$, we find that the numbers q_a are continuously distributed on the segment $[-p_0,+p_0]$, where

$$p_0=\lim_{L\to\infty}q_p=\lim_{L\to\infty}(\pi p/L).$$

Thus, $Q=2p_0$, where p_0 is the Fermi momentum. We thereby establish that the lattice is unstable against doubling of the period.

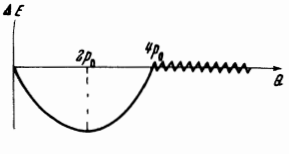
4. In the usual analysis in the Hartree-Fock approximation, we would solve the unperturbed problem and would obtain its single-electron wave functions.

$$\psi_j=\frac{1}{\sqrt{L}}\exp\left(i2\pi j\frac{x}{L}\right).$$

We would then introduce a perturbation $\delta V=\alpha\cos[2\pi L^{-1}(2n+1)x]$ (if the number of electrons in our case is $N=4n+2$, this perturbation corresponds to doubling of the period), and we then calculate in second order of perturbation theory the correction to the ground-state energy

$$\Delta E=-2\alpha^2ml^2N\ln N,\qquad l=L/N. \tag{17}$$

It is seen from (16) that when $N\to\infty$ this correction diverges, meaning inapplicability of perturbation theory or, in other words, the instability of the unperturbed ground state against doubling of the period. In Sec. 3 of this paper we have solved the problem exactly and therefore we have no divergences whatever. The instability, on the other hand, is pointed out by the fact that the energy of the lattice deformed with double the period has a minimum. Since deformation is actually always present, the true ground state has double the period.



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