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Renormalization Group Theory of Peierls Transition in One-Dimensional Electron-Phonon Systems

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Abstract Peierls transition in one-dimensional electron-phonon systems is studied by renormalization group method, considering logarithmic terms up to the next divergent corrections. The results are applied to predict power low behaviors in various response functions.

§ 1. Introduction

Peierls transitions which are drived by the Kohn anomaly in phonon spectrum have been much interested. In a recent work, in paticular, Suzumura and Kurihara[1] found that the critical anomalies of phonon spectrum and other quantities in a one-dimensional model would be characterized by a universal power law near the absolute zero temperature. Their method was based on a self-consistent (renormalized) random phase approximation but the results are very similar in form to those predicted for interacting electron systems by the method of renormalization group (RG).[2,3,4]

Such a considerable resemblence between the two problems of the electron-phonon and the interacting electron systems becomes particularly clear when we notice the algebraic structures of the perturbation series being characterized in common by logarithmic singularities. In another words, the present matter is analogous to the problem of the infrared catastrophe linked with the Fermi discontinuity of an electron gas.[5]

The purpose of the present paper is to apply the RG method to the phonon softening problem for one-dimensional electron-phonon systems described by the model similar to that studied in Ref.1. Not only the phonon spectrum but also the pairing susceptibilities and other electronic responses are studied.

Since the effective electron interaction caused by exchange of Debye phonons, in a naive sense, is of attractive nature it can be guessed from the suggestions of Refs. 2 and 4 that the present system would also asymptotically be carried over into an essentially

strong coupling regime at low temperatures, no matter how weak the bare coupling were. The cross-over from an initially assumed weak electron-phonon coupling to the strong coupling regime should be taken place continuously at about a mean field Peierls transition temperature T_p. Below this temperature we have not any small parameter of the problem near the Fermi level, even if the bare coupling constant is considered to be arbitrary small. Strictly speaking, in this asymptotic region any attempt based on perturbation theories would lose its rigorous basis. However, in so far as sufficiently reliable solutions for the problem have scarcely been available it is worth while to carry out an improved perturbation analysis which would serve us to suggest the paticular features of the critical anomalies inherent in the present model.

The present paper is outlined as follows. In Sec. 2 we formulate the problem with the help of RG method. In Sec. 3, as the first order theory, the phonon self-energy is considered. In this approximation the results are found to be the same as those of the mean field theory.[6] In Sec. 4 the next order correction, the electron self-energy, is considered. Then, relying upon the formal solution for the invariant coupling various quantities are predicted in the form of power in energy or temperture scaled by T_p. In particular, the Cooper-pairing susceptibility and the density response at $2p_F$ diverge at $T=0$. The part of the results agrees with those of Ref. 1. In conclusion (Sec. 5) the behavior of other physical properties are discussed and the role of long wave length phonon is also examined briefly.

§ 2. Description of the model and RG method

The system under consideration is the one-dimensional electron-phonon system characterized by the interaction ;[7]

$$H_{e\ p}=\sum_{pq\sigma} g_q \{C^+_{p+q\sigma}\ C_{p\sigma}(d^+_q+d_{\ q})+\mathrm{c,\ c}\} \tag{2-1}$$

where $c^+{}_{p\sigma}$ ($c_{p\sigma}$) is the creation (annihilation) operator for an electron with momentum p and spin component σ. d^+_q is the phonon creation operator with momentum q. The model is similar to that considered in Ref. 1. Since we are interested in the role played by the phonon with momentum near $2p_F$ it can be assumed that the coupling constant g and phonon frequency ω_0 are independent of momentum acting within some range D of energy.

Now let us write the Green's functions and vertex function as ;

$$\begin{aligned}\Gamma(\tilde{p})&=g\tilde{\Gamma}(\tilde{p}/D,\ D,\ g)\\ G(\tilde{p})&=d_1(\tilde{p}/D,\ D,\ g)\ G_0(p)\\ D(\tilde{p})&=d_2(\tilde{p}/D,\ D,\ g)\ D_0(p)\end{aligned} \tag{2-2}$$

where $\tilde{p}$ denotes frequency and momentum arguments. The renormalization group for this model is defined by a conventional way: For an arbitrary change of energy scale the electron and phonon Green's functions G and D, the e-p vertex and the coupling constant g are multiplied by constant;

$$d_1 \to Z_1^{-1}\, d_1,\ d_2 \to Z_2^{-2}\, d_2,\ \tilde{\Gamma} \to Z_3^{-2}\, \tilde{\Gamma},\ g \to Z_4 g \tag{2-3}$$

The invariance under transformation (2-3) implies that the multiplicative constants Z_i are subject to a relation; $Z_4 = Z_1 Z_2 Z_3$. This argument suggests that the proper choice of invariant coupling (IC) is

$$\Psi(x, \lambda) = \lambda\, d_1^2\ (x, \lambda)\, d_2(x, \lambda) \tilde{\Gamma}(x, \lambda) \tag{2-4}$$

where x is a characteristic energy of problem defined in the next section, and $\lambda = -\upsilon_F g^2$ (υ_F is the density of states at the Fermi energy).

Then we can follow the usual procedure to get various renormalized quantities which was explained in detail in the preceding contexts.[2,3,4]*

Actually in performing calculation some complexity arises because the problem involves two different cut-off parameters, i.e. the electron band width of the order of E_F and cut-off in the phonon momentum p_c multiplied by electron velocity v. However, since p_c is of order of the Fermi momentum it is sufficient to assume, within logarithmic accuracy, only a single cut-off parameter D to represent the order of E_F and vp_c.

§ 3. First order renormalization

Let us study the first order renormalization. The first logarithmic correction arises from the polarization function of $2p_F$ phonon as shown in Fig. 1. It is expressed as

$$\Pi(\omega, k) = 2g^2 \frac{T}{2\pi} \Sigma \int dp\ G_0(p + \frac{k}{2})\, G_0(p - \frac{k}{2}) \tag{3-1}$$

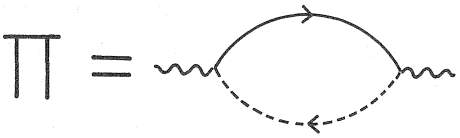


Fig. 1 Phonon self energy.
Wave line represents phonon with momentum near $2p_F$.
Solid line represents electron with momentum $\sim p_F$.
Broken line represents electron with momentum $\sim -p_F$.

*) In these literatures the method by the Lie equation have been used exclusively. However, it can be easily shown that a different formulation by the Callan-Symansik method leads to the equivalent results.

This is a logarithmic integral in the arguments ω, k' and T where $k'=k\pm 2k_F$. If $|\omega\pm vk'| \gg T$ we obtain

$$\Pi(\omega,k)\simeq\frac{1}{2}\upsilon_F g^2\{\ln x^2-i\pi\theta(x^2)\} \tag{3-2}$$

where $x^2=|\omega^2-(vk')^2|/D^2$. If $\omega\pm vk' \gg T$, x^2 in logarithm is replaced by T^2/D^2 and the sharp discontinuity in the imaginary part represented by $\theta(x^2)$ is smeared out with a tail, extending up to the point $\omega=k'=0$.

Using this correction as the input we have the Lie equation for IC as;

$$x\frac{\partial\Psi}{\partial x}=\Psi^2 \tag{3-3}$$

which solves to yield

$$\Psi=\lambda/\{1-\lambda(\ln x-\frac{i}{2}\pi\theta(x^2))\} \tag{3-4}$$

If $\omega=k'=0$ this function diverges at temperature T_p, where

$$T_p=D\exp(-1/|\lambda|) \tag{3-5}$$

This is just the Peierls transition temperature predicted by a mean field theory.[6]

§ 4. Next order renormalization

In the next order approximation, we must take into account the electron self-energy correction, shown in Fig. 2. It is expressed as

$$\Sigma(\varepsilon,p)=-(\frac{T}{2\pi})^2\Sigma\int dkdq'\ G_0(p-k)\,G_0(q')\,G_0(q'+k)\,D^2{}_0(k) \tag{4-1}$$

where $D_0(\omega,k)=-\omega^2{}_0/(\omega^2+\omega^2{}_0)$

The calculation of (4-1) is straightforward but tedious. However, the argorithm is considerably simplified if we notice that the integration is dominated by the contribution from the low frequency phonons with $\omega \ll \omega_0 \sim \omega_D$. Thus, it is sufficient to appro-

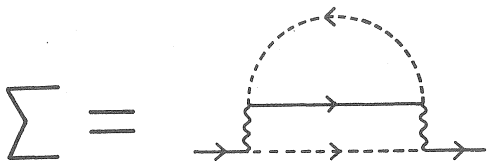


Fig. 2 Electron self energy.

ximate by $D_0(\omega, k)\sim -1$ in order to estimate correctly the dominant logarithmic term. Then it becomes

$$\Sigma(\epsilon,p) -\frac{1}{8}g^4 \nu_F^2 G_0^{-1}(\epsilon,p)\{\ln x'^2 - i\pi\theta(x'^2)\}, \quad \text{if } |\epsilon \pm (vp')| \gg T \tag{4-2}$$

where $x'^2 = |\epsilon^2 - (vp')^2|/D^2$ with $p' = p \pm p_F$. At finite temperatures the argument made in Sec. 3 about the behavior of Π holds also for (4-2) as well.

Together with Eqs. (3-1) and (3-2) this gives the Lie equation;

$$x\frac{\partial \Psi}{\partial x} = \Psi^2 + \frac{1}{2}\Psi^3 \tag{4-3}$$

and the solution;

$$\ln x = F(\Psi) - F(x)$$
$$F(\Psi) = -1/\Psi + \frac{1}{2}\ln|(\Psi+2)/\Psi| \tag{4-4}$$

(See Fig. 3) The curve for $\Psi(x)$ displays a smooth behavior and tends to the fixed point -2 as $x\to 0$. Note that the electron self-energy term on the right hand side of Eq. (4-3) is always negative for the present case (i.e. $\Psi<0$), and therefore, it counteracts to suppress the singular growth of IC due to the first term.

The Lie equations for d_1 and d_2 are

$$x\frac{\partial}{\partial x}\ln d_1 = \frac{1}{4}\Psi^2 \tag{4-5}$$

$$x\frac{\partial}{\partial x}\ln d_2 = \Psi \tag{4-6}$$

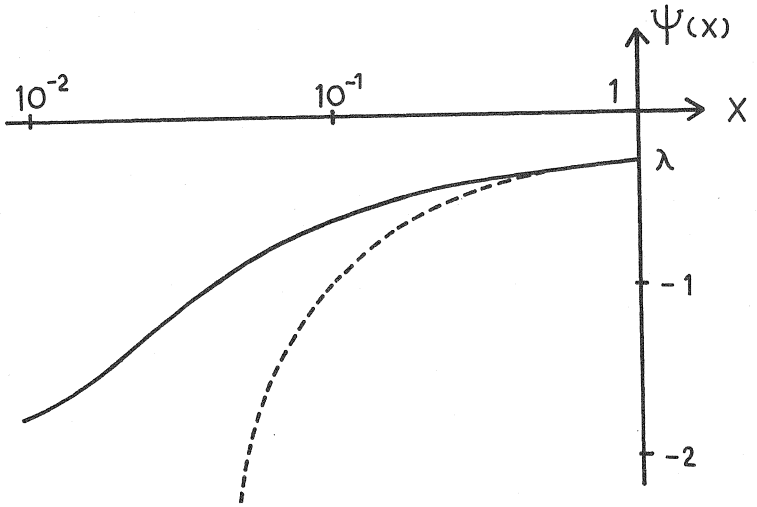


Fig. 3 Graph of the invariant coupling.

The solutions of Eqs. (4-5) and (4-6) are found in the form ;

$$d_1(x)=x\,|\,\Psi(x)/\lambda\,|^{1/2}\,\exp\,(1/\Psi(x)-1/\lambda) \tag{4-7}$$

$$d_2(x)=x^{\,2}\,\exp\,2(1/\lambda-1/\Psi(x)) \tag{4-8}$$

As $x\to 0$, these solutions behave asymptotically as

$$G=G_0\,e^{-1/2}\,|\,2\ln\,(T_p/D)\,|^{1/2}\,\tilde{x} \tag{4-9}$$

$$D=D_0\,e\,\tilde{x}^{-2} \tag{4-10}$$

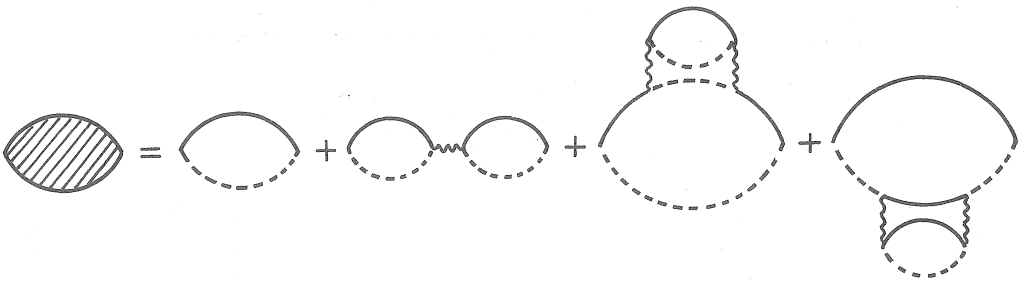
where $\tilde{x}=(\omega^2-(vp')^2)^{1/2}/T_p$ or T/T_p. Eq. (4-10) implies the softening of phonon spectrum at wave vector of $2p_F$. Note that the scaling parameter for these asymptotic expressions is T_p instead of the original cut-off energy D.

Using the form of electron Green's function (4-9), the density of states $\nu(\omega)/\nu_F$ for the electron can be written asymptotically as

$$\nu(\omega)/\nu_F\simeq\omega/T_p \tag{4-11}$$

The result is quite similar to that of Suzumura and Kurihara.[1] Note that for commensurate case the vertex correction arises in the first order renormalization which would strongly affect the property of the system as discussed in Ref. 1.

Now, let us consider the anomalous responses of the system. In addition to the Peierls instability we should expect that the system would exhibit various types of electronic instabilities. Here we examine the critical behavior of the fluctuations of singlet and triplet Cooper pairing, staggered spin- and charge-densities with $2p_F$ momentum. Their definitions are given in Ref. 4. The perturbational expansion for these quantities is written as ;



Here omitting detailed derivation we immediately write down the following equations for them

$$x\frac{\partial}{\partial x}\ln\bar{\Pi}^S = \psi+\frac{1}{2}\psi^2 \tag{4-12}$$

$$x\frac{\partial}{\partial x}\ln\bar{\Pi}^T = -\psi+\frac{1}{2}\psi^2 \tag{4-13}$$

$$x\frac{\partial}{\partial x}\ln\bar{\chi} = \frac{1}{2}\psi^2 \tag{4-14}$$

$$x\frac{\partial}{\partial x}\ln\bar{N} = 2\psi+\frac{1}{2}\psi^2 \tag{4-15}$$

where the quantities with a bar ($\bar{\Pi}$ etc.) are the three pole vertices related to each responses, defined by $\bar{\Pi}(x)=\frac{\partial\Pi(x)}{\partial \ln x}$, and so on. The asymptotic expressions are obtained in the form;

$$\begin{aligned}&\Pi^S(\omega,k) \propto \nu_F \ln\tilde{x} \quad , \quad \chi(\omega,k\pm 2p_F)\propto\tilde{x}^2\\ &\Pi^T(\omega,k)\propto\tilde{x}^4 \quad , \quad N(\omega,k\pm 2p_F)\propto\tilde{x}^{-2}\end{aligned} \tag{4-16}$$

In the limit $x\to 0$, N tends to diverge, Π^T and χ to converge to cusp minimum. The logarithmic singularity obtained for Π^S is due to the casual cancellation of the first and second order corrections leaving only the zeroth order anomaly inherent in a 1-D free electron system.

In the same way the long wave length susceptibilities[4,8] can be obtained. Here we write down only the results

$$\begin{aligned}N(\omega,k) &\sim N_0(\omega,k)\tilde{x}.\\ \chi(\omega,k) &\sim \chi_0(\omega,k)\end{aligned} \tag{4-17}$$

These quantities do not diverge, as it should be.

§ 5. Discussions and Conclusions

Here we briefly consider the role of phonons with long wavelength. Since calculation can show that the corrections due to these phonons are also logarithmic but the effect is reduced by the small factor of m/M, where m is the mass of the electron and M of the ion.[10] Repeating the manipulations as in the preceding sections we find that the magnitudes of IC and the exponents for the power of various quantities are shifted only by small amounts of order $(m/M)g^2$. Therefore, all the conclusions above derived hold without an essencial change.

Now, it is interesting to comment on the imaginary parts of the various response functions obtained in the preceding sections.[8] In simulating them with the imaginary parts in the perturbation expressions (3-1), (3-2) and similar forms for response functions (which were explicitly not written down) we can easily obtain the imaginary parts of the renormalized functions. The remarkable feature of the imaginary parts thus obtained is that they have the sharp edge at $\omega=\pm\,|\,vp\,|$. For example, from the power

law $F(\omega,k)\propto(x/T_p)^{\alpha}$ (see Sec. 4) we obtain

$$\text{Im } F(\omega,k)\propto\theta(x)\,(x/T_p)^{\alpha}$$

These arguments are applied to predict the characters of some other physical properties. For example, the electron transport life time by impurity scatterings with a potential U and concentration c, which is expressed by,[9]

$$1/\tau=\lim_{\omega\to 0}(c/\omega)\,U^2v^2\sum_{p,p'}(p-p')\,\text{Im } N(p,p',\omega)$$

should increase anomalously according to Eqs. (4-16) and (4-17). Thus the system becomes insulating at low temperatures.

In summary we would like to emphasize the following;

a) The problem of one-dimensional electron system asymptotically carried over to the strong coupling regime. The characteristic temperature determined by $\Psi(T)\sim 1$ is the mean field transition temperature T_p.

b) If we rely upon the formal solutions the Green's functions of electron and phonon and also pairing and staggered response functions are characterized by the power form with energy (temperature) argument scaled by T_p. Although these agree qualitatively with those of Ref. 1, the numerical results for the exponents can not be taken literaly because of the strong-coupling nature of the problem.

c) The vanishing of the density of states at the Fermi energy according to Eq. (4-11) implies break-down of the Fermi liquid theory. Analogous situations have been known in contexts of many other infrared problem.[2,4,5]

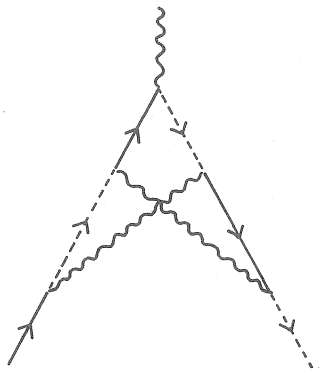


Fig. 4 Graph of a contribution $g^{2n}\ln^2 x$.

Finally we should remark a drawback in the present work that it fails to take into account some sort of graphs with the same order of divergences as exemplified in Fig. 4. The difficulty arises because the perturbational scheme of the renormalization enables to treat only the hierarchy of terms which are generated by repeating primitive

divergences in the form $g^{2n}\ln x$. For example, the graph in Fig. 4 gives a contribution $g^{2n}\ln^2 x$ and thus it does not give rise to any generating term.

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