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THE INFLUENCE OF THE ELECTRON CORRELATIONS ON THE PEIERLS TRANSITION

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Abstract The problem of the Peierls instability are considered for two models weakly interacting Fermi-particles. It is shown that the influence of the interaction is essential different for the system of spinless particles and for the Hubbard model.

INTRODUCTION

According to well-known Peierls theory[1], one-dimensional metal is unstable with respect to lattice distortions. This theory implies a number of important consequences for one-dimensional systems theory[2]. In particular it serves as a basis for the conception of solitons as a special kind of excited states of polyacetylene[3].

However, it is necessary to point out that Peierls conclusion applies to the system of non-interacting electrons. Though not once attempts have been undertaken to consider the influence of interaction on Peierls instability based either on different approximate methods[4-6] or on the results of numerical calculations of finite chains, this question has not been completely solved as yet.

The given paper will consider the problem of Peierls instability for two models of weakly interacting

Fermi-particles: spinless lattice Fermi-gas with Hamiltonian:

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

and Habbard model

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

There will be considered the case of half-filled band where according to Peierls theory doubling of chain period (i.e. dimerization) takes place. The δ value involved in (1) and (2) is dimensionless amplitude of periodic distortion. It should be noted, that Hamiltonian (1) can be expressed through spin operators thus describing spin-Peierls system with anisotropic interaction.

The purpose of investigation of one-dimensional system instability with regard to chain distortion comes to finding out the dependence of the ground state energy E on δ. Since lattice elastic energy is $E_{elast} = N\varkappa\delta^2/2$ (where $\varkappa$ - dimensionless force constant) the distortion is energetically favourable if the value of $\mathcal{E}(\delta) + E_{elast}$ has minimum at $\delta \neq 0$.

For $g = 0$

$$\mathcal{E}(\delta) \sim \delta^2 \ln \delta \qquad (3)$$

and it is clear that there is minimum when $\delta \ll 1$. This is the very statement which constitutes the essence of Peierls theorem.

The calculation of $\mathcal{E}(\delta)$ value we shall carry on with the help of perturbation theory on g. Unlike di-

agrams for $E_0(0)$ $\mathcal{E}(\delta)$ diagrams contain the lines corresponding to the "normal" average

$$\langle a_k^+ a_k \rangle = u_k^2 = \frac{1}{2}(1+\cos k/\varepsilon(k))$$

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

as well as the lines responding to the "anomalous" average

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

The number of the latter is always even in the diagram. All the $\mathcal{E}(\delta)$ diagrams can be obtained from the diagram for $E_0(0)$ by means of all kind of substitutions of the normal lines for the anomalous ones. For instance, the second order diagram given on Fig. 1 has been obtained from the corresponding $E_0(0)$ diagram by substituting a pair of normal lines for anomalous ones (double lines on Fig. 1).

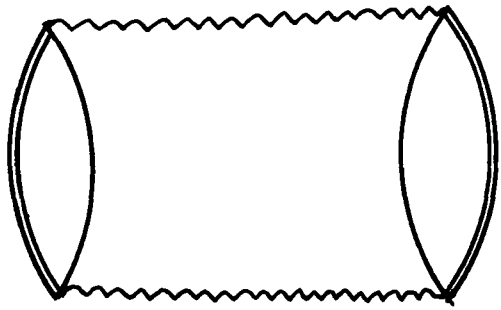

FIGURE 1 Second-order $\mathcal{E}(\delta)$ diagram.

The diagram on Fig. 1 contributes into $\mathcal{E}(\delta) \sim \delta^2 g^2 \ln^3 \delta$.

The analysis of the perturbation series shows that generally n-th order leading contribution to $\mathcal{E}(\delta) \sim \delta^2 \times g^n \ln^{n+1}\delta$. It is not difficult to conclude that diagrams $\mathcal{E}(\delta)$ giving such kind of contributions possess the following qualities: 1) they contain a pair of anomalous lines; 2) with the anomalous lines being broken the rest of the diagram with the four ends can be devided into two part by cutting it along twoinner lines (such kind of diagrams are so-called "parquet" diagrams).

Summation of these $\mathcal{E}(\delta)$ diagrams will be done below (it is assumed that $g \ll 1$). For this purpose it is convenient to express their sum through the vertex

$$\gamma(k_1\sigma_1, k_2\sigma_2; k_3\sigma_3, k_4\sigma_4) \quad (k = k, \omega),$$

(σ - spin index)[9]:

$$\mathcal{E}(\delta) = -i(8\pi^2)^{-1} \sum_{\sigma_1\sigma_2} \sum_{k_1 k_2} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \, \tilde{G}(k_1,\omega_1)\tilde{G}(k_2,\omega_2) \times \quad (4)$$

$\times \gamma(k_1\sigma_1, k_2\sigma_2; k_1+\pi\sigma_1, k_2+\pi, \sigma_2)$, where $\tilde{G}(k,\omega)$ - Green's function, corresponding to the anomalous average:

$$\tilde{G}(k,\omega) = \frac{v_k^2}{\omega - \mathcal{E}(k) + i\delta} + \frac{u_k^2}{\omega + \mathcal{E}(k) - i\delta}$$

This equation is schematically presented on Fig. 2. As is seen from (4) the variables of the vertex are chosen according to the condition:

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

The general scheme of summing up such diagrams is well-known[10,11]. The approximation shown in[10,12] was used

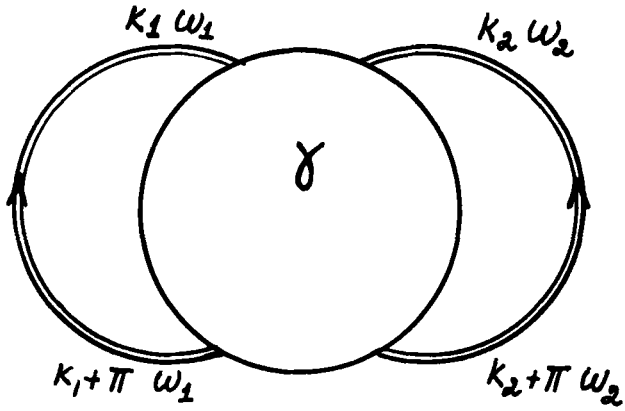

FIGURE 2 General $\mathcal{E}(\delta)$ diagram in parquet approximation.

for the calculation of Green's functions with the purpose of investigation of the instabilities arising in one-dimensional system under the influence of interaction between electrons, but when $\delta = 0$. Such kind of approach, when $\mathcal{E}(\delta)$ has not been calculated, does not allow to consider the question of how the corresponding transition actually takes place. All diagrams of the vertex part can be divided into 4 classes[10]: γ_1 diagrams being reduced from K_1, K_2 to K_3, K_4 (i.e. diagrams which can be divided into two parts containing K_1, K_2 and K_3, K_4 by cutting a diagram along two inner lines): γ_2 diagrams, being driven from K_1, K_3 to K_2, K_4 : γ_3 diagrams being reduced from K_1, K_4 to K_2, K_3 and the irreducible ones (as a kind of the latter the vertex of the first order should be chosen). In particular for

the spinless model $\gamma_{ik} = g(\cos(k_i - k_2) - \cos(k_i - k_4))$ and for Hubbard model

$$\gamma_{ik} = g(\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} - \delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})$$

In this case the vertex of γ_1, γ_2 and γ_3 are determined by solving a system of non-linear integral equations [10,13]. It should be also noted that since the variables of the vertex are connected by the following condition $k_1 + k_2 = k_3 + k_4$, each of the vertex depends on 3 variables which can be easily chosen by the following way (to simplify the notes we shall omit the spin indexes so far): $\gamma_1 = \gamma_1(k_1, k_3, Q)$, $Q = k_1 + k_2$; $\gamma_2 = \gamma_2(k_1, k_4, q)$, $q = k_1 - k_3$; $\gamma_3 = \gamma_3(k_1, k_3, \ell)$, $\ell = k_1 - k_4$ (6)

The leading logarithmic contribution to (4) is made by integration over the moments through the region in the vicinity of $k_1, k_2 \simeq \pm\pi/2$. In accordance with this $\gamma(k_1\sigma_1, k_2\sigma_2; k_3\sigma_3, k_4\sigma_4)$ behaviour is of importance only with $\simeq \pm\pi/2$ moments. According to (5) to calculate $\varepsilon(\delta)$ it is necessary to known only the following vertices: $\gamma^{+--+} = \gamma^{-++-}$ and $\gamma^{++--} = \gamma^{--++}$, where the signs $\pm$ correspond to the $\pm\pi/2$ moments. It is evident that the γ_1^{++--} vertex does not result in the high power of logarithm in the corresponding order of the perturbation theory, hence they can be omitted. Thus, (4) comprise the following vertex

$$\gamma_1^1 = \gamma_1^{+--+};\ \gamma_3^1 = \gamma_3^{++--};\ \gamma_2^1 = \gamma_2^{++--};\ \gamma_2^2 = \gamma_2^{+--+}$$

When calculating γ_1^1 and γ_3^1 functions within logarithmic accuracy one can assume $\delta = 0$ (this fact can be easily verified for the lowerest order diagrams). According to (5) and (6) the γ_1^1 vertex involved in (4) is the function of k_1 and k_2: $\gamma_1^1 = \gamma_1^1(k_1, k_2, k_1 + k_2)$. According to logarithmic character of γ_1^1

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

Similerly,

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

Taking into account (5), when calculating γ_2^1 and γ_2^2 functions involved in (4) we can not assume $\delta = 0$. For instance the contribution of the second order γ_2^1 diagram (Fig. 3) $\sim g^2 \ln\delta$.

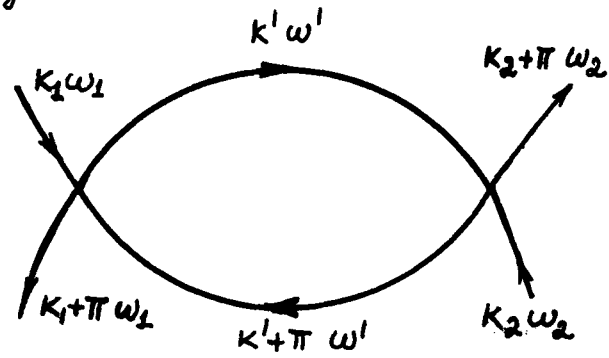

FIGURE 3 Second-order vertex γ_2 diagram.

Calculation of the higher order diagram contribution indicates that if the arguments of γ_2 are connected through (5) condition then

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

Bearing in mind all the mentioned above the expression of (4) can be put down in the following way:

$$\varepsilon(\delta) = \frac{\delta^2}{4\pi^2}\sum_{\sigma_1\sigma_2}\int_0^{\Phi} dt_1 \int_0^{\Phi} dt_2 \{\gamma_1^1(\min(t_1,t_2)) - \gamma_3^1(\min(t_1,t_2)) + \gamma_2^2(t_1,t_2,\Phi) - \gamma_2^1(t_1,t_2,\Phi)\}, \quad (7)$$

where $\varphi = -\ln\delta$ with logarithmic substitution $t_i = -\ln(\delta k_i)$ made in (7). Thus the γ_1^1 and γ_3^1 vertex involved in (7) are the functions of single variable and can be obtained through Sudakov's technique[14], while γ_2^1 and γ_2^2 functions are the functions of three variables and can be obtained by the technique developed in[11].

SPINLESS MODEL

At first we should consider spinless lattice fermigas. The system of equations for the vertex considered as functions of single variable takes the form:

$$\begin{aligned}
\gamma_1^1(\alpha)+\gamma_1^2(\alpha) &= -\frac{1}{2}\int_0^\alpha (\gamma_2^2(t)+\gamma_3^2(t)+\gamma_1^1(t)+\gamma_1^2(t))^2 dt \\
\gamma_1^2(\alpha)-\gamma_1^1(\alpha) &= -\frac{1}{2}\int_0^\alpha (4g+\gamma_3^2(t)-\gamma_2^2(t)+\gamma_1^2(t)-\gamma_1^1(t))^2 dt \\
\gamma_3^1(\alpha)+\gamma_3^2(\alpha) &= \int_0^\alpha (2g+\gamma_1^2(t)+\gamma_2^1(t)+\gamma_3^1(t)+\gamma_3^2(t))^2 dt \\
\gamma_3^2(\alpha)-\gamma_3^1(\alpha) &= \int_0^\alpha (2g+\gamma_1^2(t)-\gamma_2^1(t)+\gamma_3^2(t)-\gamma_3^1(t))^2 dt
\end{aligned} \tag{8}$$

with

$$\gamma_1^2(t) = \gamma_1^{+-+-}(t)\,;\quad \gamma_3^2(t) = \gamma_3^{+-+-}(t)$$

To find γ_1 and γ_3 from these equations it is necessary to determine γ_2 as a function of single variable. Formally this function satisfies the following equations:

$$\begin{aligned}
\gamma_2^1(\alpha)+\gamma_2^2(\alpha) &= -\int_0^\alpha (-2g+\gamma_1^1(t)+\gamma_3^1(t)+\gamma_2^1(t)+\gamma_2^2(t))^2 dt \\
\gamma_2^2(\alpha)-\gamma_2^1(\alpha) &= -\int_0^\alpha (-2g+\gamma_1^1(t)-\gamma_3^1(t)+\gamma_2^2(t)-\gamma_2^1(t))^2 dt
\end{aligned} \tag{9}$$

The vertex γ_2, involved in (7) are being derived from the equations:

$$\begin{aligned}
\Gamma_+(t_1,t_2,\varphi) &= -\int_0^\varphi X_+(\min(t_1,t'))\left(X_+(\min(t',t_2)+\Gamma_+(t',t_2,\varphi)\right)dt' \\
\Gamma_-(t_1,t_2,\varphi) &= -\int_0^\varphi X_-(\min(t_1,t'))\left(X_-(\min(t',t_2)+\Gamma_-(t',t_2,\varphi)\right)dt'
\end{aligned} \tag{10}$$

with $\Gamma_\pm(t_1,t_2,\varphi) = \gamma_2^2(t_1,t_2,\varphi) \pm \gamma_2^1(t_1,t_2,\varphi)$

$$X_{\pm}(t) = -2g + \gamma_1^1(t) \pm \gamma_3^1(t)$$

The way to derive equations (10)[11] is based on the generalization of Sudakov's approach. The solution of the system of equations (8)-(9) takes the form:

$$\gamma_1^1(\alpha) = -\gamma_1^2(\alpha) = \gamma_3^2(\alpha) = -\gamma_2^2(\alpha) = -4g^2\alpha;\ \gamma_2^1(\alpha) = \gamma_3^1(\alpha) = 0 \quad (11)$$

Substituting (11) in (10) we find out that

$$\gamma_2^1(t_1,t_2,\Phi) = 0;\ \gamma_2^2(t_1,t_2,\Phi) = -4g^2\min(t_1,t_2) - g\{\exp(2g(\max(t_1,t_2) - \min(t_1,t_2))) - 1\} - g\{\exp(4g\Phi - 2gt_1 - 2gt_2) - 1\} \quad (12)$$

The substitution of (11) and (12) in (7) and taking into account the term of the zero order produces:

$$\mathcal{E}(\delta) = -(4g)^{-1}(\exp(4g\Phi) - 1) \quad (13)$$

The given derivation of the expression for $\mathcal{E}(\delta)$ (13) is of rather a methodical character. The point is that this formula can be obtained by the most straight forward way. Namely, Hamiltonian (1) can be reduced to the Hamiltonian with linear spectrum model using the substitution of fermi-operators:

$$a_k = c_{1k} \quad k \simeq \pi/2;\ a_k = c_{2k} \quad k \simeq -\pi/2$$

As a result of this the Hamiltonian one will be transformed into the Hamiltonian of Thirring's massive model:

$$\hat{H} = \sum k(c_{1k}^{+}c_{1k} - c_{2k}^{+}c_{2k}) - i\delta\sum(c_{1k}^{+}c_{2k} - c_{2k}^{+}c_{1k}) + 2gN^{-1}\sum c_{1k+q}^{+}c_{1k}c_{2k'-q}^{+}c_{2k'} \quad (14)$$

It is well-known that one should take care while transforming such kind of Hamiltonian as type (1) into the Hamiltonian of the model with linear spectrum (anyway, it is valid if ever only under condition if $g \ll 1$).

In this case however the immediate check will show that the diagram contributions into $\mathcal{E}(\delta)$ for (1) and (14) are the same within the leading logarithmic approximation, though $E_0(0)$ is different for these two models! As for Hamiltonian (14) the exact solution for the ground state energy and the spectrum of excitations[15] is known.

Making use of the results[15] with $g \ll 1$ gives (13). As it follows from (13) with $g\varphi \ll 1$ $\mathcal{E}(\delta)$ coinside with (3), that is if $\delta \gg exp(-\pi/2|g|)$ the account of interaction effects does not influence upon Peierl's result. If $\delta \longrightarrow 0$ ($g\varphi \gg 1$) than

$$\mathcal{E}(\delta) = -(4g)^{-1}\,\delta^{2-2g/\pi}; \quad g>0$$

$$\mathcal{E}(\delta) = -\delta^2/4|g| \quad ; \quad g<0$$

Thus, the system is unstable with respect to transition into Peierls state if the interaction is repulsive. The spectrum of the Hamiltonian (1) has not gap with $\delta = 0$. While there appears a gap with $\delta \neq 0$. The value of the gap Δ can be expressed through the vertex:(graphically the equation (16) is shown on Fig. 4):

$$\Delta = 2\delta - \int_0^{\varphi} \left(\gamma_3^1(t_2) - \gamma_1^1(t_2) + \gamma_2^1(\varphi, t_2, \varphi) - \gamma_2^2(\varphi, t_2, \varphi)\right) dt_2 \quad (16)$$

The substitution of (11) and (12) into this equation gives:

$$\Delta = 2\delta\, exp(2g\varphi)$$

$\Delta = 2\delta$ with $g\varphi \ll 1$, which is equivalent to the approximation of non-interacting particles. With $\delta \longrightarrow 0$

$$\Delta = 2\delta^{1-g/\pi} \quad (17)$$

The expression of the gap for the massive Thirring model[15] with $g \ll 1$ comes to (17).

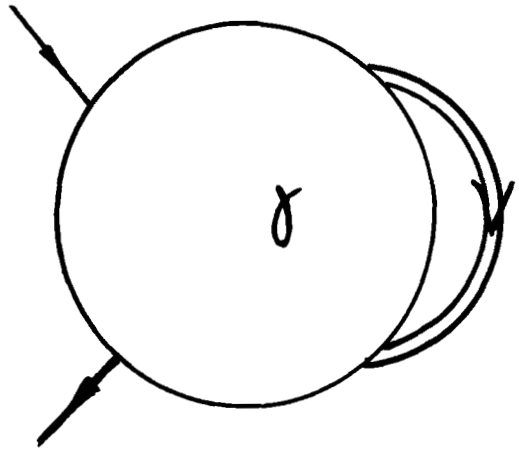

FIGURE 4 General Δ diagram.

THE HABBARD MODEL

The vertex involved in the expression for $\xi(\delta)\nabla$ can be obtained in a way similar to that of the spinless case. We will not write out the corresponding equations for γ (of type (8)-(10)) which are rather tedious for the Habbard model. We will show only the expression for the function under integration in (7), summed up through spin indexes:

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

$$=-\frac{g(\min(t_1,t_2))}{f(\min(t_1,t_2))}f(\max(t_1,t_2))+\frac{g(t_1)}{f(t_1)}\frac{g(t_2)}{f(t_2)}\int_{\max(t_1,t_2)}^{\Phi}f^2(t')\,dt' \qquad (18)$$

where

$$g(t)=6g^2t(1-4g^2t^2)^{-1};\quad f(t)=(1-4g^2t^2)^{-3/4}$$

Calculating the integral in (7) and considering zero order term we finally arrive at:

$$\mathcal{E}(\delta) = -\delta^2 \Phi \pi^{-1} \left(1-(g\Phi/\pi)^2\right)^{-1/2} \qquad (19)$$

In the region of $\delta \gg \delta_0$ ($\delta_0 = exp(-\pi/|g|)$ (19) coincides with (3), which means the consideration of the interaction effects does not modify the dependence of $\mathcal{E}(\delta)$ obtained with $g = 0$. With $\delta \to \delta_0$ $\mathcal{E}(\delta)$ is singular. Such singularity arise due to the approximate character of calculations: only the highest powers of logarithms in each order of perturbation theory are considered. Nowadays the strict determination upon behaviour of $\mathcal{E}(\delta)$ with $\delta \to 0$ is hardly solvable problem. In particular it is not clear whether the account of the higher order corrections to be effective. The fact is the effective electron interaction becomes rather strong with $\delta \to 0$, thus unperturbation approaches should be used in solving the above mentioned problem.

The expression (19) is also applicable through out the region $\delta < \delta_0$ if the following hypothesis is assumed.

First of all we should note that contrary to (1) the Habbard model possesses the gap in the spectrum of one-particle excitations even with $\delta = 0$. With preexpronent factor omitted this gap is the same as δ_0 for which $\mathcal{E}(\delta)$ is singular. According to our hypothesis the method of regularization of the expression (19) consists in changing a momentum cut-off arising while calculating the vertex part and integral in (7) so that it would be determined by the gap Δ in the spectrum of excitatious rather than δ. To put it otherwise $\tilde{\Phi} = -\ln \Delta$ substitutes Φ in all the expressions, with Δ being

found from the equation similar to (16) (or Fig. 4), which looks like as follows for the Habbard model:

$$\Delta = 2\delta f(\tilde{\Phi})$$

$\tilde{\Phi}$, found from this equation should then be inserted in (19). It is evident that $\mathcal{E}(\delta)$ found in this way is regular at $\delta \geq 0$.

The solution of self-consistent equation (20) with $\delta \gg \delta_0$ is as follows: $\Delta = 2\delta$

With $\delta \ll \delta_0$

$$\Delta = \delta_0 + (2\delta)^{4/3} \delta_0^{-1/3} \pi / 2|g|$$

As for $\mathcal{E}(\delta)$ with $\delta \gg \delta_0$:

$$\mathcal{E}(\delta) = \delta^2 \pi^{-1} \ln \delta \qquad (21)$$

though with $\delta \ll \delta_0$

$$\mathcal{E}(\delta) = -\delta^{4/3} (\delta_0/2)^{2/3} / |g| \qquad (22)$$

Since is not an analytical function of g can not be obtained within the framework of the pertubation theory. (21) and (22) expressions indicate that the Habbard model is unstable to Peierls transition, and the tendency to dimerization becomes stronger if there is weak interaction between electrones.

In connection with the (22) formula we should point out that the dependence $\mathcal{E}(\delta) \sim -\delta^{4/3}$ was obtained in[16] for Heisenberg model (spin-Peierls system), which is the limit case of the Habbard model with —

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