Peierls instability in weakly nonideal one-dimensional systems

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The problem of the Peierls instability in one-dimensional systems with weak coupling (in particular, in the Hubbard model) is considered. It is found that, depending on the deformation parameter δ, there exist two regimes of behavior of the system. When the Peierls gap is greater than the correlation gap, perturbation theory in the coupling constants is applicable. In the opposite case, the strong-coupling regime sets in. The ground-state energy $\sim -\delta^{4/3}$, and this dependence has a universal character.

According to the well known theorem of Peierls,[1] a one-dimensional metal is unstable against distortions of the lattice. The dielectric state which then arises possesses a number of unusual physical properties. In particular, in polymers with conjugated bonds, such as, e.g., polyacetylene, the transition to the Peierls-dielectric state leads to alternation of the C–C-bond lengths, and, as a consequence, to the appearance of excited states of a special kind—solitons.[2]

It is necessary to note that Peierls' conclusion referred to a system of noninteracting electrons. It is known, however, that electron-electron interactions play an important role in one-dimensional systems and can themselves form a gap in the excitation spectrum. There arises the far from trivial problem of taking simultaneous account of these two effects leading to instability. The use of the mean-field approximation[3–6] for the solution of this problem shows that these two instabilities cannot coexist, and, under certain conditions, the Peierls transition is suppressed. The mean-field approximation is, however, too crude. Variational calculations[7–9] indicate that the Peierls instability and electron correlation are not competing effects, and, in reality, correlations enhance the tendency toward a transition to the Peierls state. This conclusion was also confirmed later in other papers using perturbation theory relative to the mean-field,[10] calculations by the Monte Carlo method,[11] and exact calculations on finite systems.[12] At the same time, exact results for this problem were not obtained.

In the present paper the problem of the Peierls instability will be considered for the case of small electron-electron coupling constants. It will be shown that in those cases when there is no correlation gap the situation is a zero-charge situation and it is legitimate to use perturbation theory. But if there is a correlation gap in the excitation spectrum the system can be in either the weak-coupling or the strong-coupling regime. In this case correlation effects enhance the tendency toward a Peierls transition. Preliminary results of the work have been published in Refs. 13 and 14.

DERIVATION OF EXPRESSIONS FOR THE DEFORMATION ENERGY AND GAP

In studying the problem of the Peierls instability we shall start from the Hamiltonian of an electron-phonon system in the adiabatic approximation (as follows from Refs. 15 and 16, small departures from adiabaticity should not fundamentally change the character of the Peierls transition, although this question requires further investigation):

$$\hat{H}=\hat{H}_0+\hat{H}_1+\hat{V}, \qquad \hat{H}_0=-\sum_{k,\sigma}\cos k\, a_{k\sigma}^{+}a_{k\sigma}, \tag{1}$$

$$\hat{H}_1=(2N)^{-1}\sum_{k,k',q,\sigma,\sigma'} v(q)\, a_{k+q\sigma}^{+}a_{k'-q\sigma'}^{+}a_{k'\sigma'}a_{k\sigma},$$

$$\hat{V}=i\delta\sum \sin k\, a_{k\sigma}^{+}a_{k+\pi\sigma}+N\varkappa\delta^2/2, \tag{2}$$

where $v(q)$ is the Fourier transform of the interaction potential, $\delta \ll 1$ is the dimensionless deformation parameter, and $\varkappa$ is the dimensionless elastic constant. The second term in (2) is the energy associated with the elasticity of the chain.

Besides (2), which corresponds to alternation of the bond lengths, it is also interesting to consider another type of distortion, corresponding to the interaction of intramolecular vibrations with the local electron density (alternation of the lattice-site energies):

$$\hat{V}=\delta\sum_{k,\sigma} a_{k\sigma}^{+}a_{k+\pi\sigma}+N\varkappa\delta^2/2. \tag{3}$$

We shall be interested mainly in the case of a half-filled band, for which, according to the Peierls theorem, a doubling of the period of the chain (dimerization) occurs.

The problem of investigating the instability of a one-dimensional system against deformation of the chain reduces to finding the dependence of the ground-state energy E_0 on δ. Deformation is energetically favored if the quantity

$$N\varepsilon(\delta)+E_{el}; \qquad \varepsilon(\delta)=(E_0(\delta)-E_0(0))/N$$

has a minimum for $\delta \neq 0$. For $v(q)=0$,

$$\varepsilon(\delta)\sim\delta^2\ln\delta$$

and it is clear that there is a minimum for $\delta \ll 1$. This assertion constitutes the Peierls theorem. Since $E_{el}\propto\delta^2$, deformation is favored if as $\delta\to 0$ we have $\varepsilon(\delta)\propto -\delta^{\mu}$ with $\mu<2$. But if $\mu=2$, whether or not dimerization is favored is determined by comparing the corresponding coefficients and, in principle, the Peierls transition can be suppressed. The main task

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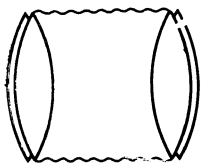

FIG. 1. Second-order diagram for $\varepsilon(\delta)$. The double lines on the diagram correspond to anomalous pairings.

of our paper is to calculate $\varepsilon(\delta)$. Since the interaction is weak, it is natural to try to use perturbation theory in $\hat{H}_1$ for this purpose.

Unlike the diagrams for $E_0(0)$ the diagrams for $\varepsilon(\delta)$ contain not only lines corresponding to "normal" pairings

$$\langle a_{k\sigma}^{+}a_{k\sigma}\rangle = u_k^2 = (1+\cos k/\varepsilon(k))/2; \quad \langle a_{k\sigma}a_{k\sigma}^{+}\rangle = v_k^2 = 1-u_k^2;$$
$$\varepsilon(k) = (\cos^2 k+\delta^2\sin^2 k)^{1/2} \quad (\varepsilon(k) = (\cos^2 k+\delta^2)^{1/2})$$

but also lines corresponding to "anomalous" pairings

$$\langle a_{k\sigma}^{+}a_{k+\pi\sigma}\rangle = i\delta\sin k/2\varepsilon(k) \quad (\delta/2\varepsilon(k)).$$

The number of the latter in the diagram is always even. All the diagrams for $\varepsilon(\delta)$ can be obtained from diagrams for $E_0(0)$ by all possible replacements of normal lines by anomalous lines. (In the brackets we indicate the corresponding expressions for the model (3).) For example, the second-order diagram is depicted in Fig. 1 and is proportional to $\delta^2 g^2 \ln^3\delta$. Analysis of the perturbation-theory series shows that, in general, in the n-th order the leading contribution to $\varepsilon(\delta)$ is proportional to

$$\varepsilon(\delta) \propto \delta^2 g^n \ln^{n+1}\delta.$$

It is not difficult to convince oneself that the diagrams that make such contributions to $\varepsilon(\delta)$ possess the following properties: 1) They contain a pair of anomalous lines; 2) if we break the anomalous lines, the remaining part of the diagram with four free ends can be divided into two parts by cutting it through two internal lines (such four-point diagrams, as is well known, belong to the so-called class of "parquet" diagrams). Below we shall sum these diagrams for $\varepsilon(\delta)$. For this it is convenient to express their sum in terms of the vertex part $\gamma(k_1\sigma_1, k_2\sigma_2; k_3\sigma_3, k_4\sigma_4)$ (here $k = (k, \omega)$, and δ is the spin index[13]):

$$\varepsilon(\delta) = -i(8\pi^2)^{-1}\sum_{\sigma_1\sigma_2}\sum_{k_1k_2}\int_{-\infty}^{\infty}d\omega_1\int_{-\infty}^{\infty}d\omega_2 G(k_1,\omega_1)G(k_2,\omega_2)$$
$$\times\gamma(k_1\sigma_1, k_2\sigma_2; k_1+\pi, \sigma_1, k_2+\pi, \sigma_2), \qquad (4)$$

where $G(k, \omega)$ is the Green function corresponding to the anomalous pairing:

$$G(k, \omega) = iu_k v_k((\omega-\varepsilon(k)+i\lambda)^{-1}-(\omega+\varepsilon(k)-i\lambda)^{-1}), \quad \lambda\to 0.$$

This relation is represented schematically in Fig. 2.

As can be seen from (4), the variables of the vertex part are chosen in accordance with the condition

$$k_3 = k_1+\pi, \quad \omega_3 = \omega_1, \quad \sigma_3 = \sigma_1,$$
$$k_4 = k_2+\pi, \quad \omega_4 = \omega_2, \quad \sigma_4 = \sigma_2. \qquad (5)$$

The general scheme of the summation of such diagrams is well known.[17,18] In Refs. 18 and 19 the indicated approximation was used to calculate the Green functions with the aim of investigating the instabilities that arise in a one-dimensional system under the influence of interaction between the electrons, but with $\delta = 0$.

The set of all diagrams for the vertex part can be divided into four classes[17]: diagrams γ_1 that are reducible from k_1, k_2 to k_3, k_4 (i.e., diagrams that can be divided into two parts, containing k_1, k_2 and k_3, k_4, by cutting two internal lines of the diagram); diagrams γ_2 that are reducible from k_1, k_3 to k_2, k_4, diagrams γ_3 that are reducible from k_1, k_4 to k_2, k_3, and irreducible diagrams (an example of such a diagram is the first-order vertex part). The vertex parts γ_1, γ_2, and γ_3 are then determined from the solution of a system of coupled nonlinear integral equations.[17,20]

We note also that since the arguments of the vertex part are connected by the relation $k_1 + k_2 = k_3 + k_4$, each of the vertex parts depends on three variables, which are conveniently chosen as follows (to simplify the writing, we omit the spin indices for now):

$$\gamma_1 = \gamma_1(k_1, k_3, Q), \quad Q = k_1+k_2,$$
$$\gamma_2 = \gamma_2(k_1, k_4, \zeta), \quad \zeta = k_1-k_3, \qquad (6)$$
$$\gamma_3 = \gamma_3(k_1, k_3, \eta), \quad \eta = k_1-k_4.$$

The leading logarithmic contribution to the integral (4) is made by the region of momenta $k_1, k_2 \cong \pm\pi/2$. Accordingly, the behavior of $\gamma(k_1\sigma_1, k_2\sigma_2; k_3\sigma_3, k_4\sigma_4)$ is important only for momenta $\cong \pm\pi/2$. According to (5), to calculate $\varepsilon(\delta)$ it is necessary to know only the following vertex parts:

$$\gamma^{+--+} = \gamma^{-++-}, \quad \gamma^{++--} = \gamma^{--++},$$

where the signs $\pm$ correspond to momenta $\pm\pi/2$. It is also not difficult to convince oneself that the vertex parts $\gamma_1^{+\,+\,-\,-}$ and $\gamma_3^{+\,-\,-\,+}$ in (4) do not give the highest power of the logarithm in the corresponding order of perturbation theory and so can be omitted.

Thus, the following vertex parts contribute to (4):

$$\gamma_1^{\,1} = \gamma_1^{\,+--+}, \quad \gamma_3^{\,1} = \gamma_3^{\,++--}, \quad \gamma_2^{\,1} = \gamma_2^{\,++--}, \quad \gamma_2^{\,2} = \gamma_2^{\,+--+}.$$

In calculating the functions γ_1^1 and γ_3^1 we can, with logarithmic accuracy, take $\delta = 0$ (this fact is easily verified for the lowest-order diagrams). According to (5) and (6), the vertex part γ_1^1 appearing in (4) is a function of k_1 and k_2:

$$\gamma_1^{\,1} = \gamma_1^{\,1}(k_1, k_1, k_1+k_2).$$

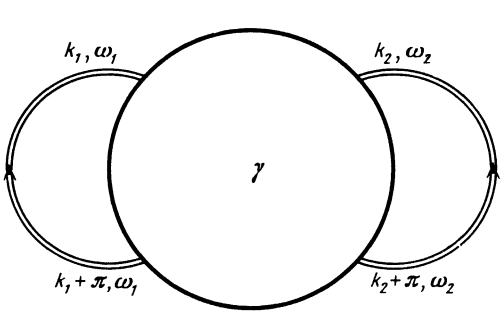

FIG. 2. Equation for $\varepsilon(\delta)$ (diagrammatic).

In accordance with the logarithmic character of γ_1^1,

$$\gamma_1^1(k_1,\ k_1,\ k_1+k_2)=\gamma_1^1(\min\{\ln|k_1|,\ \ln|k_2|\}).$$

Analogously,

$$\gamma_3^1=\gamma_3^1(\min\{\ln|k_1|,\ \ln|k_2|\}).$$

As regards the functions γ_2^1 and γ_2^2 appearing in (4), by virtue of (5) we cannot set $\delta=0$ when calculating them.

Calculation of the contributions of higher-order diagrams shows that if the arguments of γ_2 are related by the condition (5), then

$$\gamma_2^{1,2}=\gamma_2^{1,2}(\ln|k_1|,\ln|k_2|,\ln\delta).$$

Taking the aforementioned considerations into account, we can write the expression (4) in the form

$$\varepsilon(\delta)=\delta^2\sum_{\sigma,\sigma_1}\int_0^\Phi dt_1\int_0^\Phi dt_2\{\gamma_1^1(\min(t_1,t_2))-\gamma_3^1(\min(t_1,t_2))+\gamma_2^2(t_1,t_2,\Phi)-\gamma_2^1(t_1,t_2,\Phi)\},\quad(7)$$

where $\Phi=-(2\pi)^{-1}\ln\delta$, and in (7) we have changed to the logarithmic variables $t_i=-\ln\delta k_i$.

Thus, the vertex parts γ_1^1 and γ_3^1 appearing in (7) are functions of one variable. As regards the functions γ_2^1 and γ_2^2, they are functions of three variables, and to find them one can use the method developed in Ref. 18.

We shall transform the expression (7) to a more compact form. For this, in order to avoid unnecessarily cumbersome calculations, we shall carry out this transformation for the spinless variant of the model (1) with the potential $\nu(q)=g\cos q$ (nearest-neighbor interaction), with $g\ll 1$. We write (7) in the form

$$\varepsilon(\delta)=-\delta^2\int_0^\Phi dt_1\int_0^\Phi dt_2\,F(t_1,t_2,\Phi),\quad(8)$$

$$F(t_1,t_2,\Phi)=2g-\gamma_1^1(\min(t_1,t_2))+\gamma_3^1(\min(t_1,t_2))-\gamma_2^2(t_1,t_2,\Phi)+\gamma_2^1(t_1,t_2,\Phi)\quad(9)$$

(in (8) we have added to $\varepsilon(\delta)$ the term of first order in g).

Writing out the equations for γ_1, γ_2, and γ_3, we can show that $F(t_1,t_2,\Phi)$ satisfies the equation

$$F(t_1,t_2,\Phi)=r(\min(t_1,t_2))+\int_0^\Phi r(\min(t_1,t'))F(t',t_2,\Phi)\,dt',\qquad r(t)=2g-\gamma_1^1(t)+\gamma_3^1(t).\quad(10)$$

The solution of (10) can be found by the method developed in Ref. 18 and has the form

$$F(t_1,t_2,\Phi)=h(\min(t_1,t_2))f(\max(t_1,t_2))+h(t_1)h(t_2)\int_{\max(t_1,t_2)}^\Phi f^2(t)\,dt,\quad(11)$$

$$h(t)=\varphi(t)\exp\left(-\int_0^t\varphi(t')\,dt'\right),\qquad f(t)=\exp\left(\int_0^t\varphi(t')\,dt'\right).\quad(12)$$

The function $\varphi(t)=F(t,t,t)$ is the solution of the equation

$$\varphi(t)=r(t)+\int_0^t\varphi^2(t')\,dt'.\quad(13)$$

Substituting (11) into (8) and adding to (8) the zeroth-order term $(\varepsilon(\delta)|_{g=0})$, we obtain

$$\varepsilon(\delta)=-\delta^2\int_0^\Phi f^2(t)\,dt.\quad(14)$$

Thus, the problem of calculating $\varepsilon(\delta)$ reduces to the determination of the function $\varphi(t)$.

The spectrum of the spinless Hamiltonian (1) with $\delta=0$ is gapless. For $\delta\neq 0$ there is a gap in the excitation spectrum. The magnitude Δ of the gap can be expressed in terms of the vertex part (the corresponding equation is represented graphically in Fig. 3):

$$\Delta=2\delta+2\delta\int_0^\Phi[2g+\gamma_3^1(t)-\gamma_1^1(t)+\gamma_2^1(\Phi,t,\Phi)-\gamma_2^2(\Phi,t,\Phi)]\,dt.\quad(15)$$

Substituting the expression (9) into (15) and making use of the relations (11)–(13), we obtain

$$\Delta(\delta)=2\delta f(\Phi).\quad(16)$$

The formulas (14) and (16) express the electron part of the deformation energy and the "Peierls" gap in terms of the solutions of "parquet" equations.

THE SPINLESS MODEL

The parquet equations for the spinless case have the form

$$\begin{aligned}
\gamma_1^1(t)+\gamma_1^2(t)&=-(1/2)\int_0^t[\gamma_2^2(t')+\gamma_3^2(t')+\gamma_1^1(t')+\gamma_1^2(t')]^2dt',\\
\gamma_1^2(t)-\gamma_1^1(t)&=-1/2\int_0^t[4g+\gamma_3^2(t')-\gamma_2^2(t')+\gamma_1^2(t')-\gamma_1^1(t')]^2dt',\\
\gamma_3^2(t)\pm\gamma_3^1(t)&=\int_0^t[2g+\gamma_1^2(t')\pm\gamma_2^1(t')+\gamma_3^2(t')\pm\gamma_3^1(t')]^2\,dt',\\
\gamma_2^2(t)\pm\gamma_2^1(t)&=-\int_0^t[-2g+\gamma_1^1(t')\pm\gamma_3^1(t')+\gamma_2^2(t')\pm\gamma_2^1(t')]^2dt',\\
\gamma_1^2&=\gamma_1^{+-+-},\qquad \gamma_3^2=\gamma_3^{+-+-}.
\end{aligned}\quad(17)$$

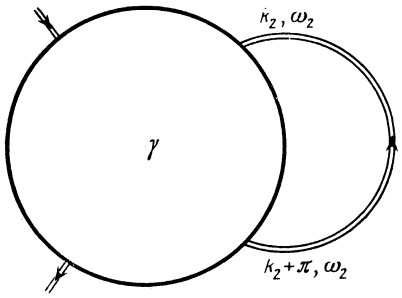

FIG. 3. Equation for the Peierls gap (diagrammatic).

The solution of the system of equations (17) has the form

$$\gamma_1^1(t)=-\gamma_1^2(t)=\gamma_3^2(t)=-\gamma_2^2(t)=4g^2t,$$
$$\gamma_2^1(t)=\gamma_3^1(t)=0.$$

As a result the functions $\varphi(t)$ and $f(t)$ are equal to

$$\varphi(t)=2g, \quad f(t)=\exp(2gt). \tag{18}$$

Substitution of (18) into (14) and (16) gives

$$\varepsilon(\delta)=-(4g)^{-1}\delta^2[\exp(4g\Phi)-1], \tag{19}$$

$$\Delta(\delta)=2\delta\exp(2g\Phi). \tag{20}$$

As follows from (19) and (20), for $g\Phi\ll 1$,

$$\varepsilon(\delta)=(2\pi)^{-1}\delta^2\ln\delta, \quad \Delta(\delta)=2\delta,$$

which corresponds to the approximation of noninteracting particles (the Peierls result). For $\delta\to 0$ ($g\Phi\gg 1$),

$$\begin{aligned}&\varepsilon(\delta)=-(4g)^{-1}\delta^{2-2g/\pi}, \quad g>0;\\ &\varepsilon(\delta)=-\delta^2/4|g|, \quad g<0,\\ &\Delta(\delta)=2\delta^{1-g/\pi}.\end{aligned} \tag{21}$$

Thus, if the interaction is repulsive, the system is certainly unstable against a transition to the Peierls state, and the magnitude of the gap increases in comparison with its value for $g=0$. In the case of attraction, suppresion of the Peierls instability is, in principle, possible.

The formulas (19) and (20) were obtained by summing parquet diagrams. These formulas can also be obtained in another, simpler way.[14] Namely, we reduce the Hamiltonian (1) to the Hamiltonian of a model with a linear spectrum, using the following replacement of the Fermi operators:

$$c_{1k}=a_k, \quad k\approx\pi/2; \quad c_{2k}=a_k, \quad k\approx-\pi/2. \tag{22}$$

As a result, (1) goes over into the Hamiltonian of the massive Thirring model:

$$\hat{H}=-\sum_k k(c_{1k}^+c_{1k}-c_{2k}^+c_{2k})+i\delta\sum_k(c_{1k}^+c_{2k}-c_{2k}^+c_{1k})$$
$$+(2g/N)\sum c_{1k+q}^+c_{1k}c_{2k'-q}^+c_{2k'}. \tag{23}$$

It is well known that the transformation of a Hamiltonian of the type (1) to the Hamiltonian of a model with a linear spectrum requires a degree of care, and in any case can be valid, if at all, only for $g\ll 1$. In the present case, however, we can convince ourselves by direct inspection that the contributions of the diagrams to $\varepsilon(\delta)$ for (1) and (23) coincide in the leading logarithmic approximation, although the contributions to $E_0(0)$ for these two models differ! For the Hamiltonian (23) the exact solution, obtained by means of the Bethe ansatz, is known for the ground-state energy and the excitation spectrum.[21] Use of the results of Ref. 21 for $g\ll 1$ leads to the expressions (19) and (20). Unfortunately, however, the model of the type (23) with spin degrees of freedom, to which the Hamiltonian (1) can be reduced, is certainly nonintegrable.

WEAK-COUPLING REGIME (PARTICLES WITH SPIN)

Summing in (7) over the spin variables and performing calculations analogous to those which led to (14) and (16), we obtain

$$\varepsilon(\delta)=-2\delta^2\int_0^\Phi f^2(t)\,dt, \tag{24}$$

$$\Delta=2\delta f(\Phi), \tag{25}$$

where $f(t)$ is defined in (12).

Omitting the cumbersome calculations, we give the expression for $\varphi(t)$:

$$\varphi(t)=-\lambda_4(t)/2-3\lambda_1(t)/2\pm\lambda_3(t), \tag{26}$$

where the upper sign corresponds to the choice of $\hat{V}$ in the form (2), and the lower sign to the choice of $\hat{V}$ in the form (3). The functions λ were found in Ref. 19 and have the form

$$\lambda_1(t)=g_1(1+2g_1t)^{-1}, \quad \lambda_4(t)=-C\operatorname{cth}C(C_1-2t),$$
$$\lambda_3(t)=\pm C\operatorname{sh}^{-1}(C_1-2t), \tag{27}$$
$$C=(g_4^2-g_1^2)^{1/2}, \quad C_1=(2C)^{-1}\ln\{(g_4-C)(g_4+C)^{-1}\},$$
$$g_1=v(\pi), \quad g_4=v(\pi)-2v(0).$$

We have confined ourselves here to the case $|g_4|\geqslant|g_1|$. Substituting (27) into (26) and using (12), we find

$$f_0(t)=(\operatorname{sh}CC_1)^{1/4}(\operatorname{sh}C(C_1-2t))^{-1/4}(1+2g_1t)^{-3/4}$$
$$\times\operatorname{th}(CC_1/2)^{\mp\varkappa/2}\operatorname{th}(C(C_1-2t)/2)^{\pm\varkappa/2}, \tag{28}$$
$$\varkappa=\operatorname{sign}g_1\operatorname{sign}g_4,$$

where the upper sign corresponds to (2), and the lower sign to (3).

In connection with formula (26) we note the following interesting fact. The representation of $\varphi(t)$ in the form (26) implies that $f(t)$ can be factorized into ρ and σ factors in accordance with the ρ,σ breakdown of the linearized Hamiltonian $\hat{H}_0+\hat{H}_1$ (1) (Ref. 22): $\hat{H}_0+\hat{H}_1\to\hat{H}_\rho+\hat{H}_\sigma$ ($[\hat{H}_\rho,\hat{H}_\sigma]=0$), where (in standard notation)

$$\hat{H}_\sigma=(2\pi v_\sigma/L)\sum_{k>0}[\sigma_1(k)\sigma_1(-k)+\sigma_2(-k)\sigma_2(k)]$$

$$-(g_{1\parallel}/L)\sum_{k>0}[\sigma_1(k)\sigma_2(-k)+\sigma_1(-k)\sigma_2(k)]$$

$$+g_{1\perp}(2\pi d)^{-2}\int_0^L dx\{\exp 2^{1/2}(\Phi_{1\sigma}^+(x)$$

$$+\Phi_{2\sigma}(x))\exp 2^{1/2}(-\Phi_{2\sigma}^+(x)-\Phi_{1\sigma}(x))+\text{H.c.}\},\qquad(29)$$

$$\hat{H}_\rho=(2\pi v_\rho/L)\sum_{k>0}[\rho_1(k)\rho_1(-k)+\rho_2(-k)\rho_2(k)]$$

$$-(g_4/L)\sum_{k>0}[\rho_1(k)\rho_2(-k)$$

$$+\rho_1(-k)\rho_2(k)]+g_3(2\pi d)^{-2}\int_0^L dx\{\exp 2^{1/2}[\Phi_{1\rho}^+(x)$$

$$+\Phi_{2\rho}(x)]\exp 2^{1/2}[-\Phi_{2\rho}^+(x)-\Phi_{1\rho}(x)]+\text{H.c.}\},$$

$$\Phi_{s\rho}^+(x)=(2\pi/L)\sum_{k>0}k^{-1}\exp(-dk/2\mp ikx)\rho_s(k),\qquad s=1,2$$

(d is a cutoff parameter), and analogously for $\Phi_{1\sigma}^{+}$ and $\Phi_{2\sigma}^{+}$. The operators $\rho_1(k)$ and $\rho_2(k)$ satisfy the following commutation relations:

$$[\rho_1(-k),\ \rho_1(k')]=[\rho_2(k),\ \rho_2(-k')]=(kL/2\pi)\delta_{k,k'},$$
$$[\rho_1(k),\ \rho_2(k')]=0$$

while the σ operators satisfy analogous relations. In writing the integral terms in $\hat{H}_\rho$ and $\hat{H}_\sigma$ we have used the boson representation of Ref. 23 for the Fermi operators of the linearized Hamiltonian:

$$\psi_s(x)=L^{-1/2}\exp(\pm ik\mp x)\exp(\Phi_s^+(x))\exp(-\Phi_s(x));\ s=1,\ 2.\qquad(30)$$

In our case, $g_{1\parallel}=g_{1\perp}=g_1=g_3$.

It is easy to see that the first term in (26) corresponds to $\hat{H}_\sigma$, while the second and third terms correspond to $\hat{H}_\rho$.

We return now to the calculation of $\varepsilon(\delta)$ and $\Delta(\delta)$, and consider certain simple particular cases that can be obtained from (28).

1. The Hubbard model ($g_1=-g_4=\gamma_0$):

$$\varepsilon_1(\delta)=-2\delta^2\Phi(1-4\gamma_0^2\Phi^2)^{-1/2},\qquad \Delta_1(\delta)=2\delta(1-4\gamma_0^2\Phi^2)^{-3/4},$$

$$\varepsilon_2(\delta)=\gamma_0^{-1}-\gamma_0^{-1}(1-2\gamma_0\Phi)^{1/2}(1+2\gamma_0\Phi)^{-1/2}$$

$$-(2\gamma_0)^{-1}\arcsin(2\gamma_0\Phi),\qquad(31)$$

$$\Delta_2(\delta)=2\delta(1-2\gamma_0\Phi)^{1/4}(1+2\gamma_0\Phi)^{-3/4}.$$

The indices 1 and 2 refer to (2) and (3), respectively.

2. The Hubbard model. The band is half-filled (umklapp processes are neglected, and so $\lambda_3=0$):

$$\varepsilon_{1,2}(\delta)=-2\delta^2\int_0^\infty\exp(4\gamma_0 t)(1+2\gamma_0 t)^{-3/2}dt,$$

$$\Delta_{1,2}(\delta)=2\delta\exp(2\gamma_0\Phi)(1+2\gamma_0\Phi)^{-3/4}.\qquad(32)$$

3. The model with Hubbard coupling γ_0 and nearest-neighbor coupling γ_1, with $\gamma_0=2\gamma_1$:

$$\varepsilon_{1,2}(\delta)=-(\delta^2/2\gamma_0)\exp(4\gamma_0\Phi)-1,\qquad \Delta_{1,2}(\delta)=2\delta\exp(4\gamma_0\Phi).\qquad(33)$$

4. The same model with $\gamma_0=-2\gamma_1$:

$$\varepsilon_1(\delta)=-(\delta^2/\gamma_0)\ln(1+4\gamma_0\Phi),\qquad \Delta_1=2\delta(1+4\gamma_0\Phi)^{-1/2},$$
$$\varepsilon_2(\delta)=-(\delta^2/4\gamma_0)((1+\gamma_0\Phi)^2-1),\qquad \Delta_2=2\delta(1+4\gamma_0\Phi)^{-3/2}.\qquad(34)$$

As can be seen from (31)–(34), for $g\Phi\ll 1$ we have

$$\varepsilon(\delta)=(\delta^2/\pi)\ln\delta,\qquad \Delta=2\delta,$$

which corresponds to the limit of noninteracting electrons. However, with decrease of δ there are two entirely different situations. For example, $\varepsilon(\delta)$ as determined from (33) remains small and proportional to $-\delta^{2-2\gamma_0/\pi}$ as $\delta\to 0$, whereas for the Hubbard model, according to (31), $\varepsilon(\delta)$ diverges as $\delta\to\delta_0=\exp(-\pi/|\gamma_0|)$. These two situations are typical in the problem of the Peierls instability. The first of them corresponds to the weak-coupling regime for all $\delta\ll 1$. The other is characterized by strengthening of the coupling upon decrease of δ. Analysis of the expressions (28) shows that the second situation is realized only when there is a correlation gap in the excitation spectrum of $\hat{H}_0+\hat{H}_1$. As can be seen from (28), (31), (32), and (34) the values δ_0 at which $\varepsilon(\delta)$ and $\Delta(\delta)$ become singular coincide with the exact values (found in Ref. 24) of the correlation gaps of the linearized Hamiltonian $\hat{H}_0+\hat{H}_1$.

Thus, if the spectrum of $\hat{H}_0+\hat{H}_1$ has no correlation gap, as in the cases 3) or 2) and 4) with $\gamma_0>0$, it is legitimate to use perturbation theory, i.e., the expressions (19) and (32)–(34) are valid for all $\delta\ll 1$ (here the behavior of $\varepsilon(\delta)$ as $\delta\to 0$ is not universal).

The presence of a correlation gap Δ_{corr} in the spectrum implies that Δ_{corr} establishes for the variable δ a scale that divides the range of variation of δ into a weak-coupling ($\delta\gg\Delta_{\text{corr}}$) and a strong-coupling ($\delta\ll\Delta_{\text{corr}}$) region. Perturbation theory is applicable only for $\delta\gg\Delta_{\text{corr}}$. In the strong-coupling region, methods based on perturbation theory in $\hat{H}_1$ are inapplicable.

THE STRONG-COUPLING REGIME

We now consider the region of parameters $\delta\ll\Delta_{\text{corr}}$, which corresponds to the strong-coupling regime. In this case it is natural to use perturbation theory not in $\hat{H}_1$, as was done earlier, but in $\hat{V}$. The difficulty, however, is that for this it is necessary to know the spectrum and wave functions of $\hat{H}_0+\hat{H}_1$, which are unknown. If these had been found, however, in the case of no correlation gap we would have obtained results coinciding with the "parquet" results as $\delta\to 0$.

It would appear that the presence of a gap simplifies the problem, since $\delta/\Delta_{\text{corr}}\ll 1$ and the excited states with $\Delta E=\Delta_{\text{corr}}$ give small contributions. It is necessary, however, to keep in mind that in the spectrum of $\hat{H}_0+\hat{H}_1$, besides such excitations there are also gapless excitations, and it is these which lead to dangerous denominators in the perturbation-theory series. It is natural, therefore, to try to sep-

arate the excitations of these two types and to reduce the problem to perturbation theory in $\hat{V}$ on the gapless excitations. It turns out that such a program can indeed be carried out.

The indicated separation can be carried out as follows. The initial Hamiltonian $\hat{H}_0 + \hat{H}_1$ can be reduced by means of the replacements (22) to a linearized Hamiltonian of the type (23), which, in turn, is reduced to (29). The Hamiltonian (29) is a sum of commuting Hamiltonians $\hat{H}_\rho$ and $\hat{H}_\sigma$. In the case of interest to us (when the spectrum of $\hat{H}_0 + \hat{H}_1$ has a correlation gap and gapless excitations), as follows from Ref. 24 one of the Hamiltonians has a spectrum that starts from the gap, while the spectrum of the other is gapless. If, for definiteness, we choose as $\hat{H}_0 + \hat{H}_1$ the Hubbard Hamiltonian with $\gamma_0 > 0$, the role of the first Hamiltonian is played by $\hat{H}_\rho$, and that of the second by $\hat{H}_\sigma$.

We write $\hat{V}$ in the ρ and σ representations. By making use of (22) (here (2) can be carried over into (3) by the replacement $g_3 \to -g_3$, as follows from the canonical transformation $\psi_1^+(x) \to \tilde{\psi}_1^+(x)$ and $\psi_2^+(x) \to i\tilde{\psi}_2^+(x)$) and (30), we obtain

$$\hat{V} = (\delta/2\pi d) \int_0^L dx\, \hat{V}_\rho(x) \hat{V}_\sigma(x),$$

$$\hat{V}_{\rho(\sigma)}(x) = \exp\{2^{-1/2}[\Phi^+_{1\rho(\sigma)}(x) + \Phi_{2\rho(\sigma)}(x)]\} \tag{35}$$

$$\times \exp\{-2^{-1/2}[\Phi^+_{2\rho(\sigma)}(x) + \Phi_{1\rho(\sigma)}(x)]\} + \text{H.c.}$$

As a result the initial Hamiltonian takes the form

$$\hat{H} = \hat{H}_\rho + \hat{H}_\sigma + \hat{V}. \tag{36}$$

In second order of perturbation theory in $\hat{V}$,

$$\varepsilon^{(2)}(\delta) = (\delta/2\pi d)^2 \sum_{n,m} (E_0 - E_n - E_m)^{-1} \int_0^L dx \int_0^{L'} dx' (V_\rho(x))_{0n}$$

$$\times (V_\rho(x'))_{n0} (V_\sigma(x))_{0m} (V_\sigma(x'))_{m0}, \tag{37}$$

where n and m label the excited states of the ρ and σ Hamiltonians, respectively.

The sum in (37) with $n = 0$ corresponds to taking the excited states of $\hat{H}_\sigma$ alone into account. But the sum with $n \neq 0$ is obviously smaller than

$$\delta^2 \Delta_{\text{corr}}^{-1} (\hat{V}^2)_{00} - (\delta/2\pi d)^2 (V_\rho)_{00}^2 \int dx \int dx' (V_\sigma(x) V_\sigma(x'))_{00}. \tag{38}$$

The first term in (38) is proportional to δ^2 while the second differs from the sum with $n = 0$ by the absence of an energy denominator. A similar analysis of higher orders of perturbation theory shows that the most divergent contributions to $\varepsilon(\delta)$ correspond to using $\hat{V}$ in the form

$$\hat{V} = (\delta/2\pi d)(V_\rho)_{00} \int dx \hat{V}_\sigma(x). \tag{39}$$

The subsequent analysis is based on the solution of the following auxiliary problem. We shall calculate the energy of the ground state of the Hamiltonian

$$\hat{H} = \hat{H}_0 + a \int_0^L dx [W_\alpha(x) + W_\alpha^+(x)],$$

$$\hat{H}_0 = 2\pi L^{-1} \sum_{k>0} [\sigma_1(k)\sigma_1(-k) + \sigma_2(-k)\sigma_2(k)], \tag{40}$$

$$\hat{W}_\alpha(x) = \exp\{\alpha^{1/2}[\Phi_{1\sigma}^+(x) + \Phi_{2\sigma}(x)]\}$$

$$\times \exp\{-\alpha^{1/2}[\Phi_{2\sigma}^+(x) + \Phi_{1\sigma}(x)\}.$$

For the quantity $\varepsilon(a) = [E_0(a) - E_0(0)]/L$ we shall have the expansion

$$\varepsilon(a) = \sum_{n=1}^{\infty} a^{2n} c_{2n}(L, \alpha), \tag{41}$$

where $c_{2n}(L, \alpha)$ are the contributions of the $2n$-th order of the perturbation-theory series and are, generally speaking, functions of L. When the time technique is used to calculate them, the problem reduces to taking integrals over x and t of averages (over the Bose vacuum of $\hat{H}_0$) of the form

$$\langle W_\alpha(x_1, 0) W_\alpha^*(x_2, t_2) \ldots W_\alpha^*(x_{2n}, t_{2n}) \rangle,$$
$$W_\alpha(x, t) = \exp(itH_0) W_\alpha(x) \exp(-itH_0). \tag{42}$$

In the average (42) there are n of each of the operators W_α and W_α^*. This average is calculated by pulling the creation operators $\Phi_{1\sigma}^+$ and $\Phi_{2\sigma}^+$ through to the left, and the annihilation operators $\Phi_{1\sigma}$ and $\Phi_{2\sigma}$ to the right. As a result, the average (42) is equal to

$$(2\pi d/L)^{2n\alpha} \prod_{i<j} \exp\left\{\alpha\sigma_{ij} \sum_{s=1}^{2} [\Phi_{s\sigma}(x_i, t_i), \Phi_{s\sigma}^+(x_j, t_j)]\right\},$$
$$\sigma_{ij} = (-1)^{i-j-1}. \tag{43}$$

In (43) the exponentials of the commutators are equal to

$$\exp\{\alpha[\Phi_{s\sigma}(x, t), \Phi_{s\sigma}^+(x', t')]\}$$
$$= \{1 - \exp[-2\pi d/L \pm i2\pi(x' - x)/L + i2\pi(t' - t)/L]\}^{-\alpha}, \tag{44}$$

where the plus and minus signs refer to $s = 1$ and $s = 2$, respectively. After taking the integrals of (43) over x and t, we obtain

$$c_{2n}(L, \alpha) \propto \int_{(2\pi/L)}^{d^{-1}} \prod_{i=2}^{2n} dk_{i1} \prod_{2<i<j} dk_{ij} dk_{ij}' (k_{21} + k_{31} + \ldots + k_{2n,1})^{-1}$$

$$\times (k_{31} + k_{32} + \ldots + k_{2n,1} + k_{2n,2})^{-1}$$

$$\times \ldots (k_{2n,1} + k_{2n,2} + \ldots + k_{2n,2n-1})^{-1}$$

$$\times \prod_{i<j} (k_{ij} k_{ij}')^{\sigma_{ij}\alpha - 1} \tag{45}$$

and the $k_{i,1}$ $(i = 2, \ldots, 2n)$ are expressed in terms of the integration variables by the relations

$$k_{21}' = k_{21} - k_{32} + k_{32}' - \ldots - k_{2n,2} + k_{2n,2}',$$

$$k_{31}' = k_{31} + k_{32} - k_{32}' - \ldots - k_{2n,3} + k_{2n,3}',$$

$$\ldots\ldots\ldots\ldots\ldots\ldots$$

$$k_{2n,1}' = k_{2n,1} + k_{2n,2} - k_{2n,2}' + \ldots + k_{2n,2n-1} - k_{2n,2n-1}'.$$

If we rescale the variables in (45) by

$$k_{ij}=(2\pi/L)\tilde{k}_{ij},$$

it is not difficult to convince oneself that

$$c_{2n}(L,\ \alpha)\infty A_{2n}+B_{2n}L^{-2+n(4-2\alpha)}, \tag{46}$$

where A_{2n} and B_{2n} are certain constants (depending on α). It follows from the expression (46) that if

$$-2+n(4-2\alpha)\leqslant 0 \tag{47}$$

for all n, then in the thermodynamic limit $c_{2n}\propto$ const and the sum (41) is a regular function of a as $a\to 0$. But if

$$-2+n(4-2\alpha)>0, \tag{48}$$

then $\varepsilon(a)$ has a singular as well as a regular part as $a\to 0$, i.e.,

$$\varepsilon(a)=\varepsilon_{\text{reg}}(a)+\varepsilon_{\text{sing}}(a). \tag{49}$$

As $a\to 0$, $\varepsilon_{\text{reg}}\propto a^2$. The behavior of $\varepsilon_{\text{sing}}(a)$ as $a\to 0$ can be established on the basis of dimensionality arguments, just as was done in the theory of the two-dimensional Coulomb gas in Ref. 25.

To this end we substitute (46) into (41). As a result we obtain

$$\varepsilon(a)=\varepsilon_{\text{reg}}(a)+|a|^{2/(2-\alpha)}R(|a|^{1/(2-\alpha)}L), \tag{50}$$

where $R(x)$ is an unknown function. It is clear, however, that in the thermodynamic limit this function should be a finite quantity, dependent on α. Thus, the singular behavior of $\varepsilon(a)$ is determined by the critical index

$$\lambda=2/(2-\alpha). \tag{51}$$

In connection with formula (51) we make the following remark. We apply to the Hamiltonian (40) the well known canonical transformation[26]

$$\tilde{H}=\exp(iS)\hat{H}\exp(-iS),$$
$$S=(2\pi/L)\varphi\sum_{k>0}k^{-1}[\sigma_1(k)\sigma_2(-k)+\sigma_1(-k)\sigma_2(k)]. \tag{52}$$

The first term of (40) then goes over into the Hamiltonian of the Tomonaga-Luttinger model, and $\alpha^{1/2}$ in the second term is replaced by $\alpha^{1/2}\exp\varphi$. If we take $\exp\varphi=\alpha^{-1/2}$ and formally go over to operators of spinless Fermi particles in accordance with the relation (30), then (40) goes over into the Hamiltonian of the massive Thirring model. Analogously, by the choice $\exp\varphi=(2/\alpha)^{1/2}$ we can formally reduce (40) to the Hamiltonian of another exactly solvable model[24]—the interacting Fermi gas with a linear spectrum. By making use of the results of Refs. 21 and 24, we obtain for λ in the first case

$$\lambda=2(1+2\pi^{-1}\operatorname{arctg}(\pi(1-\alpha^2)/2(1+\alpha^2)))^{-1}, \tag{53}$$

and in the second case

$$\lambda=(4+\alpha^2)/(4-\alpha^2). \tag{54}$$

The expressions (53) and (54) differ from the exact formula (51). This difference indicates the approximate character of the reduction of the Hamiltonian (40) to Fermi Hamiltonians. The authors of Refs. 24 and 27 also indicated the approximate character of this reduction.

We return now to the calculation of the energy of the ground state of (36) with $\hat{V}$ in the form (39). The problem in this case reduces to the corresponding problem for the Hamiltonian

$$\hat{H}_\sigma+\hat{V} \tag{55}$$

and to the calculation of the average $(V_\rho)_{00}$ over the ground state of the Hamiltonian $\hat{H}_\rho$.

We shall consider first the Hamiltonian (55). First of all we make the canonical transformation (52), which diagonalizes the bilinear part of $\hat{H}_\sigma$. This is achieved by choosing φ in the form (even though $g_{1\parallel}=g_{1\perp}$, it is convenient to distinguish these two quantities):

$$\operatorname{th}2\varphi=g_{1\parallel}/2\pi. \tag{56}$$

Here the operators in the exponentials in (29) are multiplied by $\exp\varphi$, corresponding to the replacement $2^{1/2}\to 2^{1/2}\exp\varphi$. As a result, (55) is reduced to the Hamiltonian

$$\hat{H}=\hat{H}_0+g_{1\perp}(2\pi d)^{-2}\int_0^L[W_{4\alpha}(x)+W_{4\alpha}^*(x)]\times dx+a\int_0^L[W_\alpha(x)+W_\alpha^*(x)]dx,$$
$$\hat{H}_0=2\pi L^{-1}v_\sigma\sum[\sigma_1(k)\sigma_1(-k)+\sigma_2(-k)\sigma_2(k)], \tag{57}$$
$$\alpha=\exp(2\varphi)/2,\quad a=(\delta/2\pi d)(V_\rho)_{00},$$

where $v_\sigma=1-(g_1/2\pi)^2$ (in the following we shall approximate v_σ by 1).

Expansion of the ground-state energy in a perturbation-theory series in a^2 leads to the expression (50). Allowance for the cross terms $a^2g_{1\perp}^{2n}$ gives the following contribution to $\varepsilon(a)$:

$$\varepsilon(a)=a^2\sum_{n=0}^{\infty}\tilde{c}_{2n}(L)g_{1\perp}{}^{2n}. \tag{58}$$

The dependence of the coefficients $\tilde{c}_{2n}(L)$ on L is estimated as in the derivation of (46):

$$\tilde{c}_{2n}(L)\infty L^{2+4n(1-2\alpha)-2\alpha}. \tag{59}$$

In (59) we have written out the singular part of $\tilde{c}_{2n}(L)$. It follows from (59) and (46) that

$$\tilde{c}_{2n}(L)=c_2(L)L^{4n(1-2\alpha)}.$$

Since $g_{1\parallel}>0$, the inequality

$$4n(1-2\alpha)<0$$

is fulfilled for all $n\geqslant 1$, and $\tilde{c}_{2n}/c_2$ vanishes in the thermodynamic limit. An analogous situation also obtains for the

cross terms of higher orders in a^2. Thus, in the determination of the singular part of $\varepsilon(a)$ the second term in (57) can be neglected and the critical index of $\varepsilon(a)$ is given by formula (51).

We now consider the average $(V_\rho)_{00}$ appearing in a in (57). It turns out that $(V_\rho)_{00}$ can also be calculated using dimensionality arguments, if

$$|g_3/g_4| \ll 1.$$

First of all, we diagonalize the bilinear part of $\hat{H}_\rho$; this leads to the replacements

$$2^{1/2} \to 2^{1/2} \exp\psi, \quad 2^{-1/2} \to 2^{-1/2} \exp\psi \ (\text{th}\, 2\psi = g_4/2\pi)$$

in the exponential parts of $\hat{H}_\rho$ and $\hat{V}_\rho$, respectively.

We expand $(V_\rho)_{00}$ in series in g_3:

$$(V_\rho)_{00} = \sum_n d_{2n}(L) g_3^{2n-1}. \tag{60}$$

The coefficients $d_{2n}(L)$ correspond to perturbation-theory terms arising from averages of the type

$$\langle W_{\alpha'/4}(x_1, 0) W_{\alpha'}^*(x_2, t_2) \ldots W_{\alpha'}^*(x_{2n}, t_{2n}) \rangle, \quad \alpha' = 2\exp 2\psi, \tag{61}$$

where the first operator in the average (61) corresponds to $\hat{V}_\rho$, and the others correspond to the exponential operators of $\hat{H}_\rho$.

Integrating (61) over x and t, we obtain for $d_{2n}(L)$:

$$d_{2n}(L) \propto L^{-\alpha'/4} [\tilde{A}_{2n}(g_4) + \tilde{B}_{2n}(g_4) L^{-2+4n-\alpha'(2n-1)}]. \tag{62}$$

As shown by the calculations, which, in view of their cumbersome nature, we do not give here,

$$\tilde{B}_{2n}(g_4) \propto g_4^{1-2n}. \tag{63}$$

In contrast to (46), in which the coefficients B_{2n} are nonsingular, $\tilde{B}_{2n}$ should be taken into account in the determination of the singular behavior of $(V_\rho)_{00}$. In fact, according to (63), the expansion (60) is in the parameter g_3/g_4 (and not in g_3). If this parameter is small, the singular behavior of $(V_\rho)_{00}$ can be determined as in the derivation of (50). Since $g_4 < 0$, the coefficients $d_{2n}(L)$ with n smaller than a certain $n_0 (n_0 \gg 1)$ vanish in the thermodynamic limit, while those with $n > n_0$ diverge. This means that $(V_\rho)_{00}$ as a function of g_3/g_4 has a singular structure:

$$(V_\rho)_{00} \propto |g_3/g_4|^{-\pi/2g_4}. \tag{64}$$

The fact that $(V_\rho)_{00} \neq 0$ is related physically to the presence of long-range order in the system with Hamiltonian $\hat{H}_\rho$.

Taking (50), (51), (56), and (57) into account, we obtain for $\varepsilon(\delta)$

$$\varepsilon(\delta) \propto -(V_\rho)_{00} |\delta|^\mu; \quad \mu = 2[2 - \exp(2\varphi)/2]^{-1}. \tag{65}$$

As follows from Ref. 24, the quantity appearing in the right-hand side of (64) coincides with the exact value of $\Delta_{\text{corr}}^{1/2}$ for $g_3 \ll g_4$. The calculation of the quantity $(V_\rho)_{00}$ for arbitrary relative magnitudes of g_3 and g_4 requires additional analysis, but, evidently, this quantity is always $\sim \Delta_{\text{corr}}^{1/2}$. With this assumption, formula (65) has the form

$$\varepsilon(\delta) \propto -\Delta_{\text{corr}}^{2/3} \delta^{4/3 + 4g_1/\pi}. \tag{66}$$

We note that in the derivation of formula (66) it was assumed that $g_1 > 0$ and $g_4 < 0$. It is easy to see that a change of sign of the interaction corresponds to the replacements $\rho \leftrightarrow \sigma$ and $g_{1\parallel} \leftrightarrow g_4$. In particular, for the Hubbard model,

$$\varepsilon(\delta) \propto -\delta^{4/3 + 4|\gamma_0|/\pi}.$$

The expression (66) solves the problem of the Peierls instability in the strong-coupling regime. One should also expect that the resulting Peierls gap $\Delta(\delta) \propto \delta^{2/3}$.

CONCLUSION

It follows from the above account that the problem of the Peierls instability of weakly nonideal Fermi systems whose spectrum does not have a correlation gap can be solved in the framework of perturbation theory in the coupling constant. The dependence $\varepsilon(\delta)$ for such systems does not have a universal character. The Peierls transition in them can be suppressed only in the case when the interaction is attractive.

The behavior of systems whose spectrum has a correlation gap for $\delta = 0$ has either a weak-coupling or a strong-coupling regime, depending on the relative magnitudes of δ and Δ_{corr}. For $\delta \to 0$ the dependence $\varepsilon(\delta)$ has a universal character and is characterized by a critical index equal to 4/3. Such systems are unstable against a transition to the Peierls state.

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