Peierls instability in 1D Fermi systems with a weak interaction

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The Peierls instability in a 1D Fermi system with a weak interaction and a half-filled band is analyzed. The effects of the interaction on the Peierls transition in the model of spinless particles are quite different from the effects in the model of particles with a spin.

According to the well-known Peierls theorem,[1] a one-dimensional (1D) metal is unstable with respect to lattice distortions. This theorem has several important consequences for the theory of 1D systems.[2] In particular, the concept of solitons as a particular type of excited state of polyacetylene is based on this theorem.[3]

It should be noted, however, that the Peierls theorem applies to a system of noninteracting electrons. Although several attempts have been made to take into account the effect of an interaction on the Peierls instability by a variety of approximate methods[4] or through numerical calculations for finite chains,[5,6] this question has not yet been finally resolved.

In this letter we take up the problem of the Peierls instability for two models of weakly interacting Fermi particles: a spinless lattice Fermi gas with a Hamiltonian

$$\hat{H} = -\sum_{-\pi<k<\pi} \cos k\, a_k^+ a_k + i\delta \sum_{-\pi<k<\pi} \sin k\, a_k^+ a_{k+\pi} + (g/2N) \sum \cos q\, a_{k_1+q}^+ a_{k_2-q}^+ a_{k_2} a_{k_1} \tag{1}$$

and the Hubbard model,

$$\hat{H} = -\sum_{k,\sigma} \cos k\, a_{k\sigma}^+ a_{k\sigma} + i\delta \sum_{k,\sigma} \sin k\, a_{k\sigma}^+ a_{k+\pi\sigma} + (g/N) \sum a_{k_1+q\alpha}^+ a_{k_1\alpha} a_{k_2-q\beta}^+ a_{k_2\beta} \,. \tag{2}$$

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We consider the case of a half-filled band, in which there is a doubling of the period of the chain according to the Peierls theorem. The quantity δ in (1) is the strain parameter. We might also note that Hamiltonian (1) can be expressed in terms of spin operators and can thus describe a spin-Peierls system with an anisotropic interaction.

The problem of analyzing the instability of a 1D system with respect to a deformation of the chain reduces to one of finding the δ dependence of the ground-state energy E_0. Since the elastic energy of the lattice is $E_{el} = \kappa\delta^2/2$ (κ is the dimensionless elastic modulus), a deformation is preferred from the energy standpoint if the quantity

$$\epsilon(\delta) + E_{el} \qquad (\epsilon(\delta) = E_0(\delta) - E_0(0))$$

has a minimum at $\delta \neq 0$. For $g = 0$ we have $\epsilon(\delta) \sim \delta^2 \ln\delta$, and there is clearly a minimum at $\delta \ll 1$. This assertion is the Peierls theorem.

Analysis of the perturbation-theory series in g for the ground-state energy for (1) and (2) shows that the leading contribution to $\epsilon(\delta)/\delta^2$ in nth order is $\sim g^n \ln^{n+1}\delta (\delta \ll 1)$. We will briefly describe a method for summing the most divergent terms of the perturbation-theory series. It is usually assumed that the approximation corresponding to the retention of only contributions of this type is valid if $g \ll 1$ (a weak interaction).

It turns out that contributions on the order of $\delta^2 g^n \ln^{n+1}\delta$ to $\epsilon(\delta)$ are made by diagrams of the "parquet" type, which have a pair of lines corresponding to "anomalous" pairing, $\langle a_k^+ a_{k+\pi}\rangle$:

$$\langle a_k^+ a_{k+\pi}\rangle = i\delta \sin k/2\epsilon(k); \quad \epsilon(k) = (\cos^2 k + \delta^2 \sin^2 k)^{1/2}.$$

The sum of such diagrams is expressed in terms of the vertex part, $\gamma(k_1\sigma_1, k_2\sigma_2; k_3\sigma_3, k_4\sigma_4)$ [$k = (k,\omega)$, σ is the spin index]:

$$\epsilon(\delta) = -i(8\pi^2)^{-1} \sum_{\sigma_1\sigma_2} \sum_{k_1 k_2} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2\, G(k_1, \omega_1) G(k_2,\omega_2) \gamma(k_1\sigma_1, k_2\sigma_2; k_1 + \pi\sigma_1, k_2 + \pi\sigma_2). \tag{3}$$

Here $G(k,\omega)$ is the Green's function corresponding to the anomalous pairing.

The vertex part of (3) should be found in the parquet approximation. Finding the sum of the most divergent energy diagrams thus reduces to calculating the sum of the parquet diagrams of the vertex part. The general method for summing such diagrams is well known.[7,8] This approximation was used in Refs. 7 and 9 to study possible states of 1D systems. The set of all diagrams of the vertex part can be broken up into four classes[7]: the γ_1 diagrams, which are reducible from k_1,k_2 to k_3,k_4 (i.e., diagrams which can be broken up into two parts containing k_1,k_2 and k_3,k_4 by cutting the diagram along two interior lines); γ_2, which are reducible from k_1,k_3 to k_2,k_4; γ_3 diagrams, which are reducible from k_1,k_4 to k_2,k_3; and irreducible diagrams (as such diagram we choose the vertex part of first order). The leading logarithmic contribution to (3) comes from the region $k_1,k_2 \cong \pm\pi/2$ of the integration over the momenta. Correspondingly, the behavior of $\gamma(k_1\sigma_1,k_2\sigma_2;k_3\sigma_3,k_4\sigma_4)$ is important only at the momenta $\cong \pm\pi/2$. It

can be shown by working from (3) that $\epsilon(\delta)$ is expressed as follows in terms of γ_1, γ_2, and γ_3:

$$\epsilon(\delta) = (i\delta^2/4\pi^2) \sum_{\sigma_1\sigma_2} \int_0^{\Phi} dt_1 \int_0^{\Phi} dt_2 \{ \gamma_1^{+--+}(\min(t_1, t_2)) - \gamma_3^{++--}(\min(t_1, t_2)) + \gamma_2^{+--+}(t_1, t_2, \Phi) - \gamma_2^{++--}(t_1, t_2, \Phi) \}, \quad (4)$$

where the plus and minus signs correspond to the momenta $\pm\pi/2$, $\Phi = -\ln\delta$, and we have transformed to the logarithmic variables $t_i = -\ln(\delta k_i)$. It can be seen from (4) that γ_1^{+--+} and γ_3^{++--} are functions of a single variable (this is a familiar situation in the theory of parquet equations, in which all the momenta on which γ depends are comparable in magnitude), and γ_2^{+--+} and γ_2^{++--} are functions of three variables.

The problem of finding the function γ in (4) reduces to one of solving a system of nonlinear integral equations. We omit the intermediate calculations (which will be published separately) and proceed immediately to the final expressions for $\epsilon(\delta)$, which incorporate the term of zeroth order in g. For model (1) we find

$$\epsilon(\delta) = -(\delta^2/4g)(\exp(2g\Phi/\pi) - 1). \quad (5)$$

For the Hubbard model we find

$$\epsilon(\delta) = -(\delta^2\Phi/\pi)\,|1 - (g\Phi/\pi)|^{-1/2}. \quad (6)$$

It follows from (5) that in the case $\delta \ll 1$ for a spinless Fermi gas we would have $\epsilon(\delta) = (-4g)^{-1}\gamma^{2-2g/\pi}$, and a deformation would be preferred from the energy standpoint if $g > 0$; in the case of an attraction, the system would be stable with respect to the Peierls transition. In the Hubbard model, $\epsilon(\delta)$ diverges at $\delta_0 = \exp(-\pi/|g|)$. On the other hand, the ground-state energy for (2) must be finite at $\delta = \delta_0$. The reason for the singularity in (6) is the approximate nature of the calculations. This singularity shows that the function $\epsilon(\delta)/\delta^2$ has a minimum at $\delta = \delta_0(g)$. To determine the nature of the singularity of $\epsilon(\delta)$ at $\delta = \delta_0(g)$ requires consideration of the nonparquet diagrams. At any rate, the system is stable with respect to a transition to the Peierls state if $|\epsilon(\delta_0)/\delta_0^2|$ is less than $\kappa/2$.

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