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Theory of Fluctuations in Quasi-One-Dimensional Electron-Phonon Systems†)

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The effect of fluctuations on the Peierls transition in quasi-one-dimensional systems is investigated within a renormalized random phase approximation in the half-filled tight-binding model. The fluctuations are divided into two parts; thermal fluctuations and zero point fluctuations. It is shown that the effect of the thermal fluctuations is always dominant even if the transition temperature is extremely low.

§ 1. Introduction

The effect of fluctuations on the Peierls transition in strictly one-dimensional systems has been investigated by many authors above and below the Peierls transition temperature T_p.[1),2)]

Suzumura and Kurihara[3)] and the present authors[4)] have recently studied this problem in a renormalized random phase approximation (RRPA). We have concluded that the Peierls transition does not occur in one-dimensional systems, because zero point fluctuations break down the Peierls transition.[4)]

On the other hand the effect of fluctuations in quasi-one-dimensional systems also has been investigated.[5)~8)] In the present paper we study this problem above T_p in RRPA. We divide fluctuations into thermal and zero-point fluctuations and investigate which fluctuation becomes dominant when the magnitude d of electron hopping integral between linear chains changes.

Our theory includes electron-electron, ion-ion and electron-ion interactions in a half-filled tight-binding model. On the assumptions that the coupling strength of the electron-ion interaction is constant and phonon dispersions come only from renormalized phonon polarization parts, we can show that thermal fluctuations are dominant even if the transition temperature is extremely low. With respect to the case that the above assumptions do not hold, that is, the Coulomb interaction contributes dominantly to phonon dispersions, we shall investigate in the next paper.

When d tends to zero, T_p becomes zero, but as far as d is finite, there

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exists a finite transition temperature.

In § 2 we introduce electron and phonon Green's functions in RRPA including Umklapp processes. The dynamical dielectric function is obtained. In § 3 the electron Green's function is obtained and the single particle properties are discussed. Then we calculate a bubble diagram consisting of one-electron and one-hole Green's functions and examine the behavior of the bubble diagram with small wavenumber and small frequency. In § 4 by the use of the above results we obtain the phonon spectrum near the Peierls temperature. In § 5 we investigate the self-consistent equation of fluctuations and study which fluctuation, the zero-point fluctuation or the thermal fluctuation, becomes dominant as the parameter d increases from zero. Then we obtain the Peierls transition temperature and the magnitude of the fluctuation as functions of d. Finally we give some discussion in § 6.

§ 2. Hamiltonian and Green's functions

We start with the Hamiltonian

$$H=\sum_{\boldsymbol{k},\sigma}\varepsilon_{\boldsymbol{k}\sigma}c^{+}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}+\frac{1}{2}\sum_{\substack{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}\\ \sigma,\sigma'}}V(\boldsymbol{q})\,c^{+}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}+\boldsymbol{q}\sigma}c^{+}_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}'-\boldsymbol{q}\sigma'}$$
$$+\sum_{\boldsymbol{q},\lambda}\omega_{\boldsymbol{q}\lambda}b^{+}_{\boldsymbol{q}\lambda}b_{\boldsymbol{q}\lambda}+\sum_{\substack{\boldsymbol{k},\boldsymbol{q}\\ \sigma,\lambda}}i\alpha_{\boldsymbol{q}\lambda}(\boldsymbol{q}+\boldsymbol{K})\,c^{+}_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{K}\sigma}c_{\boldsymbol{k}\sigma}\phi_{\boldsymbol{q}\lambda}\,, \tag{1}$$

where $c^{+}_{\boldsymbol{k}\sigma}$ and $b^{+}_{\boldsymbol{q}\lambda}$ are creation operators for the electron with wavenumber $\boldsymbol{k}$ and spin σ, and the λ-polarized phonon with wavenumber $\boldsymbol{q}$, respectively, $V(\boldsymbol{q})$ is the Fourier component of the electron-electron interaction, and $\omega_{\boldsymbol{q}\lambda}$, $\alpha_{\boldsymbol{q}\lambda}(\boldsymbol{q}+\boldsymbol{K})$ and $\phi_{\boldsymbol{q}\lambda}$ are given by

$$\omega^{2}_{\boldsymbol{q}\lambda}\varepsilon_{\boldsymbol{q}\lambda}=\frac{N}{M}\sum_{\boldsymbol{K}}[(\boldsymbol{q}+\boldsymbol{K})\cdot(\boldsymbol{q}+\boldsymbol{K})U_I(\boldsymbol{q}+\boldsymbol{K})-\boldsymbol{K}\cdot\boldsymbol{K}U_I(\boldsymbol{K})]\varepsilon_{\boldsymbol{q}\lambda}\,, \tag{2}$$

$$\alpha_{\boldsymbol{q}\lambda}(\boldsymbol{q}+\boldsymbol{K})=\sqrt{\frac{N}{M}}(\boldsymbol{q}+\boldsymbol{K})\cdot\varepsilon_{\boldsymbol{q}\lambda}U_b(\boldsymbol{q}+\boldsymbol{K}), \tag{3}$$

$$\phi_{\boldsymbol{q}\lambda}=\frac{1}{\sqrt{2\omega_{\boldsymbol{q}\lambda}}}(b_{\boldsymbol{q}\lambda}+b^{\dagger}_{-\boldsymbol{q}\lambda}). \tag{4}$$

In the above equations, N is the number of ions, M the mass of an ion, $\varepsilon_{\boldsymbol{q}\lambda}$ the polarization vector of phonon. U_I and U_b are the Fourier components of ion-ion and electron-ion interactions, respectively. The electron momenta $\boldsymbol{k}$'s are considered in the extended zone scheme, but the phonon momenta $\boldsymbol{q}$'s are restricted within the first Brillouin zone. The $\boldsymbol{K}$'s are reciprocal lattice vectors. Henceforth the spin indices are abbreviated for simplicity.

Green's functions are defined by

$$G(\boldsymbol{k},i\omega_n)=-\int_0^{\beta}\langle T_\tau c_{\boldsymbol{k}}(\tau)\,c_{\boldsymbol{k}}{}^{\dagger}(0)\rangle e^{i\omega_n\tau}d\tau\,, \tag{5}$$

$$D_\lambda(\boldsymbol{q}, i\zeta_m) = -\int_0^\beta \langle T_\tau \phi_{\boldsymbol{q}\lambda}(\tau)\phi_{-\boldsymbol{q}\lambda}(0)\rangle e^{i\zeta_m\tau}d\tau\,, \tag{6}$$

where $\langle\ \rangle$ denotes the thermal average, $\omega_n=(2n+1)\pi T$ and $\zeta_m=2m\pi T$. The Green's functions $G(\boldsymbol{k}, i\omega_n)$ and $D_\lambda(\boldsymbol{q}, i\zeta_m)$ satisfy in general the Dyson equations:

$$G^{-1}(\boldsymbol{k}, i\omega_n) = G^{(0)-1}(\boldsymbol{k}, i\omega_n) - \Sigma(\boldsymbol{k}, i\omega_n), \tag{7}$$

$$D_\lambda^{-1}(\boldsymbol{q}, i\zeta_m) = D_\lambda^{(0)-1}(\boldsymbol{q}, i\zeta_m) - \Pi_\lambda(\boldsymbol{q}, i\zeta_m), \tag{8}$$

where $G^{(0)}(\boldsymbol{k}, i\omega_n)$ is the free electron Green's function, $D_\lambda^{(0)}(\boldsymbol{q}, i\zeta_m)$ the free phonon Green's function, and they are given by

$$G^{(0)}(\boldsymbol{k}, i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\boldsymbol{k}}}, \tag{9}$$

$$D_\lambda^{(0)}(\boldsymbol{q}, i\zeta_m) = -\frac{1}{\zeta_m^2 + \omega_{\boldsymbol{q}\lambda}^2}. \tag{10}$$

The quantities $\Sigma(\boldsymbol{k}, i\omega_n)$ and $\Pi_\lambda(\boldsymbol{q}, i\zeta_m)$ are the electron self-energy and the phonon self-energy, respectively.

We shall calculate the self-energy parts in a renormalized random phase approximation (RRPA), which is given by replacing the free electron Green's functions in the bubble diagram in the random phase approximation with the renormalized Green's functions.[9] In RRPA $\Sigma(\boldsymbol{k}, i\omega_n)$ and $\Pi_\lambda(\boldsymbol{q}, i\zeta_m)$ are expressed as follows:

$$\Sigma(\boldsymbol{k}, i\omega_n) = -T\sum_{\substack{\boldsymbol{q},\boldsymbol{K}\\ m}} V(\boldsymbol{q}+\boldsymbol{K})G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m)\Gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)$$
$$-T\sum_{\substack{\boldsymbol{q},\boldsymbol{K}\\ m,\lambda}} D_\lambda(\boldsymbol{q}, i\zeta_m)G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m)\alpha_{\boldsymbol{q}\lambda}^2(\boldsymbol{q}+\boldsymbol{K})\Gamma^\lambda(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m), \tag{11}$$

$$\Pi_\lambda(\boldsymbol{q}, i\zeta_m) = 2T\sum_{\substack{\boldsymbol{k},\boldsymbol{K}\\ n}} \Gamma^\lambda(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)\alpha_{\boldsymbol{q}\lambda}^2(\boldsymbol{q}+\boldsymbol{K})G(\boldsymbol{k}, i\omega_n)G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m). \tag{12}$$

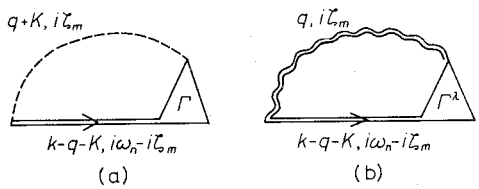

Fig. 1. Electron self-energy parts. (a) Coulomb part. (b) electron-phonon part.

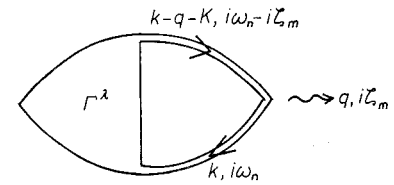

Fig. 2. Phonon self-energy.

The vertices $\Gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)$ and $\Gamma^\lambda(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)$ are expressed in RRPA as follows:

$$\Gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = 1 + \gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)V(\boldsymbol{q}+\boldsymbol{K})$$
$$+\sum_\lambda \gamma^\lambda(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)D_\lambda(\boldsymbol{q}, i\zeta_m)\alpha_{\boldsymbol{q}\lambda}^2(\boldsymbol{q}+\boldsymbol{K}), \tag{13}$$

$$\Gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = 1+\gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)\, V(\boldsymbol{q}+\boldsymbol{K}), \tag{14}$$

where

$$\gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = 2T\sum_{\boldsymbol{k}, n}\Gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)\, G(\boldsymbol{k}, i\omega_n)\, G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m), \tag{15}$$

$$\gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = 2T\sum_{\boldsymbol{k}, n}\Gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)\, G(\boldsymbol{k}, i\omega_n)\, G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m). \tag{16}$$

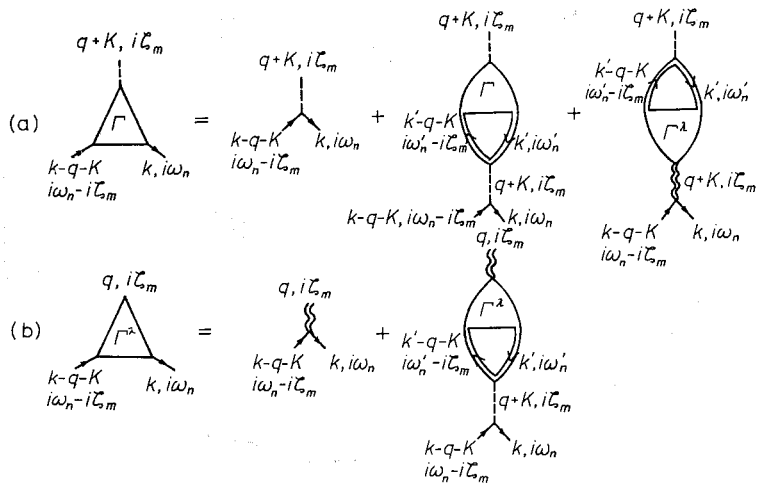

Fig. 3. Vertices. (a) electron-electron vertex Γ. (b) electron-phonon vertex Γ^{λ}.

Now we introduce the dynamical dielectric function as follows:

$$\epsilon(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = 1 - V(\boldsymbol{q}+\boldsymbol{K})\, P(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m), \tag{17}$$

where

$$P(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = 2T\sum_{\boldsymbol{k}, n} G(\boldsymbol{k}, i\omega_n)\, G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m). \tag{18}$$

Using $\epsilon(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)$, $\gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)$ and $\gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)$ can be rewritten as

$$\gamma(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = \Big[1+\sum_{\lambda}\gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)\,\alpha^2_{\boldsymbol{q}\lambda}(\boldsymbol{q}+\boldsymbol{K})\, D_{\lambda}(\boldsymbol{q}, i\zeta_m)\Big] \times \frac{1}{V(\boldsymbol{q}+\boldsymbol{K})}\left[\frac{1}{\epsilon(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)} - 1\right], \tag{19}$$

$$\gamma^{\lambda}(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m) = \frac{1}{V(\boldsymbol{q}+\boldsymbol{K})}\left[\frac{1}{\epsilon(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)} - 1\right] \tag{20}$$

and the expressions for $\Sigma(\boldsymbol{k}, i\omega_n)$ and $\Pi_{\lambda}(\boldsymbol{q}, i\zeta_m)$ become

$$\Sigma(\boldsymbol{k}, i\omega_n) = -T\sum_{\boldsymbol{q}, \boldsymbol{K}\atop m}\frac{V(\boldsymbol{q}+\boldsymbol{K})}{\epsilon(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)}\, G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m) - T\sum_{\boldsymbol{q}, \boldsymbol{K}\atop m}\frac{\sum_{\lambda}\alpha^2_{\boldsymbol{q}\lambda}(\boldsymbol{q}+\boldsymbol{K})\, D_{\lambda}(\boldsymbol{q}, i\zeta_m)}{\epsilon^2(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)}\, G(\boldsymbol{k}-\boldsymbol{q}-\boldsymbol{K}, i\omega_n - i\zeta_m), \tag{21}$$

$$\Pi_\lambda(\boldsymbol{q}, i\zeta_m) = \sum_{\boldsymbol{K}} \frac{\alpha^2_{\boldsymbol{q}\lambda}(\boldsymbol{q}+\boldsymbol{K})}{V(\boldsymbol{q}+\boldsymbol{K})} \left[\frac{1}{\epsilon(\boldsymbol{q}+\boldsymbol{K}, i\zeta_m)} - 1 \right]. \tag{22}$$

§ 3. Electron Green's function and calculation of bubble diagrams

For simplicity, we consider a half-filled conduction band with the tight-binding spectrum involving the coupling between one-dimensional chains. Then

$$\varepsilon_{\boldsymbol{k}\sigma} = -\varepsilon_{\mathrm{F}} \cos k_x a - d\varepsilon_{\mathrm{F}} (\cos k_x b + \cos k_y b), \tag{23}$$

where ε_{F} is Fermi energy, d is the strength parameter of the electron hopping integral between chains, a and b are lattice spacing constants. If we take $\boldsymbol{Q} = (\pi/b, \pi/b, 2k_{\mathrm{F}})$, then we have the relation

$$\varepsilon_{\boldsymbol{k}-\boldsymbol{Q}} = -\varepsilon_{\boldsymbol{k}}. \tag{24}$$

Near the Peierls transition temperature T_p, the phonon frequency at $\boldsymbol{q}=\boldsymbol{Q}$ is expected to become very small, so that the second term on the right-hand side of Eq. (21) becomes dominant and the first term may be neglected. In the summation of the second term, the factors other than D_λ change very little near $\boldsymbol{q}\sim\boldsymbol{Q}$ and $\zeta_m\sim 0$, and we can make the following approximation:

$$\Sigma(\boldsymbol{k}, i\omega_n) \cong \Delta^2 G(\boldsymbol{k}-\boldsymbol{Q}, i\omega_n), \tag{25}$$

$$\Delta^2 = -T \sum_{\substack{\boldsymbol{q}, m \\ \lambda}} \frac{\alpha^2_{\boldsymbol{Q}\lambda}(\boldsymbol{Q})}{\epsilon^2(\boldsymbol{Q}, 0)} [D_\lambda(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m) + D_\lambda(\boldsymbol{Q}-\boldsymbol{q}, i\zeta_m)]. \tag{26}$$

Here we neglect the Umklapp process. The quantity Δ may be thought to express the magnitude of the fluctuation.

Using Eqs. (25) and (7), one obtains

$$G(\boldsymbol{k}, i\omega_n) = -\frac{\omega_n^2 + \varepsilon_{\boldsymbol{k}}^2 - \sqrt{(\omega_n^2+\varepsilon_{\boldsymbol{k}}^2)(\omega_n^2+\varepsilon_{\boldsymbol{k}}^2+4\Delta^2)}}{2\Delta^2(i\omega_n - \varepsilon_{\boldsymbol{k}})} \tag{27}$$

from which the spectral density is obtained as

$$\rho(\boldsymbol{k}, \omega) = -\frac{1}{\pi} \operatorname{Im} G(\boldsymbol{k}, \omega + i0^+)$$

$$= \begin{cases} \dfrac{1}{2\pi\Delta^2} \sqrt{(\omega+\varepsilon_{\boldsymbol{k}})(\varepsilon_{\boldsymbol{k}}^2 + 4\Delta^2 - \omega^2)} \dfrac{}{\omega - \varepsilon_{\boldsymbol{k}}} & \text{for} \quad \varepsilon_{\boldsymbol{k}}^2 < \omega^2 < \varepsilon_{\boldsymbol{k}}^2 + 4\Delta^2, \\ 0 & \text{otherwise}. \end{cases} \tag{28}$$

The behavior of the spectral density (see Fig. 4) indicates that the electron Green's function above the transition temperature has some resemblance to the character in the ordered phase because of the effect of the fluctuations.

The electronic density of states $\rho(\omega)$ is calculated as

$$\rho(\omega) = \sum_{\boldsymbol{k}} \rho(\boldsymbol{k}, \omega)$$

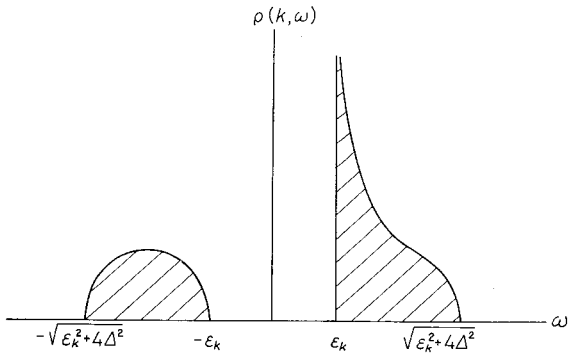

Fig. 4. Spectral density $\rho(\boldsymbol{k}, \omega)$ (schematic).

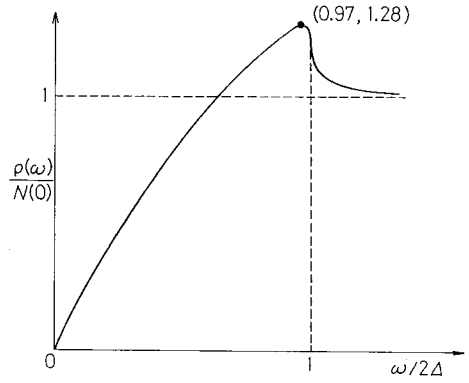

Fig. 5. Electronic density of states $\rho(\omega)$. $N(0)$ is the density of states of the free electron on the Fermi surface. There exists a maximum at $\omega/2\Delta=0.97$. The derivative diverges logarithmically at $\omega/2\Delta=1$.[10]

$$=\begin{cases}\dfrac{4}{\pi}N(0)\dfrac{|\omega|}{2\Delta}E\left(\dfrac{\omega}{2\Delta}\right) & \text{for } |\omega|<2\Delta\,, \\ \dfrac{4}{\pi}N(0)\left(\dfrac{\omega}{2\Delta}\right)^2\left[\left(\dfrac{4\Delta^2}{\omega^2}-1\right)K\left(\dfrac{2\Delta}{\omega}\right)+E\left(\dfrac{2\Delta}{\omega}\right)\right] & \text{for } |\omega|>2\Delta\,,\end{cases} \tag{29}$$

where $N(0)$ is the density of states on the Fermi surface for the free electron system and $K(k)$ and $E(k)$ are the complete elliptic integrals of the first kind and the second kind, respectively. From Eq. (29), $\rho(\omega)$ can be expressed approximately as

$$\rho(\omega)=\begin{cases}N(0)\dfrac{|\omega|}{\Delta} & \text{for } |\omega|\ll\Delta\,, \\ N(0)\left(1+\dfrac{\Delta^2}{2\omega^2}\right) & \text{for } |\omega|\gg\Delta\,,\end{cases} \tag{30}$$

which shows that if $\Delta\to 0$ then $\rho(\omega)$ approaches $N(0)$. Therefore it follows that deppressed near the Fermi surface on account of the fluctuations, the density of states has a pseudo-gap and vanishes on the Fermi surface. Note that the density of states depends implicitly on T and d through Δ.

The same results as those expressed by Eqs. (29) and (30) have been given first by Takada[10] for the superconductive transition.

Lee, Rice and Anderson[2] also have shown phenomenologically that the density of states has the pseudo-gap at temperatures below half the transition temperature, assuming the phonon Green's function to be a Lorentzian structure factor. On the other hand Rice and Strässler[5] have derived similar results, taking explicitly

account of the interchain coupling through the soft-phonon frequency. Here we have succeeded in deriving the pseudo-gap microscopically. In their works, however, the density of states remains finite on the Fermi surface and is proportional to ξ^{-1}, where ξ is the coherent length, while in our treatment the density of states always vanishes on the Fermi surface: This results from the approximation in Eq. (25) that electron with wavenumber $\boldsymbol{k}$ couples only with electron with wavenumber $\boldsymbol{k}-\boldsymbol{Q}$. Comparing our results with theirs, we find that our treatment is appropriate for $v_F\xi^{-1}\ll T$, which is satisfied in a certain region near the transition temperature.

We turn to the calculation of the bubble diagram. In order to calculate $P(\boldsymbol{Q}+\boldsymbol{q}, 0)$ given by Eq. (18) we put

$$\varepsilon_{\boldsymbol{k}-\boldsymbol{q}}=\varepsilon_{\boldsymbol{k}}+2\eta\,, \tag{31}$$

$$\begin{aligned}2\eta\equiv&-\varepsilon_F[\cos(k_z-q_z)a-\cos k_z a]\\&-d\varepsilon_F[\cos(k_x-q_x)b-\cos k_x b+\cos(k_y-q_y)b-\cos k_y b]\\\cong&-\varepsilon_F\sin q_z a-d\varepsilon_F[\cos(k_x-q_x)b-\cos k_x b\\&+\cos(k_y-q_y)b-\cos k_y b].\end{aligned} \tag{32}$$

In the following calculation, the dominant contribution of the $\boldsymbol{k}$ summation comes from the region near the Fermi surface, so that we can neglect k_z dependence of η. Inserting the expression (27) for G, and using Eq. (31) the following expression for P is obtained:

$$\begin{aligned}P(\boldsymbol{Q}+\boldsymbol{q}, 0)=&2T\sum_{\boldsymbol{k},n}\frac{-\omega_n^2-a_{\boldsymbol{k}}b_{\boldsymbol{k}}}{4\Delta^2\sqrt{(\omega_n^2+a_{\boldsymbol{k}}^2)(\omega_n^2+b_{\boldsymbol{k}}^2)}}\\&\times(\sqrt{\omega_n^2+A_{\boldsymbol{k}}^2}-\sqrt{\omega_n^2+a_{\boldsymbol{k}}^2})(\sqrt{\omega_n^2+B_{\boldsymbol{k}}^2}-\sqrt{\omega_n^2+b_{\boldsymbol{k}}^2}),\end{aligned} \tag{33}$$

where $a_{\boldsymbol{k}}=\varepsilon_{\boldsymbol{k}}-\eta$, $A_{\boldsymbol{k}}=\sqrt{a_{\boldsymbol{k}}^2+4\Delta^2}$, $b_{\boldsymbol{k}}=\varepsilon_{\boldsymbol{k}}+\eta$, $B_{\boldsymbol{k}}=\sqrt{b_{\boldsymbol{k}}^2+4\Delta^2}$. Because it is difficult to perform the summation in Eq. (33) in general, we investigate two limiting cases only, i.e., $T\ll\Delta$ and $T\gg\Delta$. Since $P(\boldsymbol{Q}+\boldsymbol{q}, 0)$ is an even function of η, in what follows we assume $\eta>0$ for simplicity.

i) *The case* $T\ll\Delta$

Because we are interested in the behavior of $P(\boldsymbol{Q}+\boldsymbol{q}, 0)$ for small $\boldsymbol{q}$, η can be assumed to be much smaller than Δ. Replacing the frequency summation in Eq. (33) by the contour integration, we obtain

$$\begin{aligned}P(\boldsymbol{Q}+\boldsymbol{q}, 0)=&\frac{1}{2\pi\Delta^4}\sum_{\boldsymbol{k}}\Bigg[\int_{|a_{\boldsymbol{k}}|}^{b_{\boldsymbol{k}}}dz\tanh\frac{z}{2T}(z^2-a_{\boldsymbol{k}}b_{\boldsymbol{k}})\sqrt{\frac{(A_{\boldsymbol{k}}^2-z^2)(B_{\boldsymbol{k}}^2-z^2)}{(z^2-a_{\boldsymbol{k}}^2)(b_{\boldsymbol{k}}^2-z^2)}}\\&+\int_{A_{\boldsymbol{k}}}^{B_{\boldsymbol{k}}}dz\tanh\frac{z}{2T}(z^2-a_{\boldsymbol{k}}b_{\boldsymbol{k}})\sqrt{\frac{(z^2-A_{\boldsymbol{k}}^2)(B_{\boldsymbol{k}}^2-z^2)}{(z^2-a_{\boldsymbol{k}}^2)(z^2-b_{\boldsymbol{k}}^2)}}\\&-\int_{|a_{\boldsymbol{k}}|}^{A_{\boldsymbol{k}}}dz\tanh\frac{z}{2T}(z^2-a_{\boldsymbol{k}}b_{\boldsymbol{k}})\sqrt{\frac{A_{\boldsymbol{k}}^2-z^2}{z^2-a_{\boldsymbol{k}}^2}}\end{aligned}$$

$$-\int_{b_k}^{B_k} dz \tanh\frac{z}{2T}(z^2-a_kb_k)\sqrt{\frac{B_k^2-z^2}{z^2-b_k^2}}\Big]. \tag{34}$$

Under the condition $|\eta|\ll\Delta$, Eq. (34) becomes

$$\begin{aligned}P(\boldsymbol{Q}+\boldsymbol{q},0)\cong\frac{1}{2\pi\Delta^4}\sum_k\Big[&\int_{|a_k|}^{b_k} dz\tanh\frac{z}{2T}\frac{4\Delta^2(z^2-a_kb_k)}{\sqrt{(z^2-a_k^2)(b_k^2-z^2)}}\\&+\int_{A_k}^{B_k} dz\tanh\frac{z}{2T}\sqrt{(z^2-A_k^2)(B_k^2-z^2)}\\&-\int_{|a_k|}^{A_k} dz\tanh\frac{z}{2T}(z^2-a_kb_k)\sqrt{\frac{A_k^2-z^2}{z^2-a_k^2}}\\&-\int_{b_k}^{B_k} dz\tanh\frac{z}{2T}(z^2-a_kb_k)\sqrt{\frac{B_k^2-z^2}{z^2-b_k^2}}\Big].\end{aligned} \tag{35}$$

Since $\tanh(z/2T)=1-2f(z)$, where $f(z)$ is the Fermi distribution function, we divide $P(\boldsymbol{Q}+\boldsymbol{q},0)$ into two parts, each being obtained by replacing the factor $\tanh(z/2T)$ in the integrand of Eq. (35) by 1 and $-2f(x)$, respectively, and denotes each function as $P_0(\boldsymbol{Q}+\boldsymbol{q},0)$ and $P_T(\boldsymbol{Q}+\boldsymbol{q},0)$.

Performing the integration with respect to z in $P_0(\boldsymbol{Q}+\boldsymbol{q},0)$ and expanding in power series of η/Δ up to second order, we obtain

$$\begin{aligned}P_0(\boldsymbol{Q}+\boldsymbol{q},0)=2\sum_k\Big\{&\frac{\eta^2}{\Delta^2}\Big(\frac{2\varepsilon_k}{b_k^2}-\frac{3\varepsilon_k^3}{2b_k^4}\Big)+\frac{\eta^2\varepsilon_k^2}{4\Delta^4B_k}\\&-\Big[\frac{1}{4A_k}-\frac{\eta}{2\Delta^2}\Big(\frac{a_k}{A_k}+\frac{3\Delta^2a_k}{2A_k^3}\Big)\Big]-\Big[\frac{1}{4B_k}+\frac{\eta}{2\Delta^2}\Big(\frac{b_k}{B_k}+\frac{3\Delta^2b_k}{2B_k^3}\Big)\Big]\Big\}.\end{aligned} \tag{36}$$

Since the dominant contribution of the $\boldsymbol{k}$ summation in Eq. (36) comes from the region near the Fermi surface, ε_k can be replaced by $\varepsilon_F a(|k_z|-k_F)-\varepsilon_F du$, where $u=\cos k_xb+\cos k_yb$. Performing the k_z summation, we obtain

$$P_0(\boldsymbol{Q}+\boldsymbol{q},0)\cong\sum_{k_x,k_y}\frac{1}{\pi\varepsilon_Fa}\Big[\Big(\frac{\eta}{\Delta}\Big)^2\ln\frac{\Delta}{\eta}-\ln\frac{\varepsilon_F}{\Delta}+\frac{\varepsilon_F^2\eta^2}{4\Delta^4}\Big] \tag{37}$$

for $\Delta^2>\eta\varepsilon_F$. Here we have neglected the higher order terms such as η/ε_F and du/ε_F.

P_0 is a even function of η and d is very small, so that we can replace η by $\bar{\eta}$, which is defined as

$$\begin{aligned}\bar{\eta}^2&=\Big(\frac{b}{2\pi}\Big)^2\int\int_{-\pi/b}^{\pi/b}dk_xdk_y\eta^2\\&=\varepsilon_F^2\sin^2q_za+\frac{1}{2}d^2\varepsilon_F^2(\sin^2q_xb+\sin^2q_yb)\\&\cong\varepsilon_F^2\Big(q_z^2a^2+\frac{1}{2}d^2q_\perp^2b^2\Big),\end{aligned} \tag{32a}$$

$$q_\perp{}^2 = q_x{}^2 + q_y{}^2 .$$

From now on we express $\bar{\eta}$ as η simply.

Summing with respect to k_x and k_y, the expression for $P_0(\boldsymbol{Q}+\boldsymbol{q}, 0)$ is obtained:

$$P_0(\boldsymbol{Q}+\boldsymbol{q}, 0) = N(0)\left[\left(\frac{\eta}{\Delta}\right)^2 \ln\frac{\Delta}{\eta} - \ln\frac{\varepsilon_F}{\Delta} + \frac{\varepsilon_F{}^2\eta^2}{4\Delta^4}\right], \tag{38}$$

where $N(0) = (\pi\varepsilon_F a b^2)^{-1}$.

Next let us consider $P_T(\boldsymbol{Q}+\boldsymbol{q}, 0)$. Because $A_{\boldsymbol{k}}$, $B_{\boldsymbol{k}} > \Delta \gg T$, and $f(z)$ is a rapidly decreasing function, the expression for $P_T(\boldsymbol{Q}+\boldsymbol{q}, 0)$ can be written as

$$P_T(\boldsymbol{Q}+\boldsymbol{q}, 0) \cong -\frac{1}{\pi\Delta^4}\sum_{\boldsymbol{k}}\left[4\Delta^2\int_{|a_{\boldsymbol{k}}|}^{b_{\boldsymbol{k}}} dz\, f(z)\frac{z^2 - a_{\boldsymbol{k}}b_{\boldsymbol{k}}}{\sqrt{(z^2 - a_{\boldsymbol{k}}{}^2)(b_{\boldsymbol{k}}{}^2 - z^2)}}\right.$$
$$\left. - 2\Delta\int_{|a_{\boldsymbol{k}}|}^{\infty} dz\, f(z)\frac{z^2 - a_{\boldsymbol{k}}b_{\boldsymbol{k}}}{\sqrt{z^2 - a_{\boldsymbol{k}}{}^2}} - 2\Delta\int_{|b_{\boldsymbol{k}}|}^{\infty} dz\, f(z)\frac{z^2 - a_{\boldsymbol{k}}b_{\boldsymbol{k}}}{\sqrt{z^2 - b_{\boldsymbol{k}}{}^2}}\right]. \tag{39}$$

Integrating first with respect to $\boldsymbol{k}$ and next with respect to z, we obtain

$$P_T(\boldsymbol{Q}+\boldsymbol{q}, 0) = -N(0)\left[\left(\frac{\eta}{\Delta}\right)^2 \ln\frac{2\eta}{2\eta+T} - \left(\frac{\eta}{\Delta}\right)^2 - \frac{3\zeta(3)}{2}\left(\frac{T}{\Delta}\right)^3\right], \tag{40}$$

where $\zeta(3)$ is the ζ-function. We have neglected the higher order terms such as du/ε_F.

Considering that $P(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ is invariant with respect to the interchange between 2η and ζ_m, from Eqs. (38) and (40) we obtain

$$p(\boldsymbol{q}, i\zeta_m) \equiv P(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m) - P(\boldsymbol{Q}, 0)$$
$$= \frac{1}{4}N(0)\left[\left(\frac{2\eta}{\Delta}\right)^2 \ln\frac{\Delta}{|2\eta| + T} + \left(\frac{\zeta_m}{\Delta}\right)^2 \ln\frac{\Delta}{|\zeta_m| + T} + \frac{\varepsilon_F{}^2}{4\Delta^2}\left(\frac{4\eta^2}{\Delta^2} + \frac{\zeta_m{}^2}{\Delta^2}\right)\right], \tag{41}$$

$$P(\boldsymbol{Q}, 0) = -2N(0)\left[\ln\frac{\varepsilon_F}{\Delta} - \frac{3\zeta(3)}{2}\left(\frac{T}{\Delta}\right)^3\right]. \tag{42}$$

ii) *The case* $\Delta \ll T$

In this case we immediately obtain

$$P(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m) \cong 2T\sum_{\boldsymbol{k}, n}\frac{1}{(i\omega_n - \varepsilon_{\boldsymbol{k}})(i\omega_n - i\zeta_m + \varepsilon_{\boldsymbol{k}-\boldsymbol{q}})} \tag{43}$$

which gives

$$p(\boldsymbol{q}, i\zeta_m) = N(0)\left[\psi\left(\frac{1}{2} + \frac{\zeta_m + 2i\eta}{4\pi T}\right) + \psi\left(\frac{1}{2} + \frac{\zeta_m - 2i\eta}{4\pi T}\right) - 2\psi\left(\frac{1}{2}\right)\right]$$
$$\cong -2N(0)\left\{-\frac{\pi}{8}\frac{|\zeta_m|}{T} + \frac{7\zeta(3)}{16\pi^2}\left[\left(\frac{\zeta_m}{T}\right)^2 - \left(\frac{2\eta}{T}\right)^2\right]\right\}, \tag{44}$$

where $\psi(x)$ is the di-gamma function. For later convenience, we give the expression for $P(\boldsymbol{Q}, 0)$ up to order $(\Delta/T)^2$:

$$P(\boldsymbol{Q}, 0) = -2N(0)\left[\ln\frac{2\gamma\varepsilon_{\mathrm{F}}}{\pi T} - \frac{7\zeta(3)}{4\pi^2}\left(\frac{\Delta}{T}\right)^2\right], \tag{45}$$

where γ is Euler constant.

§ 4. Phonon Green's function

In this section we derive the expression for the phonon Green's function by using the expressions for P derived in the previous section. We consider only the longitudinal mode.

Let us introduce the quantity $\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ as

$$D^{-1}(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m) = -\zeta_m{}^2 - \Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m). \tag{46}$$

Then $\Omega(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ is expressed from Eq. (8) as

$$\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m) = \omega^2_{\boldsymbol{Q}+\boldsymbol{q}} + \Pi(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m), \tag{47}$$

where $\omega^2_{\boldsymbol{Q}+\boldsymbol{q}}$ and $\Pi(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ are given in Eqs. (2) and (22), respectively, as the summations over all reciprocal lattice vectors. Since the summands decrease rapidly as $\boldsymbol{q}+\boldsymbol{K}$ increases, we retain only first two terms in the summation and neglect the other terms. Then $\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ is written as

$$\begin{aligned}&\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)\\ &= \omega^2_{\boldsymbol{Q}+\boldsymbol{q}} + \frac{\alpha^2(\boldsymbol{Q}+\boldsymbol{q})}{V(\boldsymbol{Q}+\boldsymbol{q})}\left[\frac{1}{\epsilon(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)} - 1\right] + \frac{\alpha^2(\boldsymbol{Q}-\boldsymbol{q})}{V(\boldsymbol{Q}-\boldsymbol{q})}\left[\frac{1}{\epsilon(\boldsymbol{Q}-\boldsymbol{q}, i\zeta_m)} - 1\right],\end{aligned} \tag{48}$$

$$\omega^2_{\boldsymbol{Q}+\boldsymbol{q}} = \frac{N}{M}\{[(\boldsymbol{Q}+\boldsymbol{q})\cdot\boldsymbol{\varepsilon}_{\boldsymbol{Q}+\boldsymbol{q}}]^2 U_I(\boldsymbol{Q}+\boldsymbol{q}) + [(\boldsymbol{Q}-\boldsymbol{q})\cdot\boldsymbol{\varepsilon}_{\boldsymbol{Q}+\boldsymbol{q}}]^2 U_I(\boldsymbol{Q}-\boldsymbol{q})\}, \tag{49}$$

where $\varepsilon_{\boldsymbol{q}} = \boldsymbol{q}/|\boldsymbol{q}|$ and $\alpha(\boldsymbol{q}) = \sqrt{N/M}\,\boldsymbol{q}\cdot\varepsilon_{\boldsymbol{q}} U_I(\boldsymbol{q})$. Expanding $\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ in power series of $\boldsymbol{q}$ and retaining terms up to second order, we obtain

$$\begin{aligned}\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m) = \Omega^2(\boldsymbol{Q}, 0) + \frac{2N}{M}\Big\{&q^2\left(U_I - \frac{PU_b{}^2}{\epsilon^2}\right)\\ &+ 2\frac{(\boldsymbol{q}\cdot\boldsymbol{Q})^2}{Q^2}\left(U_I + \frac{2V^2U_b{}^2P^3}{\epsilon^3}\right) + \frac{1}{2}Q^2(\boldsymbol{q}\cdot\nabla_{\boldsymbol{Q}})^2\left(U_I + \frac{PU_b{}^2}{\epsilon}\right)\\ &+ 2(\boldsymbol{q}\cdot\boldsymbol{Q})(\boldsymbol{q}\cdot\nabla_{\boldsymbol{Q}})\left[U_I + \frac{PU_b{}^2}{\epsilon}\left(1 - \frac{PV}{\epsilon}\right)\right] + \frac{Q^2U_b{}^2}{\epsilon^2}p(\boldsymbol{q}, i\zeta_m)\Big\},\end{aligned} \tag{50}$$

$$\Omega^2(\boldsymbol{Q}, 0) = \frac{2N}{M}Q^2\left(U_I + \frac{PU_b{}^2}{\epsilon}\right), \tag{51}$$

where we have omitted the arguments of $U_I(\boldsymbol{Q})$, $U_b(\boldsymbol{Q})$, $V(\boldsymbol{Q})$, $P(\boldsymbol{Q}, 0)$ and $\epsilon(\boldsymbol{Q}, 0)$. The operator $\nabla_{\boldsymbol{Q}}$ operates U_I and U_b.

The condition for the occurrence of the phonon softening at $\boldsymbol{q}=\boldsymbol{Q}$, $\Omega^2(\boldsymbol{Q}, 0) = 0$, depends on the behavior of $U_I(\boldsymbol{Q})$, $U_b(\boldsymbol{Q})$, $V(\boldsymbol{Q})$ and $P(\boldsymbol{Q}, 0)$. If the ion-ion and the electron-ion interaction are taken as Coulombic, i.e., $z^{-2}U_I(\boldsymbol{Q}) = z^{-1}U_b(\boldsymbol{Q})$

$=V(\boldsymbol{Q})=4\pi e^2/Q^2$, where ze is the charge of the ion, $\Omega^2(\boldsymbol{Q},0)$ is written as $2Nz^2Q^2V(\boldsymbol{Q})/M\epsilon$ and no phonon softening occurs. This situation holds in the jellium model.[8]

In the expression (50) for $\Omega^2(\boldsymbol{Q}+\boldsymbol{q},i\zeta_m)$ the anisotropy of the conduction band appears through $\epsilon(\boldsymbol{Q},0)$, $P(\boldsymbol{Q},0)$ and $p(\boldsymbol{q},i\zeta_m)$, among which the term involving the factor $p(\boldsymbol{q},i\zeta_m)$ is of the lowest order. Since we are interested in the effect of the anisotropy of the conduction band on the Peierls transition, we retain only the first and last terms in Eq. (50). We shall investigate the effect of the Coulomb interaction in the next paper.

Thus $\Omega^2(\boldsymbol{Q}+\boldsymbol{q},i\zeta_m)$ is written down as

$$\Omega^2(\boldsymbol{Q}+\boldsymbol{q},i\zeta_m)\cong\omega_0^2t+\frac{1}{4}\omega_0^2\left\{\left(\frac{2\eta}{\Delta}\right)^2\ln\frac{\Delta}{|2\eta|+T}+\left(\frac{\zeta_m}{\Delta}\right)^2\ln\frac{\Delta}{|\zeta_m|+T}+\frac{1}{4}\left(\frac{\varepsilon_F}{\Delta}\right)^2\left[\left(\frac{2\eta}{\Delta}\right)^2+\left(\frac{\zeta_m}{\Delta}\right)^2\right]\right\}\quad\text{for}\quad T\ll\Delta\,,\tag{52}$$

$$\Omega^2(\boldsymbol{Q}+\boldsymbol{q},i\zeta_m)\cong\omega_0^2t+2\omega_0^2\left\{\frac{\pi}{8}\frac{|\zeta_m|}{T}-\frac{7\zeta(3)}{16\pi^2}\left[\left(\frac{\zeta_m}{T}\right)^2-\left(\frac{2\eta}{T}\right)^2\right]\right\}\qquad\text{for}\quad T\gg\Delta\,,\tag{53}$$

$$\Omega^2(\boldsymbol{Q},0)=\omega_{\boldsymbol{Q}}^2+\frac{\epsilon\omega_0^2}{N(0)}P=\omega_0^2t\,,\tag{54}$$

$$\omega_0^2=\frac{2NQ^2U_b^2}{M\epsilon^2}N(0)\,.\tag{55}$$

§ 5. Self-consistent equations

In Eq. (24) we divide $T\sum_m D(\boldsymbol{q},i\zeta_m)$ into two parts: $TD(\boldsymbol{q},0)$ and $T\sum_{m\neq0}D(\boldsymbol{q},i\zeta_m)$. The first part $TD(\boldsymbol{q},0)$ corresponds to the thermal fluctuation and the second one $T\sum_{m\neq0}D(\boldsymbol{q},i\zeta_m)$ to the zero point fluctuation. We can replace $T\sum_{m\neq0}D(\boldsymbol{q},i\zeta_m)$ by $\int d\zeta_m D(\boldsymbol{q},i\zeta_m)/2\pi$ for very low temperatures discussed now.

Then the equation for Δ^2 can be expressed as

$$\Delta^2=\Delta_Z^2+\Delta_T^2=\frac{\omega_0^2}{\pi\varepsilon_F^2}\left[\int_0^{\kappa_1}d\xi\int_0^{\kappa_2}\rho d\rho\int_{-\infty}^{\infty}\frac{d\zeta_m}{2\pi}\frac{1}{\zeta_m^2+\Omega^2(\boldsymbol{Q}+\boldsymbol{q},i\zeta_m)}+T\int_0^{\kappa_1}d\xi\int_0^{\kappa_2}\rho d\rho\frac{1}{\Omega^2(\boldsymbol{Q}+\boldsymbol{q},0)}\right],\tag{56}$$

where κ_1 and κ_2 are cutoff parameters, $\xi=\varepsilon_F aq_z$ and $\rho^2=(1/2)\varepsilon_F^2b^2q_\perp^2$. These quantities Δ_Z and Δ_T correspond to the zero point fluctuation and the thermal one, respectively. We put

$$\Omega^2(\boldsymbol{Q}+\boldsymbol{q},i\zeta_m)=\omega_0^2[t+\sigma(\xi^2+d^2\rho^2)+\sigma'\zeta_m^2],\tag{57}$$

where σ and σ' are functions of ζ_m, ξ and ρ. However because of the condition $\kappa_1^2 \gg d^2\kappa_2^2$, the dominant contribution to Δ^2 comes from small ζ_m and ξ regions. In this case we can take σ and σ' as constants and we have

$$\left.\begin{aligned} &\sigma=\sigma'\cong\frac{1}{8\Delta^2}\ln\frac{\Delta}{T} \quad \text{for} \quad T\ll\Delta\exp\left[-\left(\frac{\varepsilon_F}{\Delta}\right)^2\right], \\ &\sigma=\sigma'\cong\frac{\varepsilon_F^2}{16\Delta^4} \quad \text{for} \quad \Delta\exp\left[-\left(\frac{\varepsilon_F}{\Delta}\right)^2\right]\ll T\ll\Delta, \\ &\sigma=-\sigma'\cong\frac{7\zeta(3)}{8\pi^2T^2} \quad \text{for} \quad \Delta\ll T. \end{aligned}\right\} \tag{58}$$

Of course we must note that for $\Delta\ll T$ Eq. (53) has been obtained by expanding the first line in Eq. (44) in power series of ζ_m/T and η/T. For $\zeta_m\neq 0$, since ζ_m/T is larger than unity, this expansion cannot be used. In this case, $\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ depends logarithmically on ζ_m. Therefore in the first term of Eq. (56), ζ_m dependence of $\Omega^2(\boldsymbol{Q}+\boldsymbol{q}, i\zeta_m)$ can be neglected compared with ζ_m^2 for the case $\Delta\ll T$.

Under the condition $\kappa_1^2\gg d^2\kappa_2^2+t/\sigma$ we obtain

$$\Delta_Z^2\cong\frac{\omega_0}{4\pi\varepsilon_F^2d^2\sqrt{\sigma(1+\omega_0^2\sigma')}}\left(\frac{1}{2}d^2\kappa_2^2+\frac{t}{2\sigma}\ln\frac{t}{t+d^2\kappa_2^2\sigma}+d^2\kappa_2^2\ln\frac{2\kappa_1}{\sqrt{t/\sigma+d^2\kappa_2^2}}\right), \tag{59}$$

$$\Delta_T^2\cong\frac{T}{2\pi\varepsilon_F^2\sigma d^2}\left[d^2\frac{\kappa_2^2}{\kappa_1}+\pi\left(\sqrt{\frac{t}{\sigma}+d^2\kappa_2^2}-\sqrt{\frac{t}{\sigma}}\right)\right]. \tag{60}$$

From the discussion above the factor $\sqrt{1+\omega_0^2\sigma'}$ in Eq. (59) can be replaced by $\sqrt{\omega_0^2\sigma}$ for $T\ll\Delta$ and by 1 for $T\gg\Delta$.

Using Eqs. (56), (58), (59) and (60), Δ is self-consistently determined as a function of T.

Below we determine the Peierls transition temperature T_p, at which the complete phonon softening, $\Omega(\boldsymbol{Q}, 0)=0$, occurs, as a function of the interchain coupling parameter d from Eqs. (54) and (56).

i) $T_p\ll\Delta_p$

In this case, putting $t=0$, Δ_Z^2 and Δ_T^2 are expressed as

$$\Delta_Z^2\cong\frac{\kappa_2^2}{4\pi\varepsilon_F^2\sigma}\ln\frac{\kappa_1}{d\kappa_2}, \tag{61}$$

$$\Delta_T^2\cong\frac{\kappa_2^2}{2\varepsilon_F^2\sigma}\frac{T_p}{\kappa_1}\frac{\kappa_1}{d\kappa_2}. \tag{62}$$

Here we introduce dimensionless parameters as follows:

$$x=\frac{\kappa_1}{d\kappa_2}, \quad y=\frac{T_p}{\varepsilon_F}, \quad z=\frac{\Delta_p}{\varepsilon_F}, \quad a=\left(\frac{\kappa_2}{\varepsilon_F}\right)^2, \quad \alpha=\frac{3}{2}\zeta(3), \tag{63}$$

where Δ_p is the fluctuation at $T=T_p$.

a) $T_p \ll \Delta_p \exp[-(\varepsilon_F/\Delta_p)^2]$

In this case we can take $\sigma \cong (8\Delta_p^2)^{-1} \ln \Delta_p/T_p$ from Eq. (58). Using Eqs. (54), (42), (56), (61) and (62), we obtain

$$\ln \frac{z}{y} \approx \frac{2a}{\pi} \ln x + 4a \frac{\varepsilon_F}{\kappa_1} xy, \tag{64}$$

$$\ln \frac{z}{z_0} + \alpha \left(\frac{y}{z}\right)^3 \simeq 0, \tag{65}$$

where

$$\ln \frac{1}{z_0} \equiv \frac{\omega_Q^2}{2\epsilon\omega_0^2} \equiv \frac{1}{\lambda}. \tag{66}$$

λ is the dimensionless electron-phonon coupling constant.

The region of x corresponding to this case is given by

$$\frac{\kappa_1}{4a\varepsilon_F z_0} \exp\left(\frac{1}{z_0^2}\right) < x. \tag{67}$$

In this region the thermal fluctuation is dominant and T_p and Δ_p are determined as*)

$$y \simeq \frac{\kappa_1}{4a\varepsilon_F x} \ln(z_0 x), \quad T_p \simeq \frac{\kappa_2}{4a} d \ln\left(\frac{1}{e^{1/\lambda} d}\right), \tag{68}$$

$$z \simeq z_0, \quad \Delta_p \simeq \varepsilon_F e^{-1/\lambda}. \tag{69}$$

As d tends to zero, then x becomes infinity and T_p becomes zero as expected, but Δ_p is almost independent of d.

b) $\Delta_p \exp[-(\varepsilon_F/\Delta_p)^2] \ll T_p \ll \Delta_p$

In this case we can put $\sigma \simeq \varepsilon_F^2/16\Delta_p^4$ from Eq. (58). Using Eqs. (54), (56), (61) and (62), we obtain

$$\frac{1}{z^2} \simeq 4\pi a \ln x + 8a \frac{\varepsilon_F}{\kappa_1} xy, \tag{70}$$

$$\ln \frac{z}{z_0} + \alpha \left(\frac{y}{z}\right)^3 \simeq 0. \tag{71}$$

The region of x corresponding to this case is given by

$$\frac{\kappa_1}{8a\varepsilon_F z_0^3} \ll x \ll \frac{\kappa_1}{8a\varepsilon_F z_0^3} \exp\left(\frac{1}{z_0^2}\right). \tag{72}$$

In this region the thermal fluctuation is dominant. T_p and Δ_p are obtained as

$$y \simeq \frac{\kappa_1}{8a\varepsilon_F z_0^2 x}, \quad T_p \simeq \frac{\varepsilon_F^2 \kappa_1}{8\kappa_2^2 x} e^{2/\lambda}, \tag{73}$$

*) At first we have solved Eqs. (64) and (65), assuming the zero point fluctuation to be dominant by mistake. This mistake has been pointed out by Dr. Suzumura.

$$z \simeq z_0 , \quad \Delta_p \simeq \varepsilon_F e^{-1/\lambda} . \tag{74}$$

ii) $\Delta_p \ll T_p$

In this case the zero point fluctuation and the thermal one are given by

$$\Delta z^2 \simeq \frac{\omega_0 \kappa_2^2}{4\pi \varepsilon_F^2 \sqrt{\sigma}} \ln \frac{\kappa_1}{d\kappa_2} , \tag{75}$$

$$\Delta_T{}^2 \simeq \frac{\kappa_2^2}{2\varepsilon_F^2 \sigma} \frac{T_p}{\kappa_1} \frac{\kappa_1}{d\kappa_2} , \tag{76}$$

where $\sigma = 7\zeta(3)/8\pi^2 T_p^2$ from Eq. (58). In this case the thermal fluctuation is dominant. From Eqs. (45), (54) and (76) we obtain

$$z^2 \simeq \frac{a\varepsilon_F}{\sigma_0 \kappa_1} x y^3 , \tag{77}$$

$$\ln \frac{\pi y}{2\gamma z_0} + \sigma_0 \left(\frac{z}{y} \right)^2 \simeq 0 , \tag{78}$$

where $\sigma_0 = 7\zeta(3)/4\pi^2$. Solving these equations we obtain

$$y \simeq \frac{2\gamma z_0}{\pi} \exp\left(-\frac{2\gamma a z_0 \varepsilon_F}{\pi \kappa_1} x \right), \quad T_p \simeq \frac{2\gamma}{\pi} \varepsilon_F e^{-1/\lambda} \exp\left(-\frac{2\gamma \kappa_2 z_0}{\pi \varepsilon_F d} \right), \tag{79}$$

$$z \simeq \sqrt{\frac{a\varepsilon_F}{\sigma_0 \kappa_1}} x y^3 , \qquad \Delta_p \simeq \frac{2\gamma}{\pi} \varepsilon_F e^{-1/\lambda} \sqrt{\frac{2\gamma z_0 \kappa_2}{\pi \sigma_0 \varepsilon_F d}} . \tag{80}$$

The region of x is as follows:

$$x \ll \frac{\sigma_0 \kappa_1}{2\gamma z_0 a \varepsilon_F} . \tag{81}$$

To understand the features of the results obtained above, we put $\kappa_1 = \varepsilon_F$, $\kappa_2 = 1/2\,\varepsilon_F$. Then the above results can be summarized as Table I, from which we can find the following properties:

Firstly thermal fluctuations are dominant in quasi-one-dimensional systems even if T_p is extremely low and therefore in real crystals the zero point fluctuations play no role in the Peierls transition. Secondly when d tends to zero, T_p becomes zero, but as far as d is finite, there exists a finite transition temperature. Mean-

Table I. Summary of results.

d	$d < 4\exp\left(-\frac{3}{\lambda} - e^{2/\lambda}\right)$	$4\exp\left(-\frac{3}{\lambda} - e^{2/\lambda}\right) < d < 4\exp\left(-\frac{3}{\lambda}\right)$	$2.66\exp\left(-\frac{1}{\lambda}\right) < d$
T_p/ε_F	$0.5d \ln \frac{1}{d}$	$0.25\exp\left(\frac{2}{\lambda}\right) \cdot d$	$1.13\exp\left(-\frac{1}{\lambda} - 0.54\, e^{-1/\lambda} d^{-1}\right)$
Δ_p/ε_F	$\exp\left(-\frac{1}{\lambda}\right)$		$1.85\exp\left(-\frac{3}{2\lambda}\right) d^{-1/2}$

while it should be noted that in exactly one-dimensional systems the zero point fluctuations break down the Peierls transition in which case one cannot put $t=0$ in Eqs. (59) and (60).[40]

§ 6. Concluding remarks

We have investigated the effect of fluctuations on the Peierls transition in quasi-one-dimensional systems in the renormalized random phase approximation which is given by replacing the free electron Green's function in bubble diagrams in the random phase approximation with the renormalized Green's function. It has shown that the electronic density of states has a pseudo-gap near the Fermi surface due to fluctuations and that the thermal fluctuations play a dominant role even if T_p is extremely low.

So far we have investigated the effect of fluctuations at $T=T_p$, where $\Omega(\boldsymbol{Q}, 0)=0$. Near the transition point it is expected that while thermal fluctuations are dominant at temperatures where $T_p \gg \Omega(\boldsymbol{Q}, 0)$, zero point fluctuations are dominant at temperatures where $T_p \ll \Omega(\boldsymbol{Q}, 0)$. In strictly one-dimensional systems $\Omega(\boldsymbol{Q}, 0)$ tends to zero as T approaches zero. As we examined before (cf. Ref. 4)), when T decreases the ratio $T/\Omega(\boldsymbol{Q}, 0)$ decreases and consequently zero point fluctuations break down the Peierls transition.

In § 4 we have assumed that the main contribution to the phonon dispersion comes from the bubble diagram so that the density of states available to the nesting of wavenumber $\boldsymbol{Q}=(\pi/b, \pi/b, 2k_F)$ becomes maximum and d plays an important role. In the case where the terms except for the last term in Eq. (50) are dominant, d is unimportant. Thus instead of d, a new parameter denoting the one-dimensionality of the system should be introduced, which is determined by the other terms except for the last term and is of order $Q_x/Q_z \sim a/b$. Even in this case, however, our result is valid by looking upon d as the new parameter. We shall discuss this in detail in the next paper.

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