

Theory of Polaron Mobility

Yukio ŌSAKA

Department of Physics, Tōhoku University, Sendai

(Received September 25, 1959)

(Revised manuscript received December 20, 1960)

The polaron mobility is calculated by making use of the general theory of electrical conductivity. We take the states determined by Feynman's trial action as the unperturbed states and treat the difference between the true action and the trial action as a perturbation. Numerical values of the polaron mobility at very low temperatures are given and are discussed in comparison with the results obtained by Shultz and by Morita.

§ 1. Introduction

We have investigated the static properties of polaron at finite temperatures in the previous paper¹⁾ (hereafter referred to as I). We shall investigate the polaron mobility in the present paper. In the same way as in I, we calculate the polaron mobility by using Feynman's path-integral method. In the polaron problem, the interaction between an electron and lattice vibrations is so large that the usual perturbation theoretic treatment fails. Therefore the calculation of the mobility in the present paper will be based on the general theory of electrical conductivity recently developed by many authors,²⁾ which is applicable to a system which does not allow us to set up the Boltzmann equation. We take the states determined by Feynman's trial action as unperturbed states and treat the difference between the trial action and the true action as a perturbation which yields a decay of electronic current correlation.

The following assumptions will be made in the present paper. i) The electrical conductivity is determined by the asymptotic form of a correlation function of electronic current. ii) This asymptotic form has the property of exponential decay in time. These assumptions are valid in the case of weak interaction. It is not sure whether or not they are applicable to the present problem which includes the case of strong interaction. In the present treatment, however, the states determined by Feynman's trial action instead of the states of a free electron are chosen as the unperturbed states. It is expected that the perturbation in the former case may be made weaker than in the latter case and that the above mentioned assumptions may be valid. In fact the self-energy of polaron at 0°K calculated by using these assumptions agrees with that obtained by Feynman³⁾ as will be shown in § 3. Therefore, the approxi-

mation used in the present calculation for the mobility may not be so bad even for strong interactions.

In §2, the calculation of electrical conductivity, using the path-integral method, is discussed. Then, it is applied to the calculation of the polaron mobility in the case of a weak interaction. In §3, we shall calculate the polaron mobility in the case of strong interaction based on the evaluation in §2. In §4, the result will be discussed in comparison with the results by Shultz and by Morita.

§ 2. Calculation of the polaron mobility

(in the case of weak interaction)

In this paper, we take the units so that $\hbar=1$, the electron mass $m=1$, and the optical phonon frequency $=1$.

The conductivity σ is generally expressed by a current correlation function $\chi(t)$ in the following way :

$$\sigma = \beta \int_0^{\infty} \chi(t) dt, \quad (1)$$

$$\chi(t) = \langle j_x(t) j_x + j_x j_x(t) \rangle / 2, \quad (2)$$

where $\beta=1/kT$, j_x is the x component of electronic current operator and

$$j_x(t) = e^{-iHt} j_x e^{iHt},$$

H being the Hamiltonian of the system. In this equation and in what follows $\langle A \rangle$ denotes $\text{Tr } \rho A / \text{Tr } \rho$ where ρ is the density matrix defined by $e^{-\beta H}$. The following equation is easily derived :

$$\begin{aligned} & \text{Tr}(e^{-\beta H} e^{-iHt} j_x e^{iHt} j_x) \\ &= -e^2 \iint d\mathbf{X}_1 d\mathbf{X}_2 (\partial/\partial X_{2x}^{\beta-\lambda}) (\partial/\partial X_{1x}^{\lambda}) \left\{ \iint d\mathbf{Q}_1 d\mathbf{Q}_2 \rho(\mathbf{X}_1 \mathbf{Q}_1, \mathbf{X}_2 \mathbf{Q}_2; \beta-\lambda) \right. \\ & \left. \times \rho(\mathbf{X}_2 \mathbf{Q}_2, \mathbf{X}_1 \mathbf{Q}_1; \lambda) \right\}, \quad (3) \end{aligned}$$

where e is the electronic charge, $\lambda=-it$, and \mathbf{X} is the electron coordinate, \mathbf{Q} denotes the many-dimensional coordinates of phonons, and $\partial/\partial X_{2x}^{\beta-\lambda}$ operates only on \mathbf{X}_2 in $\rho(\mathbf{X}_1 \mathbf{Q}_1, \mathbf{X}_2 \mathbf{Q}_2; \beta-\lambda)$ and not on \mathbf{X}_2 in $\rho(\mathbf{X}_2 \mathbf{Q}_2, \mathbf{X}_1 \mathbf{Q}_1; \lambda)$. In what follows, we try to rewrite the density matrices by the use of the path-integral method.

Let us take the Hamiltonian as follows :

$$H = (p^2/2) + \sum_{\mathbf{k}} M\omega_{\mathbf{k}} q_{\mathbf{k}} \gamma_{\mathbf{k}} + \sum_{\mathbf{k}} M\omega_{\mathbf{k}}^2 q_{\mathbf{k}}^2/2 + \sum_{\mathbf{k}} p_{\mathbf{k}}^2/2M, \quad (4)$$

where $\gamma_{\mathbf{k}}(\mathbf{X})$ is some function of the electronic coordinate \mathbf{X} , and $p_{\mathbf{k}}$ are the coordinate and its conjugate momentum of the \mathbf{k} -th normal mode of lattice

vibrations, respectively, and M is the reduced mass of the lattice ions. In the polaron problem, $\gamma_k = (2^{3/2}\alpha\pi/V)^{1/2} \cdot 1/k \cdot e^{ik \cdot X}$ and $\omega_k = 1$ for all k , where V is the volume of the crystal and α is the coupling constant used in I. The density matrix ρ in the path-integral representation is given by

$$\rho(\mathbf{X}_1 \mathbf{Q}_1, \mathbf{X}_2 \mathbf{Q}_2; u) \left\{ \prod_k (M\omega_k/2\pi \sinh \omega_k u) \right\}^{-1/2} \\ = \int \exp \left[- \left\{ \int_0^u \frac{1}{2} \dot{\mathbf{X}}^2(t) dt + \sum_k P(q_{1k}, q_{2k}, \mathbf{X}(t)) \right\} \right] \mathfrak{D}(\mathbf{X}(t) : \mathbf{X}_2(u), \mathbf{X}_1(0)), \quad (5)$$

where

$$P(q_{1k}, q_{2k}, \mathbf{X}(t)) = [(q_{1k}^2 + q_{2k}^2) \cosh \omega_k u - 2q_{1k} \cdot q_{2k} \\ + 2A_k \cdot q_{1k} + 2B_k \cdot q_{2k} + 2C_k] / 2 \sinh \omega_k u, \quad (6a)$$

and

$$A_k = \int_0^u \gamma_k(\mathbf{X}(t)) \sinh \omega_k t dt, \quad B_k = \int_0^u \gamma_k(\mathbf{X}(t)) \sinh \omega_k (u-t) dt, \\ C_k = - \int_0^u dt \int_0^t ds \gamma_k(\mathbf{X}(t)) \gamma_k(\mathbf{X}(s)) \sinh \omega_k (u-t) \sinh \omega_k s. \quad (6b)$$

$\mathfrak{D}(\mathbf{X}(t) : \mathbf{X}_2(u), \mathbf{X}_1(0))$ means that the path-integration must be carried out under the conditions $\mathbf{X}(0) = \mathbf{X}_1$ and $\mathbf{X}(u) = \mathbf{X}_2$.

Using (5) and (6), we obtain, after some calculations, the following equation for the polaron problem:

$$(e^{\beta/2}/e^\beta - 1)^{-3N} \int d\mathbf{Q}_1 d\mathbf{Q}_2 \rho(\mathbf{X}_1 \mathbf{Q}_1, \mathbf{X}_2 \mathbf{Q}_2; \beta - \lambda) \rho(\mathbf{X}_2 \mathbf{Q}_2, \mathbf{X}_1 \mathbf{Q}_1; \lambda) \\ = \iint \exp \left[- \int_0^{\beta-\lambda} \frac{1}{2} \dot{\mathbf{X}}'^2(t) dt - \int_0^\lambda \frac{1}{2} \dot{\mathbf{X}}''^2(t) dt + Q(\mathbf{X}' \mathbf{X}'') \right] \mathfrak{D}(\mathbf{X}'(t) : \mathbf{X}_2(\beta - \lambda), \mathbf{X}_1(0)) \\ \times \mathfrak{D}(\mathbf{X}''(t) : \mathbf{X}_1(\lambda), \mathbf{X}_2(0)), \quad (7a)$$

where N is the total number of unit cells in the crystal and

$$Q(\mathbf{X}', \mathbf{X}'') = Q_1(\mathbf{X}' \mathbf{X}''; \beta, \lambda) + S_{cross}(\mathbf{X}' \mathbf{X}''; \beta, \lambda).$$

Q_1 and S_{cross} are given by

$$Q_1(\mathbf{X}' \mathbf{X}''; \beta, \lambda) V (e^\beta - 1) / 2^{3/2} \alpha \pi \\ = \sum_w \frac{1}{w^2} \left[\int_0^\lambda d\tau \int_0^\tau d\sigma I_w(\mathbf{X}''(\tau), \mathbf{X}''(\sigma); 1) + \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma I_w(\mathbf{X}''(\tau), \mathbf{X}'(\sigma); 1) \right], \quad (7b)$$

$$S_{cross}(\mathbf{X}'\mathbf{X}''; \beta\lambda) V(e^\beta - 1)/2^{3/2} \alpha \pi = \left[\sum_w \frac{1}{\omega^3} \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma I_w(\mathbf{X}'(\tau), \mathbf{X}''(\sigma); 1) \right], \quad (7c)$$

where

$$I_w(\mathbf{x}(\tau), \mathbf{y}(\sigma); \chi) = e^{\chi(\beta-\tau+\sigma)-i\mathbf{w}(\mathbf{x}(\tau)-\mathbf{y}(\sigma))} + e^{\chi(\tau-\sigma)+i\mathbf{w}(\mathbf{x}(\tau)-\mathbf{y}(\sigma))}. \quad (7d)$$

In this section, we hereafter confine ourselves to the case in which the interaction of the electron with phonons can be treated as a small perturbation. In order to calculate the mobility in such a case, we shall make the approximations that (1) the correlation function of electronic current is, assumed to have the property of simple exponential decay in time and that (2) all averages over the canonical distribution are replaced by those of the unperturbed system. Substituting (7a) in (3) and omitting the unimportant numerical factor $(e^{\beta/2}/e^\beta - 1)^{-3N}$ which is cancelled by the normalization factor for phonon, we get

$$\text{Tr}(e^{-\beta H} e^{-iHt} j_x e^{iHt} j_x) = -e^2 \iint d\mathbf{X}_1 d\mathbf{X}_2 (\partial/\partial X_{2x}^{\beta-\lambda}) (\partial/\partial X_{1x}^\lambda) G(\mathbf{X}_1, \mathbf{X}_2), \quad (8a)$$

where

$$\begin{aligned} G(\mathbf{X}_1, \mathbf{X}_2) = & \iint \mathfrak{D}(\mathbf{X}' : \mathbf{X}_2(\beta-\lambda)) \mathfrak{D}(\mathbf{X}'' : \mathbf{X}_1(\lambda)) \\ & \times \exp \left[- \int_0^{\beta-\lambda} \frac{1}{2} \dot{\mathbf{X}}'^2(t) dt - \int_0^\lambda \frac{1}{2} \dot{\mathbf{X}}''^2(t) dt \right] \times \left[1 + (2^{3/2} \pi \alpha / (e^\beta - 1)) V \right. \\ & \times \left\{ \sum_w \frac{1}{\omega^3} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma I_w(\mathbf{X}''(\tau), \mathbf{X}''(\sigma); 1) \right. \right. \\ & \left. \left. + \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma I_w(\mathbf{X}'(\tau), \mathbf{X}'(\sigma); 1) + \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma I_w(\mathbf{X}'(\tau), \mathbf{X}''(\sigma); 1) \right\} \right\} \left. \right]. \quad (8b) \end{aligned}$$

It should be noted here that the approximation

$$\exp[Q(\mathbf{X}', \mathbf{X}'')] \simeq 1 + Q(\mathbf{X}', \mathbf{X}'') \quad (8c)$$

was used to obtain (8b). As is seen from (7b), $Q(\mathbf{X}'\mathbf{X}'')$ is proportional to the coupling constant α which is small in the present case.

The perturbational treatment in the present path-integral method consists of replacing $\exp(\pm i\mathbf{w} \cdot (\mathbf{X}''(\tau) - \mathbf{X}''(\sigma)))$, $\exp(\pm i\mathbf{w} \cdot (\mathbf{X}'(\tau) - \mathbf{X}'(\sigma)))$, and $\exp(\pm i\mathbf{w} \cdot (\mathbf{X}'(\tau) - \mathbf{X}''(\sigma)))$ by their average values over the path with a free action $-\int_0^\lambda 1/2 \cdot \dot{\mathbf{X}}''^2(t) dt$ and $-\int_0^{\beta-\lambda} 1/2 \cdot \dot{\mathbf{X}}'^2(t) dt$. In the same way as in I, these average values are given by

$$\begin{aligned}
 &\langle e^{\pm i\mathbf{w}\cdot(\mathbf{X}'(\tau)-\mathbf{X}'(\sigma))} \rangle_{\mathbf{X}_2\mathbf{X}_1;\lambda} \\
 &= \exp(\pm i\mathbf{w}\cdot(\mathbf{X}_2-\mathbf{X}_1)(\tau-\sigma)/\lambda) \exp\left(-\frac{w^2}{2}(\tau-\sigma)\left(1-\frac{(\tau-\sigma)}{\lambda}\right)\right), \\
 &\langle e^{\pm i\mathbf{w}\cdot(\mathbf{X}'(\tau)-\mathbf{X}'(\sigma))} \rangle_{\mathbf{X}_1\mathbf{X}_2;\beta-\lambda} \\
 &= \exp(\pm i\mathbf{w}\cdot(\mathbf{X}_2-\mathbf{X}_1)(\tau-\sigma)/\beta-\lambda) \exp\left(-\frac{w^2}{2}(\tau-\sigma)\left(1-\frac{(\tau-\sigma)}{\beta-\lambda}\right)\right), \\
 &\langle e^{\pm i\mathbf{w}\cdot\mathbf{X}'(\tau)} \rangle_{\mathbf{X}_1\mathbf{X}_2;\beta-\lambda} = \exp(\pm i\mathbf{w}\cdot(\mathbf{X}_2-\mathbf{X}_1)\tau/\beta-\lambda) \exp\left(-\frac{w^2}{2}\tau\left(1-\frac{\tau}{\beta-\lambda}\right)\right), \\
 &\langle e^{\pm i\mathbf{w}\cdot\mathbf{X}'(\sigma)} \rangle_{\mathbf{X}_2\mathbf{X}_1;\lambda} = \exp(\pm i\mathbf{w}\cdot(\mathbf{X}_1-\mathbf{X}_2)\sigma/\lambda) \exp\left(\frac{w^2}{2}\sigma\left(1+\frac{\sigma}{\lambda}\right)\right). \tag{9}
 \end{aligned}$$

We shall give another method to calculate the average values of Eq. (9) in Appendix I, which will be used in the calculation in § 3. Noting that the identity

$$\begin{aligned}
 &-\iint d\mathbf{X}_1 d\mathbf{X}_2 (\partial/\partial X_{1x}^{\beta-\lambda}) f_{\beta-\lambda}(\mathbf{X}_1, \mathbf{X}_2) (\partial/\partial X_{2x}^{\lambda}) f_{\lambda}(\mathbf{X}_2, \mathbf{X}_1) \\
 &= \iint d\mathbf{K}_1 d\mathbf{K}_2 K_{1x} K_{2x} g_{\beta-\lambda}(\mathbf{K}_1, \mathbf{K}_2) g_{\lambda}(\mathbf{K}_2, \mathbf{K}_1) \tag{10a}
 \end{aligned}$$

holds with

$$f_{\lambda}(\mathbf{X}_1, \mathbf{X}_2) = (2\pi)^{-3} \int g_{\lambda}(\mathbf{K}_1, \mathbf{K}_2) e^{i(\mathbf{K}_1\mathbf{X}_1 - \mathbf{K}_2\mathbf{X}_2)} d\mathbf{K}_1 d\mathbf{K}_2$$

and that the density matrix $\rho_0(\mathbf{X}_1\mathbf{X}_2; u)$ for a free electron is $(\sqrt{2\pi/u})^3 \times \exp(-(\mathbf{X}_1-\mathbf{X}_2)^2/2u)$, and furthermore, using (8) and (9) one can obtain

$$\begin{aligned}
 \text{Tr}(e^{-\beta H} e^{-iHt} j_x e^{iHt} j_x) &= \sum_{\mathbf{k}} e^2 k_x^2 e^{-k^2 \beta/2} \left[1 + \sum_{\mathbf{w}} \{ 2^{3/2} \alpha/Vw^2 (e^{\beta} - 1) \} \right. \\
 &\times \left\{ \int_0^{\lambda} d\tau (\lambda - \tau) (e^{\beta - \tau(1 - \mathbf{k}\cdot\mathbf{w} + w^2/2)} + e^{-\tau(-1 + \mathbf{k}\cdot\mathbf{w} + w^2/2)}) \right. \\
 &+ \int_0^{\beta-\lambda} d\tau (\beta - \lambda - \tau) (e^{\beta - \tau(1 - \mathbf{k}\cdot\mathbf{w} + w^2/2)} + e^{-\tau(-1 + \mathbf{k}\cdot\mathbf{w} + w^2/2)}) \\
 &\left. \left. + \int_0^{\beta-\lambda} d\tau \int_0^{\lambda} d\sigma (e^{\beta - (\tau-\sigma)(1 - \mathbf{k}\cdot\mathbf{w} + w^2/2)} + e^{(\tau-\sigma)(-1 + \mathbf{k}\cdot\mathbf{w} + w^2/2)}) \right\} \right]. \tag{11}
 \end{aligned}$$

The first four terms appearing in brackets in the right-hand side of Eq. (11) are simplified by using the formulae for a large time t

$$\sum_{\omega} F(\omega) \left[\int_0^{\beta+it} ds (\beta + it - s) e^{-f(\omega)s} + \int_0^{-it} ds (-it - s) e^{-f(\omega)s} \right] \simeq 2\pi t \sum_{\omega} F(\omega) \delta(f(\omega)), \tag{A.2.1}$$

which will be proved in Appendix II, Here $F(\omega)$ and $f(\omega)$ are some functions of ω . The remaining terms which come from the terms S_{cross} of Eq. (7c) become quantities being independent of t for a large time t as will be shown in Appendix II. Then, one obtains

$$\text{Tr}(e^{-\beta H} e^{-iHt} j_x e^{iHt} j_x) \simeq \sum_{\mathbf{k}} e^3 k_x^2 e^{-k^2 \beta / 2} (1 - t/\tau_k) \quad (12a)$$

for a large time t , where

$$1/\tau_k = \{2\pi \cdot 2^{3/2} \alpha \pi / V(e^\beta - 1)\} \sum_{\omega} \frac{1}{\omega^2} \left\{ e^\beta \delta\left(1 - \mathbf{k} \cdot \boldsymbol{\omega} + \frac{\omega^2}{2}\right) + \delta\left(-1 + \mathbf{k} \cdot \boldsymbol{\omega} + \frac{\omega^2}{2}\right) \right\}. \quad (12b)$$

This expression of τ_k agrees with the collision time obtained by the ordinary perturbation theory with the electron-phonon interaction as a perturbing Hamiltonian. In the perturbation theory, the energy shift ΔE_n and the collision time τ_n of an unperturbed state are given, respectively, by

$$\Delta E_n = P \sum_m |\langle m | H' | n \rangle|^2 / (E_n^0 - E_m^0),$$

$$1/2\pi\tau_n = \sum_m \delta(E_n^0 - E_m^0) |\langle m | H' | n \rangle|^2,$$

where H' is the perturbing Hamiltonian and E_m^0 is the energy of the unperturbed state m . Comparing these two equations with one another, it is expected that the self energy ΔE_k corresponding to τ_k given by Eq. (12) becomes

$$\Delta E_k = \{2^{3/2} \alpha \pi / (e^\beta - 1) V\} \sum_{\omega} \{e^\beta P / (1 - \mathbf{k} \cdot \boldsymbol{\omega} + \omega^2/2) + P / (-1 + \mathbf{k} \cdot \boldsymbol{\omega} + \omega^2/2)\}. \quad (13)$$

This result also agrees with that obtained by the ordinary perturbation treatment.

Adopting the assumption that the asymptotic form of a correlation function of electronic current has the property of simple exponential decay in time and using of Eqs. (1), (2) and (12a), we get, as the expression of the mobility μ_0 ,

$$\mu_0 = e\beta \sum_{\mathbf{k}} k_x^2 e^{-(k^2/2)\beta} \int_0^\infty e^{-t/\tau_k} dt / \sum_{\mathbf{k}} e^{-(k^2/2)\beta}.$$

Substituting the value τ_k of Eq. (12b) in this equation, the mobility μ_0 at very low temperatures is given by

$$\mu_0 = e/2 \bar{n} \alpha, \quad (14)$$

where

$$\bar{n} = 1/(e^\beta - 1).$$

§ 3. Calculation of the polaron mobility

(in the case of strong interaction)

We shall calculate the polaron mobility in the case of strong interaction by using the evaluation in § 2. We take states determined by Feynman's trial action as the unperturbed states and treat the difference between it and the true action as a perturbation.

We shall start with the approximate expression

$$\text{Tr}(e^{-(\beta+it)H} j_x e^{iHt} j_x) = -e^2 \iint d\mathbf{X}_1 d\mathbf{X}_2 (\partial/\partial X_{2x}^{\beta-\lambda}) (\partial/\partial X_{1x}^\lambda) G(\mathbf{X}_1, \mathbf{X}_2), \quad (15a)$$

where

$$G(\mathbf{X}_1, \mathbf{X}_2) = \iint \mathfrak{D}(\mathbf{X}'(t) : \mathbf{X}_2(\beta-\lambda) : \mathbf{X}_1(0)) \mathfrak{D}(\mathbf{X}''(t) : \mathbf{X}_1(\lambda) : \mathbf{X}_2(0)) \\ \times \exp[S_{0,\beta-\lambda}(\mathbf{X}') + S_{0,\lambda}(\mathbf{X}'') + S_{0,\lambda,\beta-\lambda}(\mathbf{X}', \mathbf{X}'')] (1 + F(\mathbf{X}'\mathbf{X}''; \beta, \lambda)), \quad (15b)$$

and

$$F(\mathbf{X}'\mathbf{X}''; \beta, \lambda) = 2^{-3/2} \alpha (e^\beta - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma F_1(\mathbf{X}''(\tau), \mathbf{X}''(\sigma)) \right. \\ \left. + \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma F_1(\mathbf{X}'(\tau), \mathbf{X}'(\sigma)) + \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma F_1(\mathbf{X}'(\tau), \mathbf{X}''(\sigma)) \right\} \\ + C(e^{\beta_0} - 1)^{-1/2} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma F_2(\mathbf{X}''(\tau), \mathbf{X}''(\sigma)) \right. \\ \left. + \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma F_2(\mathbf{X}'(\tau), \mathbf{X}'(\sigma)) + \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma F_2(\mathbf{X}'(\tau), \mathbf{X}''(\sigma)) \right\}, \quad (15c)$$

where

$$S_{0u}(\mathbf{X}) = -\frac{1}{2} \int_0^u \dot{\mathbf{X}}^2(t) dt - C(e^{\beta_0} - 1)^{-1/2} \int_0^u d\tau \int_0^\tau d\sigma F_2(\mathbf{X}(\tau), \mathbf{X}(\sigma)), \quad (15d)$$

$$S_{0,\lambda,\beta-\lambda}(\mathbf{X}'\mathbf{X}'') = C(e^{\beta_0} - 1)^{-1/2} \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma F_2(\mathbf{X}(\tau), \mathbf{X}(\sigma)), \quad (15e)$$

$$F_1(\mathbf{x}(\tau), \mathbf{y}(\sigma)) = |\mathbf{x}(\tau) - \mathbf{y}(\sigma)|^{-1} (e^{(\beta-\tau+\sigma)} + e^{(\tau-\sigma)}), \quad (15f)$$

$$F_2(\mathbf{x}(\tau), \mathbf{y}(\sigma)) = |\mathbf{x}(\tau) - \mathbf{y}(\sigma)|^2 (e^{\alpha(\beta-\tau+\sigma)} + e^{\alpha(\tau-\sigma)}). \quad (15g)$$

Here S_{0u} denotes Feynman's trial action. To derive (15) from (3), we considered $F(\mathbf{X}'\mathbf{X}''; \beta\lambda)$ small, since it corresponds to the difference between the true action and the trial action, and we used an approximation similar to (8c)

in the case of weak interaction. C and ω are variational parameters which should be determined so as to minimize the free energy of the system.

Let us first consider the term which does not include the terms $F(\mathbf{X}'\mathbf{X}''; \beta\lambda)$ in Eq. (15b), that is,

$$\begin{aligned}
 & -e^2 \iint d\mathbf{X}_1 d\mathbf{X}_2 (\partial/\partial X_{2x}^{\beta-\lambda}) (\partial/\partial X_{1x}^\lambda) \iint \mathfrak{D} \left((\mathbf{X}'(t) : \frac{\mathbf{X}_2(\beta-\lambda)}{\mathbf{X}_1(0)}) \right) \\
 & \times \mathfrak{D} \left(\mathbf{X}''(t) : \frac{\mathbf{X}_1(\lambda)}{\mathbf{X}_2(0)} \right) e^{\bar{S}_0(\mathbf{X}'\mathbf{X}'')}, \tag{16}
 \end{aligned}$$

where

$$\bar{S}_0(\mathbf{X}'\mathbf{X}'') = S_{0,\beta-\lambda}(\mathbf{X}') + S_{0,\lambda}(\mathbf{X}'') + S_{0,\lambda,\beta-\lambda}(\mathbf{X}'\mathbf{X}'').$$

As was shown in I, the states determined by the trial action S_0 are equivalent to the states of a system with the Lagrangian

$$L_0 = (\dot{\mathbf{X}}^2 + M\dot{\mathbf{q}}^2 - \kappa(\mathbf{q} - \mathbf{X})^2)/2, \tag{17}$$

where

$$\kappa = M\omega^2 \text{ and } M = 4C/\omega^2.$$

The Hamiltonian H_0 corresponding to the Lagrangian L_0 is expressed by

$$H_0 = -\frac{1}{2m_0} \partial^2/\partial \mathbf{x}_0^2 + \left(-\frac{1}{2\eta} \partial^2/\partial \mathbf{r}^2 + \frac{\kappa}{2} \mathbf{r}^2 \right), \tag{18}$$

where the new variables \mathbf{x}_0 and \mathbf{r} defined by

$$\mathbf{x}_0 = (M\mathbf{q} + \mathbf{X})/(M+1), \quad \mathbf{r} = \mathbf{X} - \mathbf{q} \tag{19}$$

are used instead of X and q , and also

$$m_0 = \nu^2/\omega^2, \quad \eta = 4C/\nu^2.$$

The energy eigenvalues of this Hamiltonian are given by

$$E_0(\mathbf{k}, n_1 n_2 n_3) = \mathbf{k}^2/2m_0 + (n_1 + n_2 + n_3 + 3/2)\nu, \tag{20}$$

where \mathbf{k} is the wave number specifying a free motion for \mathbf{x}_0 and n_1, n_2 and n_3 are the quantum numbers of the harmonic oscillator for \mathbf{r} .

It is not so difficult to show, by performing calculations similar to that used in § 2, that

$$\begin{aligned}
 \text{the quantity (16)} &= \sum_{mm'} e^{-(\beta-\lambda)E_m^0} e^{-\lambda E_{m'}^0} (m|j_x|m') (m'|j_x|m) \\
 &= \text{Tr}(e^{-\beta H_0} e^{-iH_0 t} j_x e^{iH_0 t} j_x), \tag{21}
 \end{aligned}$$

where we simply express the eigenstates $|\mathbf{k} n_1 n_2 n_3\rangle$ and their eigenvalues $E_0(\mathbf{k} n_1 n_2 n_3)$ by $|m\rangle$ and E_m^0 , respectively. Using Eq. (21) and noting that

$$\partial/\partial \mathbf{X} = (m_0)^{-1} \partial/\partial \mathbf{x}_0 + \partial/\partial \mathbf{r}, \tag{22}$$

we obtain that

$$\begin{aligned}
 \text{the quantity (16)} &= \sum_{\mathbf{k} n_1 n_2 n_3} e^2 \exp\{-\beta E_0(\mathbf{k} n_1 n_2 n_3)\} [kx^2/m_0^2 \\
 &+ (\kappa\eta)^{1/2} (n_1 + 1)e^{-\lambda\nu}/2 + (\kappa\eta)^{1/2} n_1 e^{\lambda\nu}/2]. \tag{23}
 \end{aligned}$$

Next, we consider the term including $F(\mathbf{X}'\mathbf{X}''; \beta\lambda)$ in Eq. (15). This quantity is transformed into

$$\begin{aligned}
 & -e^2 \iint d\mathbf{X}_1 d\mathbf{X}_2 (\partial/\partial X_{2x}^{\beta-\lambda}) (\partial/\partial X_{1x}^\lambda) \left[\iint \mathfrak{D}(\mathbf{X}'(t) : \mathbf{X}_2(\beta-\lambda) : \mathbf{X}_1(0)) \mathfrak{D}(\mathbf{X}''(t) : \mathbf{X}_1(\lambda) : \mathbf{X}_2(0)) \right] e^{\bar{S}_0(\mathbf{X}', \mathbf{X}'')} \\
 & \times \left[\sum_u C_u^2 (e^\beta - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma I_u(\mathbf{X}''(\tau), \mathbf{X}''(\sigma) : 1) + \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma I_u(\mathbf{X}'(\tau), \mathbf{X}'(\sigma) : 1) \right. \right. \\
 & + \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma I_u(\mathbf{X}'(\tau), \mathbf{X}''(\sigma) : 1) \left. \left. + \sum_u D_u^2 (e^{\beta\omega} - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma I_u(\mathbf{X}''(\tau), \mathbf{X}''(\sigma) ; \omega) \right. \right. \right. \\
 & \left. \left. + \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma I_u(\mathbf{X}'(\tau), \mathbf{X}'(\sigma) ; \omega) + \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma I_u(\mathbf{X}'(\tau), \mathbf{X}''(\sigma) ; \omega) \right\} \right], \quad (24)
 \end{aligned}$$

where we used the notation of Eq. (7d) and the identities

$$\begin{aligned}
 |\mathbf{X}_1 - \mathbf{X}_2|^{-1} &= 4\pi \sum_u e^{i\mathbf{u} \cdot (\mathbf{X}_1 - \mathbf{X}_2)} / V u^2, \\
 |\mathbf{X}_1 - \mathbf{X}_2|^2 &= -8\pi^3 \sum_u \delta(\mathbf{u}) \mathcal{V}_u^2 e^{i\mathbf{u} \cdot (\mathbf{X}_1 - \mathbf{X}_2)} / V
 \end{aligned}$$

and the definitions

$$C_u = \sqrt{2^{3/2} \pi \alpha / V u}, \quad D_u = -i \sqrt{2^3 \pi^3 C \delta(\mathbf{u}) \mathcal{V}_u^2 / V}. \quad (25)$$

Now we replace $e^{\pm i\mathbf{u} \cdot (\mathbf{X}''(\tau) - \mathbf{X}'(\sigma))}$, $e^{\pm i\mathbf{u} \cdot (\mathbf{X}'(\tau) - \mathbf{X}'(\sigma))}$ and $e^{\pm i\mathbf{u} \cdot (\mathbf{X}'(\tau) - \mathbf{X}''(\sigma))}$ by their average values $\overline{e^{\pm i\mathbf{u} \cdot (\mathbf{X}''(\tau) - \mathbf{X}'(\sigma))}}$, $\overline{e^{\pm i\mathbf{u} \cdot (\mathbf{X}'(\tau) - \mathbf{X}'(\sigma))}}$ and $\overline{e^{\pm i\mathbf{u} \cdot (\mathbf{X}'(\tau) - \mathbf{X}''(\sigma))}}$ taken along the path with the action $S_{0, \beta-\lambda}(\mathbf{X}') + S_{0, \lambda}(\mathbf{X}'') + S_{0, \lambda, \beta-\lambda}(\mathbf{X}'\mathbf{X}'')$ as was done in § 2. These average values are calculated as follows. Noting that

$$\begin{aligned}
 & \iint \mathfrak{D}(\mathbf{X}'(t) : \mathbf{X}_2(\beta-\lambda) : \mathbf{X}_1(0)) \mathfrak{D}(\mathbf{X}''(t) : \mathbf{X}_1(\lambda) : \mathbf{X}_2(0)) e^{\bar{S}_0(\mathbf{X}', \mathbf{X}'')} \\
 & = \sum_{mm'} \iint d\mathbf{q}_1 d\mathbf{q}_2 e^{-(\beta-\lambda)E_m^0 + \lambda E_{m'}^0} \phi_m^{0*}(\mathbf{X}_1 \mathbf{q}_1) \phi_m^0(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^{0*}(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^0(\mathbf{X}_1 \mathbf{q}_1),
 \end{aligned}$$

where $\phi_m^0(\mathbf{X}_1 \mathbf{q}_1)$ is the eigen-function of H_0 , and making use of Eqs. (A.1.1) and (A.1.2), it is shown that

$$\begin{aligned}
 & \left[\iint \mathfrak{D}(\mathbf{X}'(t) : \mathbf{X}_2(\beta-\lambda) : \mathbf{X}_1(0)) \mathfrak{D}(\mathbf{X}''(t) : \mathbf{X}_1(\lambda) : \mathbf{X}_2(0)) e^{\bar{S}_0(\mathbf{X}', \mathbf{X}'')} \right] \overline{e^{\pm i\mathbf{u} \cdot (\mathbf{X}''(\tau) - \mathbf{X}'(\sigma))}} \\
 & = \sum_{mm'} \iint d\mathbf{q}_1 d\mathbf{q}_2 e^{-(\beta-\lambda)E_m^0 + \lambda E_{m'}^0} \phi_m^{0*}(\mathbf{X}_1 \mathbf{q}_1) \phi_m^0(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^{0*}(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^0(\mathbf{X}_1 \mathbf{q}_1) \\
 & \times \langle m' | e^{\pm i\mathbf{u} \cdot \mathbf{X}(\tau)} e^{\mp i\mathbf{u} \cdot \mathbf{X}(\sigma)} | m' \rangle, \quad (26a)
 \end{aligned}$$

$$\begin{aligned}
 & \left[\iint \mathfrak{D}(\mathbf{X}'(t) : \mathbf{X}_2(\beta-\lambda) : \mathbf{X}_1(0)) \mathfrak{D}(\mathbf{X}''(t) : \mathbf{X}_1(\lambda) : \mathbf{X}_2(0)) e^{\bar{S}_0(\mathbf{X}', \mathbf{X}'')} \right] \overline{e^{\pm i\mathbf{u} \cdot (\mathbf{X}'(\tau) - \mathbf{X}''(\sigma))}} \\
 & = \sum_{mm'} e^{-(\beta-\lambda)E_m^0 + \lambda E_{m'}^0} \phi_m^{0*}(\mathbf{X}_1 \mathbf{q}_1) \phi_m^0(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^{0*}(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^0(\mathbf{X}_1 \mathbf{q}_1) \\
 & \times \langle m | e^{\pm i\mathbf{u} \cdot \mathbf{X}(\tau)} e^{\mp i\mathbf{u} \cdot \mathbf{X}(\sigma)} | m \rangle, \quad (26b)
 \end{aligned}$$

and

$$\begin{aligned}
 & \left[\iint \mathfrak{D} \left(\mathbf{X}'(t) : \begin{matrix} \mathbf{X}_2(\beta - \lambda) \\ \mathbf{X}_1(0) \end{matrix} \right) \mathfrak{D} \left(\mathbf{X}''(t) : \begin{matrix} \mathbf{X}_1(\lambda) \\ \mathbf{X}_2(0) \end{matrix} \right) e^{\delta_0(\mathbf{X}', \mathbf{X}'')} \right] e^{\pm i\mathbf{u} \cdot (\mathbf{X}'(\tau) - \mathbf{X}''(\sigma))} \\
 &= \lim_{\sigma' \rightarrow 0, \tau' \rightarrow 0} \sum_{m, m'} \iint d\mathbf{q}_1 d\mathbf{q}_2 e^{-(\beta - \lambda)E_m^0 + \lambda E_{m'}^0} \phi_m^{0*}(\mathbf{X}_1 \mathbf{q}_1) \phi_m^0(\mathbf{X}_2 \mathbf{q}_2) \\
 & \times \phi_{m'}^{0*}(\mathbf{X}_2 \mathbf{q}_2) \phi_{m'}^0(\mathbf{X}_1 \mathbf{q}_1) \langle m | e^{\pm i\mathbf{u} \cdot \mathbf{X}(\tau)} e^{\mp i\mathbf{u} \cdot \mathbf{X}(\sigma')} | m \rangle \langle m' | e^{\pm i\mathbf{u} \cdot \mathbf{X}(\sigma')} e^{\mp i\mathbf{u} \cdot \mathbf{X}(\sigma)} | m' \rangle,
 \end{aligned} \tag{26c}$$

where

$$e^{\pm i\mathbf{u} \cdot \mathbf{X}(\tau)} = e^{H_0 \tau} e^{\pm i\mathbf{u} \cdot \mathbf{X}} e^{-H_0 \tau}.$$

The quantity (24) can be replaced, using of Eq. (26), by

$$\begin{aligned}
 & \sum_{\mathbf{u}} C_{\mathbf{u}}^2 (e^\beta - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma (e^{(\beta - \tau + \sigma)} f_{\mathbf{u}}^{\lambda, +}(\tau, \sigma) + e^{(\tau - \sigma)} f_{\mathbf{u}}^{\lambda, -}(\tau, \sigma)) \right. \\
 & + \int_0^{\beta - \lambda} d\tau \int_0^\tau d\sigma (e^{(\beta - \tau + \sigma)} f_{\mathbf{u}}^{\beta - \lambda, +}(\tau, \sigma) + e^{(\tau - \sigma)} f_{\mathbf{u}}^{\beta - \lambda, -}(\tau, \sigma)) \\
 & + \left. \int_0^{\beta - \lambda} d\tau \int_0^\lambda d\sigma (e^{(\beta - \tau + \sigma)} g_{\mathbf{u}}^{\lambda, \beta - \lambda, +}(\tau, \sigma) + e^{(\tau - \sigma)} g_{\mathbf{u}}^{\lambda, \beta - \lambda, -}(\tau, \sigma)) \right\} \\
 & + \sum_{\mathbf{u}} D_{\mathbf{u}}^2 (e^{\beta\omega} - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma (e^{\omega(\beta - \tau + \sigma)} f_{\mathbf{u}}^{\lambda, +}(\tau, \sigma) + e^{\omega(\tau - \sigma)} f_{\mathbf{u}}^{\lambda, -}(\tau, \sigma)) \right. \\
 & + \int_0^{\beta - \lambda} d\tau \int_0^\tau d\sigma (e^{\omega(\beta - \tau + \sigma)} f_{\mathbf{u}}^{\beta - \lambda, +}(\tau, \sigma) + e^{\omega(\tau - \sigma)} f_{\mathbf{u}}^{\beta - \lambda, -}(\tau, \sigma)) \\
 & + \left. \int_0^{\beta - \lambda} d\tau \int_0^\lambda d\sigma (e^{\omega(\beta - \tau + \sigma)} g_{\mathbf{u}}^{\lambda, \beta - \lambda, +}(\tau, \sigma) + e^{\omega(\tau - \sigma)} g_{\mathbf{u}}^{\lambda, \beta - \lambda, -}(\tau, \sigma)) \right\},
 \end{aligned} \tag{27a}$$

where

$$\begin{aligned}
 f_{\mathbf{u}}^{\lambda, \pm}(\tau, \sigma) &= \sum_{\mathbf{k} n_1 n_2 n_3} e^{-\beta E_0(\mathbf{k} n_1 n_2 n_3)} e^2 \{ k_x^2 / m_0^2 + \sqrt{\kappa\eta} (n_1 + 1) e^{-\lambda\nu} / 2 \\
 & + \sqrt{\kappa\eta} n_1 e^{\lambda\nu} / 2 \} h_{\mathbf{u}}^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau\sigma),
 \end{aligned} \tag{27b}$$

$$\begin{aligned}
 f_{\mathbf{u}}^{\beta - \lambda, \pm}(\tau, \sigma) &= \sum_{\mathbf{k} n_1 n_2 n_3} e^{-\beta E_0(\mathbf{k} n_1 n_2 n_3)} e^2 \{ k_x^2 h_{\mathbf{u}}^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau\sigma) / m_0^2 \\
 & + (n_1 + 1) \sqrt{\kappa\eta} e^{-\lambda\nu} h_{\mathbf{u}}^{\pm}(\mathbf{k}, n_1 + 1, n_2 n_3; \tau\sigma) / 2 \\
 & + n_1 \sqrt{\kappa\eta} e^{\lambda\nu} h_{\mathbf{u}}^{\pm}(\mathbf{k}, n_1 - 1, n_2 n_3; \tau\sigma) / 2 \},
 \end{aligned} \tag{27c}$$

and

$$\begin{aligned}
 g_u^{\lambda, \beta-\lambda, \pm}(\tau, \sigma) &= \lim_{\tau' \rightarrow 0, \sigma' \rightarrow 0} \sum_{\mathbf{k} n_1 n_2 n_3} e^{-\beta E_0(\mathbf{k} n_1 n_2 n_3)} e^{\pm} \\
 &\times \{k_x^2 h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau \tau') h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \sigma' \sigma) / m_0^2 + (n_1 + 1) \sqrt{\kappa \eta} e^{-\lambda \nu} \\
 &\times h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau \tau') h_u^{\pm}(\mathbf{k}, n_1 + 1, n_2 n_3; \sigma' \sigma) / 2 + n_1 \sqrt{\kappa \eta} e^{\lambda \nu} \\
 &\times h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau \tau') h_u^{\pm}(\mathbf{k}, n_1 - 1, n_2 n_3; \sigma' \sigma) / 2\}, \tag{27d}
 \end{aligned}$$

and notation

$$h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau \sigma) = (\mathbf{k} n_1 n_2 n_3 | e^{\pm i \mathbf{u} \cdot \mathbf{X}(\tau)} e^{\mp i \mathbf{u} \cdot \mathbf{X}(\sigma)} | \mathbf{k} n_1 n_2 n_3) \tag{27e}$$

is employed, for simplicity.

For convenience of calculations in what follows, let us consider operators $X_s(\tau)$ and $e^{i X_0(\tau) \cdot \mathbf{u}}$ defined below. $X_s(\tau)$ is defined by

$$X_s(\tau) = x_{0s}(\tau) + \eta r_s(\tau) = x_{0s}(\tau) + \sqrt{\eta / 2\nu} (b_s^* e^{-\nu \tau} + b_s e^{\nu \tau}), \tag{28}$$

where the suffix s stands for one of x, y and z -components, b_s^* and b_s denote the creation and annihilation operators of the harmonic oscillator for r_s . In Eq. (28), the first equality comes from Eq. (18) and the second equality from the definition

$$r_s(\tau) = (b_s^*(\tau) + b_s(\tau)) / \sqrt{2\nu \eta}.$$

$e^{i x_0(\tau) \cdot \mathbf{u}}$ is defined by

$$e^{i x_0(\tau) \cdot \mathbf{u}} = e^{H_0 \tau} e^{i x_0 \cdot \mathbf{u}} e^{-H_0 \tau} = \exp\left(\frac{p_0^2 - (\mathbf{p}_0 - \mathbf{u})^2}{2m_0}\right) e^{i x_0 \cdot \mathbf{u}}, \tag{29}$$

where \mathbf{p}_0 is the momentum conjugate to the coordinate \mathbf{x}_0 . It is shown, according to Eqs. (28) and (29), that

$$\begin{aligned}
 h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau \sigma) &= \exp\{(k^2 - (\mathbf{k} \mp \mathbf{u})^2)(\tau - \sigma) / 2m_0\} \exp(-\eta u^2 / 2\nu) \\
 &\times \langle n_1 n_2 n_3 | \prod_s \exp(\mp i \sqrt{\eta} u_s b_s^* e^{\nu \tau} / \sqrt{2\nu}) \exp(\pm i \sqrt{\eta} u_s b_s e^{-\nu \tau} / \sqrt{2\nu}) \\
 &\times \prod_{s'} \exp(\pm i \sqrt{\eta} u_{s'} b_{s'}^* e^{\nu \sigma} / \sqrt{2\nu}) \exp(\mp i \sqrt{\eta} u_{s'} b_{s'} e^{-\nu \sigma} / \sqrt{2\nu}) | n_1 n_2 n_3 \rangle. \tag{30}
 \end{aligned}$$

If we are concerned only with the phenomena at low temperatures, it is sufficient to carry out the evaluation of Eq.(30) in the case of $n_1 = n_2 = n_3 = 0$. In such a case, we have

$$\begin{aligned}
 h_u^{\pm}(\mathbf{k} n_1 n_2 n_3; \tau \sigma)_{n_1 = n_2 = n_3 = 0} &= \exp\{(k^2 - (\mathbf{k} \pm \mathbf{u})^2)(\tau - \sigma) / 2m_0\} \\
 &\times \exp(-\eta u^2 / 2\nu) \sum_{l_s=0}^{\infty} \prod_s (\eta u_s^2)^{l_s} \exp(-\nu l_s(\tau - \sigma)) / l_s! (2\nu)^{l_s}, \tag{31a}
 \end{aligned}$$

$$\begin{aligned}
 h_u^{\pm}(\mathbf{k}, n_1 + 1, n_2 n_3; \tau \sigma)_{n_1 = n_2 = n_3 = 0} &= \exp\{(k^2 - (\mathbf{k} \pm \mathbf{u})^2)(\tau - \sigma) / 2m_0\} \exp(-\eta u^2 / 2\nu) \\
 &\times [\eta u_x^2 \sum_{l_s=0}^{\infty} \prod_s (\eta u_s^2)^{l_s} e^{-\nu(l_s - 1)(\tau - \sigma)} / 2\nu l_s!
 \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{l_1=0, l_2=0, l_3=0}^{\infty} (l_1+1)^2 (\eta)^{l_1+l_2+l_3} (u_x)^{2l_1} (u_y)^{2l_2} (u_z)^{2l_3} \\
 &\times e^{-\nu(l_1+l_2+l_3)(\tau-\sigma)} / (l_1+1)! l_2! l_3! (2\nu)^{l_1+l_2+l_3}]. \tag{31b}
 \end{aligned}$$

According to Eqs. (23), (27), (28), (29), (31a) and (31b), Eq. (15a) is rewritten, in the case of $n_1=n_2=n_3=0$, as

$$\begin{aligned}
 &\text{Tr}(e^{-(\beta+i t)H} j_x e^{iHt} j_x) \\
 &= \sum_k e^{-k^2 \beta / 2m_0} e^2 \{k_x^2 / m_0^2 + \sqrt{\kappa \eta} e^{-\lambda \nu} / 2\} + \sum_k e^{-k^2 \beta / 2m_0} e^2 k_x^2 / m_0^2 \\
 &\times \left[\sum_u C_u^2 (e^\beta - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma (e^{(\beta-\tau+\sigma)} B_{uk}^+(\tau-\sigma) + e^{(\tau-\sigma)} B_{uk}^-(\tau-\sigma)) \right. \right. \\
 &+ \left. \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma (e^{(\beta-\tau+\sigma)} B_{uk}^+(\tau-\sigma) + e^{(\tau-\sigma)} B_{uk}^-(\tau-\sigma)) \right\} \\
 &+ \sum_u D_u^2 (e^{\omega\beta} - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma (e^{\omega(\beta-\tau+\sigma)} B_{uk}^+(\tau-\sigma) + e^{\omega(\tau-\sigma)} B_{uk}^-(\tau-\sigma)) \right. \\
 &+ \left. \left. \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma (e^{\omega(\beta-\tau+\sigma)} B_{uk}^+(\tau-\sigma) + e^{\omega(\tau-\sigma)} B_{uk}^-(\tau-\sigma)) \right\} \right] \\
 &+ \sum_k e^{-k^2 \beta / 2m_0} e^2 \sqrt{\kappa \eta} e^{-\lambda \nu} / 2 \\
 &\times \left[\sum_u C_u^2 (e^\beta - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma (e^{(\beta-\tau+\sigma)} B_{uk}^+(\tau-\sigma) + e^{(\tau-\sigma)} B_{uk}^-(\tau-\sigma)) \right. \right. \\
 &+ \left. \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma (e^{(\beta-\tau+\sigma)} C_{uk}^+(\tau-\sigma) + e^{(\tau-\sigma)} C_{uk}^-(\tau-\sigma)) \right\} \\
 &+ \sum_u D_u^2 (e^{\omega\beta} - 1)^{-1} \left\{ \int_0^\lambda d\tau \int_0^\tau d\sigma (e^{\omega(\beta-\tau+\sigma)} B_{uk}^+(\tau-\sigma) + e^{\omega(\tau-\sigma)} B_{uk}^-(\tau-\sigma)) \right. \\
 &+ \left. \int_0^{\beta-\lambda} d\tau \int_0^\tau d\sigma (e^{\omega(\beta-\tau+\sigma)} C_{uk}^+(\tau-\sigma) + e^{\omega(\tau-\sigma)} C_{uk}^-(\tau-\sigma)) \right\} \right] \\
 &+ \sum_k e^{-k^2 \beta / 2m_0} e^2 k_x^2 / m_0^2 \\
 &\times \left[\sum_u C_u^2 (e^\beta - 1)^{-1} \left\{ \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma (e^{(\beta-\tau+\sigma)} \overline{B}_{uk}^+(\tau, \sigma) + e^{(\tau-\sigma)} \overline{B}_{uk}^-(\tau, \sigma)) \right\} \right. \\
 &+ \left. \sum_u D_u^2 (e^{\omega\beta} - 1)^{-1} \left\{ \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma (e^{\omega(\beta-\tau+\sigma)} \overline{B}_{uk}^+(\tau, \sigma) + e^{\omega(\tau-\sigma)} \overline{B}_{uk}^-(\tau, \sigma)) \right\} \right] \\
 &+ \sum_k e^{-k^2 \beta / 2m_0} \sqrt{\kappa \eta} e^{-\lambda \nu} / 2
 \end{aligned}$$

$$\begin{aligned} & \times \left[\sum_{\mathbf{u}} C_{\mathbf{u}}^2 (e^\beta - 1)^{-1} \left\{ \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma (e^{(\beta-\tau+\sigma)} \overline{C_{\mathbf{u}\mathbf{k}}^+}(\tau, \sigma) + e^{(\tau-\sigma)} \overline{C_{\mathbf{u}\mathbf{k}}^-}(\tau, \sigma)) \right\} \right. \\ & \left. + \sum_{\mathbf{u}} D_{\mathbf{u}}^2 (e^{\alpha\beta} - 1)^{-1} \left\{ \int_0^{\beta-\lambda} d\tau \int_0^\lambda d\sigma (e^{\alpha(\beta-\tau+\sigma)} \overline{C_{\mathbf{u}\mathbf{k}}^+}(\tau, \sigma) + e^{\alpha(\tau-\sigma)} \overline{C_{\mathbf{u}\mathbf{k}}^-}(\tau, \sigma)) \right\} \right], \end{aligned} \tag{32a}$$

where

$$\begin{aligned} B_{\mathbf{u}\mathbf{k}}^\pm(\tau - \sigma) &= \exp\{(k^2 - (\mathbf{k} \mp \mathbf{u})^2)(\tau - \sigma)/2m_0\} \exp(-\eta u^2/2\nu) \\ & \times \sum_{l_1, l_2, l_3=0}^\infty f_{\mathbf{u}}(l_1 l_2 l_3) e^{-\nu(l_1+l_2+l_3)(\tau-\sigma)}, \end{aligned} \tag{32b}$$

$$\begin{aligned} \overline{B_{\mathbf{u}\mathbf{k}}^\pm}(\tau, \sigma) &= \exp\{(k^2 - (\mathbf{k} \mp \mathbf{u})^2)(\tau - \sigma)/2m_0\} \exp(-\eta u^2/2\nu) \\ & \times \left(\sum_{l_1, l_2, l_3=0}^\infty f_{\mathbf{u}}(l_1 l_2 l_3) e^{-\nu(l_1+l_2+l_3)\tau} \right) \left(\sum_{l_1', l_2', l_3'=0}^\infty f_{\mathbf{u}}(l_1' l_2' l_3') e^{\nu(l_1'+l_2'+l_3')\sigma} \right), \end{aligned} \tag{32c}$$

$$\begin{aligned} C_{\mathbf{u}\mathbf{k}}^\pm(\tau - \sigma) &= \exp\{(k^2 - (\mathbf{k} \mp \mathbf{u})^2)(\tau - \sigma)/2m_0\} \exp(-\eta u^2/2\nu) \\ & \times \left\{ (\eta u_x^2/2\nu) \sum_{l_1, l_2, l_3=0}^\infty f_{\mathbf{u}}(l_1 l_2 l_3) e^{-\nu(l_1+l_2+l_3-1)(\tau-\sigma)} + \sum_{l_1, l_2, l_3=0}^\infty g_{\mathbf{u}}(l_1 l_2 l_3) e^{-\nu(l_1+l_2+l_3)(\tau-\sigma)} \right\}, \end{aligned} \tag{32d}$$

$$\begin{aligned} \overline{C_{\mathbf{u}\mathbf{k}}^\pm}(\tau, \sigma) &= \exp\{(k^2 - (\mathbf{k} \mp \mathbf{u})^2)(\tau - \sigma)/2m_0\} \exp(-\eta u^2/2\nu) \\ & \times \left(\sum_{l_1, l_2, l_3=0}^\infty f_{\mathbf{u}}(l_1 l_2 l_3) e^{-\nu(l_1+l_2+l_3)\tau} \right) \left\{ (\eta u_x^2/2\nu) \right. \\ & \left. \times \sum_{l_1', l_2', l_3'=0}^\infty f_{\mathbf{u}}(l_1' l_2' l_3') e^{\nu(l_1'+l_2'+l_3'-1)\sigma} + \sum_{l_1', l_2', l_3'=0}^\infty g_{\mathbf{u}}(l_1' l_2' l_3') e^{\nu(l_1'+l_2'+l_3')\sigma} \right\}, \end{aligned} \tag{32e}$$

and

$$f_{\mathbf{u}}(l_1 l_2 l_3) = (\eta/2\nu)^{l_1+l_2+l_3} (u_x)^{2l_1} (u_y)^{2l_2} (u_z)^{2l_3} / l_1! l_2! l_3!, \tag{32f}$$

$$g_{\mathbf{u}}(l_1 l_2 l_3) = (\eta/2\nu)^{l_1+l_2+l_3} (u_x)^{2l_1} (u_y)^{2l_2} (u_z)^{2l_3} (l_1+1)^2 / (l_1+1)! l_2! l_3!. \tag{32g}$$

The second and third term in the right-hand of Eq. (32a) are simplified by using Eqs. (A.2.1), (A.2.2) and (A.2.3), and is proportional to t . The fourth and fifth term become a constant quantities independent of t for a large time t , as will be shown in Appendix II, and can be omitted.

According to the discussion mentioned just above, we can obtain

$$\begin{aligned} \text{Tr}(e^{-(\beta+it)H} j_x e^{iHt} j_x) &= \sum_{\mathbf{k}} e^{-k^2 \beta/2m_0} e^2 \left[(1 - |t|/\tau(\mathbf{k}, 0)) k_x^2/m_0^2 \right. \\ & \left. + \sqrt{\kappa\eta} e^{\delta\nu t} \{ 1 + it(\Delta E(k, 1) - \Delta E(k, 0)) - |t|(1/\tau(\mathbf{k}, 0) + 1/\tau(\mathbf{k}, 1))/2 \} \right] \\ & \simeq \sum_{\mathbf{k}} e^{-k^2 \beta/2m_0} e^2 \left[e^{-(|t|/\tau(\mathbf{k}, 0))} / m_0^2 \right. \\ & \left. + \sqrt{\kappa\eta} e^{i(\nu + \Delta E(k, 1) - \Delta E(k, 0))t} e^{-(|t|/2)(1/\tau(\mathbf{k}, 0) + 1/\tau(\mathbf{k}, 1))} \right], \end{aligned} \tag{33a}$$

in the case of $n_1=n_2=n_3=0$, where

$$\begin{aligned} 1/2\pi\tau(\mathbf{k}, 0) = & \sum_{u l_1 l_2 l_3} C_u^2 e^{-u^2 \eta/2\nu} f_u(l_1 l_2 l_3) (e^\beta - 1)^{-1} (\delta_u^+(1, \nu; l_1 l_2 l_3) \\ & + e^\beta \delta_u^-(1, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} D_u^2 e^{-u^2 \eta/2\nu} f_u(l_1 l_2 l_3) (e^{\omega\beta} - 1)^{-1} \\ & \times (\delta_u^+(\omega, \nu; l_1 l_2 l_3) + e^{\omega\beta} \delta_u^-(\omega, \nu; l_1 l_2 l_3)), \end{aligned} \quad (33b)$$

where we have used the notation $\epsilon_k = \mathbf{k}^2/2m_0$ and the abbreviations are

$$\delta_u^\pm(x, y; l_1 l_2 l_3) = \delta(\epsilon_k \pm x - \epsilon_{k \pm u} - (l_1 + l_2 + l_3)y). \quad (33c)$$

and

$$\Delta E(\mathbf{k}, 0) = \sum_{u l_1 l_2 l_3} C_u^2 e^{-u^2 \eta/2\nu} f_u(l_1 l_2 l_3) (e^\beta - 1)^{-1} (p_u^+(1, \nu; l_1 l_2 l_3) + e^\beta p_u^-(1, \nu; l_1 l_2 l_3)), \quad (33d)$$

where the abbreviations are

$$p_u^\pm(xy; l_1 l_2 l_3) \equiv P/(\epsilon_k \pm x - \epsilon_{k \pm u} - (l_1 + l_2 + l_3)y), \quad (33e)$$

$$\begin{aligned} 1/2\pi\tau(\mathbf{k}, 1) = & \sum_{u l_1 l_2 l_3} C_u^2 e^{-u^2 \eta/2\nu} (\eta u_x^2/2\nu) f_u(l_1 l_2 l_3) (e^\beta - 1)^{-1} (\delta_u^+(1, \nu; l_1 l_2 l_3) \\ & + e^\beta \delta_u^-(1, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} D_u^2 e^{-u^2 \eta/2\nu} (\eta u_x^2/2\nu) f_u(l_1 l_2 l_3) \\ & \times (\delta_u^+(\omega, \nu; l_1 l_2 l_3) + e^{\omega\beta} \delta_u^-(\omega, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} C_u^2 e^{-u^2 \eta/2\nu} g_u(l_1 l_2 l_3) \\ & \times (\delta_u^+(1, \nu; l_1 l_2 l_3) + e^\beta \delta_u^-(1, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} D_u^2 e^{-u^2 \eta/2\nu} g_u(l_1 l_2 l_3) \\ & \times (\delta_u^+(\omega, \nu; l_1 l_2 l_3) + e^{\omega\beta} \delta_u^-(\omega, \nu; l_1 l_2 l_3)), \end{aligned} \quad (33f)$$

$$\begin{aligned} \Delta E(\mathbf{k}, 1) = & \sum_{u l_1 l_2 l_3} C_u^2 e^{-u^2 \eta/2\nu} (\eta u_x^2/2\nu) f_u(l_1 l_2 l_3) (e^\beta - 1)^{-1} (p_u^+(1, \nu; l_1 l_2 l_3) \\ & + e^\beta p_u^-(1, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} D_u^2 e^{-u^2 \eta/2\nu} (\eta u_x^2/2\nu) f_u(l_1 l_2 l_3) \\ & \times (p_u^+(\omega, \nu; l_1 l_2 l_3) + e^{\omega\beta} p_u^-(\omega, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} C_u^2 e^{-u^2 \eta/2\nu} g_u(l_1 l_2 l_3) \\ & \times (p_u^+(1, \nu; l_1 l_2 l_3) + e^\beta p_u^-(1, \nu; l_1 l_2 l_3)) + \sum_{u l_1 l_2 l_3} D_u^2 e^{-u^2 \eta/2\nu} g_u(l_1 l_2 l_3) \\ & \times (p_u^+(\omega, \nu; l_1 l_2 l_3) + e^{\omega\beta} p_u^-(\omega, \nu; l_1 l_2 l_3)). \end{aligned} \quad (33g)$$

The terms including D_u of $\tau(\mathbf{k}, 0)$ and $\tau(\mathbf{k}, 1)$ are shown to be zero, by taking into account that D_u^2 contains a $\delta(\mathbf{u})$ (see Eq. (25)) and $\nu \neq \omega$. We retain these terms, however, in order to make it easy to get insight into a relation between the energy shift and the collision time.

It is noted that $\Delta E(\mathbf{k}, 0)$ and $\tau(\mathbf{k}, 0)$ correspond to the energy shift and the collision time of the state $|\mathbf{k}, n_1=n_2=n_3=0\rangle$, respectively, and $\Delta E(\mathbf{k}, 1)$ and $\tau(\mathbf{k}, 1)$ the energy shift and the collision time of the state $|\mathbf{k}, n_1=1, n_2=n_3=0\rangle$ respectively. The energy shift $\Delta E(\mathbf{k}, 0)$ at $\mathbf{k}=0$ near 0°K is given, after some mathematical manipulations, by

$$\begin{aligned}
 \Delta E(\mathbf{k}=0, 0) &= - \sum_u C_u^2 \int_0^\infty \exp[-u^2 \{ \eta(1 - e^{-\nu t}) / 2\nu + t / 2m_0 \}] e^{-t} dt \\
 &- \sum_u D_u^2 \int_0^\infty \exp[-u^2 \{ \eta(1 - e^{-\nu t}) / 2\nu + t / 2m_0 \}] e^{-\omega t} dt, \\
 &= -\alpha\nu / \sqrt{\pi} \omega \left\{ \int_0^\infty d\tau e^{-\tau} / \sqrt{\tau(1 + (\nu^2 - \omega^2)(1 - e^{-\nu\tau}) / \nu\omega^2\tau)} \right\} + (3C/\nu\omega).
 \end{aligned} \tag{34}$$

The energy of the ground state determined by the trial action is $(3/2)(\nu - \omega)$, which has been calculated by Feynman.³⁾ Therefore, the self-energy of the polaron state at 0°K is $(3/2)(\nu - \omega) + \Delta E(\mathbf{k}=0, 0)$. This result agrees with that obtained by Feynman, that is, the approximation in our calculation of mobility may be considered to correspond to that which gives Feynman's result for the self-energy at 0°K.

Further, $\Delta E(\mathbf{k}=0, 1)$ near 0°K is given by

$$\begin{aligned}
 \Delta E(\mathbf{k}=0, 1) &= - \sum_u C_u^2 \int_0^\infty (1 + (\eta u_x^2 / \nu)) \exp[-u^2 \{ \eta(1 - e^{-\nu t}) / 2\nu + t / 2m_0 \}] e^{-(\nu+1)t} dt \\
 &- \sum_u D_u^2 \int_0^\infty (1 + (\eta u_x^2 / \nu)) \exp[-u^2 \{ \eta(1 - e^{-\nu t}) / 2\nu + t / 2m_0 \}] e^{-(\nu+\omega)t} dt.
 \end{aligned} \tag{35}$$

Explicit calculation of Eq. (35) is not necessary, because the contribution to the mobility at very low temperature from the term including $\Delta E(\mathbf{k}=0, 1)$ is neglected as we shall mention below.

We can calculate conductivity using Eqs. (1), (2) and Eq. (33) in the same way as the derivation of Eq. (14). Near 0°K, we are interested in the collision time for the state $k=0$. If we put $\tau(\mathbf{k}=0, 0) = \tau_0$ and $\tau(\mathbf{k}=0, 1) = \tau_1$, we get

$$\begin{aligned}
 1/\tau_0 &= 2\sqrt{m_0}\alpha / (e^\beta - 1), \\
 1/\tau_1 &= (2\sqrt{m_0}\alpha / (e^\beta - 1)) (1 + 2(\eta m_0)^2 / 5\nu^2).
 \end{aligned} \tag{36}$$

Using Eqs. (1), (33a) and (36), we get the mobility μ near 0°K given by

$$\begin{aligned}
 \mu &= (\mu_0 \exp(m_0\eta/\nu) / m_0^{3/2}) + (\beta\sqrt{\kappa\eta} e/2) \\
 &\times (1/\tau_1 + 1/\tau_0) / 2 \{ (\nu + \Delta E(1, 0) - \Delta E(0, 0))^2 + (1/\tau_1 + 1/\tau_0)^2 / 4 \},
 \end{aligned} \tag{37}$$

where μ_0 is the mobility given by Eq. (14). The second term in the right-hand side of Eq. (37) can be neglected compared with the first term at very low temperatures. Therefore, we get

$$\lim_{\beta \rightarrow \infty} (\mu / \mu_0) = \exp(m_0\eta/\nu) / (m_0)^{3/2}. \tag{38}$$

§ 4. Discussion

We compare the polaron mobility at 0°K obtained in the preceding section with those obtained by Shultz⁴⁾ and by Morita⁵⁾ which are shown in Fig. 1. Their results are given over a wide range of the magnitude of coupling constant. The present result is numerically given in Table I.

The treatment used by Shultz is as follows. He considers the "extended Hamiltonian" which gives the same energy-shift as that obtained by Feynman at $k=0$. He says that the use of this Hamiltonian in a time-dependent formalism with the appropriate boundary conditions gives the same results as the evaluation of the path-integration in all orders of the difference between true action and trial action. He calculates the self-energy for all k to the first approximation of the damping theory, using this "extended" Hamiltonian. Then, he calculates the polaron mobility, using this self-energy as the unperturbed energy of the polaron and treating the interaction between electron and phonons as the perturbation determining polaron mobility. It seems rather difficult, however, to give the concrete justification of Shultz' treatment using the damping theory. The equivalence of the path-integration and his "extended" Hamiltonian is not verified in all the orders of the difference between true action and trial action. Therefore, the approximation contained in his result of the polaron mobility is not evident.

As was mentioned before, the approximation used in the present calculation for the polaron mobility at 0°K gives the same self-energy as that obtained

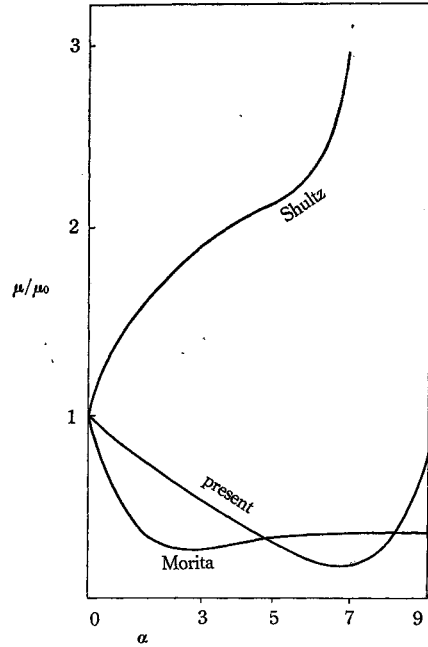


Fig. 1. Theoretical Value of Polaron mobility.

Table I

α	ν	ω	m_0	μ/μ_0
3	3.4	2.55	1.78	0.530
5	4.02	2.13	3.56	0.282
7	5.81	1.60	13.2	0.170
9	9.85	1.28	59.2	0.808
11	15.5	1.15	181.	45.5

Parameters at 0°K

by Feynman. Our result of the collision time (33b) includes the absorption and emission of phonons followed by the excitation of the internal state of the polaron at a finite temperature. Our result is similar to Morita's result up to $\alpha=7$, if the effective mass is put to unity in his formulation. According to the present result, the mobility of the polaron increases steeply at a large coupling constant even though the increase is slower than the result obtained by Shultz where the increase begins already at a smaller coupling constant. This increase is expected because when the coupling becomes strong the wave length of phonons, which contribute effectively to the polaron scattering, decreases more steeply than the localization length of the polaron, so that the polaron becomes insensitive to the scattering by phonons. This effective wave length is proportional to $1/\alpha^2$ and the localization length of the polaron to $1/\alpha$, as Shultz already suggested. This fact is based on the assumption that the polaron mobility is determined by the scattering of the polaron which is accompanied with phonon cloud. It has to be noted, however, that the polaron mobility related to the electronic current is determined by the scattering of the electronic part of the polaron. There will remain some problem in the behaviour of the mobility for a large coupling constant.

At finite temperatures, the deviation from $(e^\beta - 1)$ of the temperature dependence of the mobility comes from the temperature dependence of the variational parameters ν and ω , that is, the temperature change of the polaron state. Moreover, other mechanisms for the scattering, for example, the internal excitation and the spontaneous emission of phonons that occur only at finite temperatures, change the temperature dependence of the mobility. Also the second term in the right-hand side of Eq. (37), which is neglected at very low temperature, has a contribution to the mobility at finite temperature.

The author wishes to express his thanks to Prof. A. Morita and Prof. C. Horie for their valuable discussions. This study was financed by the Scientific Research Fund of the Ministry of Education.

Appendix I

In this appendix, we shall prove the following two equations :

$$\int e^{[S_0(\mathbf{X}') + i\omega \cdot \mathbf{X}'(\tau) - \mathbf{X}'(\sigma)]} \mathfrak{D} \left(\mathbf{X}'(t) ; \begin{matrix} \mathbf{X}_2(u) \\ \mathbf{X}_1(0) \end{matrix} \right) \\ = \sum_m \int d\mathbf{q} e^{-u\mathbf{X}_m^0} \phi_m^{0*}(\mathbf{X}_1 \mathbf{q}) \phi_m^0(\mathbf{X}_2 \mathbf{q}) (m | e^{i\omega \cdot \mathbf{X}(\tau)} e^{-i\omega \cdot \mathbf{X}(\sigma)} | m), \quad (\text{A} \cdot 1 \cdot 1)$$

$$\int e^{[S_0(\mathbf{X}') + i\omega \cdot \mathbf{X}(\tau)]} \mathfrak{D} \left(\mathbf{X}'(t) ; \begin{matrix} \mathbf{X}_2(u) \\ \mathbf{X}_1(0) \end{matrix} \right) \\ = \lim_{\sigma \rightarrow 0} \sum_m \int d\mathbf{q} e^{-u\mathbf{X}_m^0} \phi_m^{0*}(\mathbf{X}_1 \mathbf{q}) \phi_m^0(\mathbf{X}_2 \mathbf{q}) (m | e^{i\omega \cdot \mathbf{X}(\tau)} e^{-i\omega \cdot \mathbf{X}(\sigma)} | m), \\ = \lim_{\sigma \rightarrow 0} \int e^{[S_0(\mathbf{X}') + i\omega(\mathbf{X}'(\tau) - \mathbf{X}'(\sigma))]} \mathfrak{D} \left(\mathbf{X}'(t) ; \begin{matrix} \mathbf{X}_2(u) \\ \mathbf{X}_1(0) \end{matrix} \right), \quad (\text{A} \cdot 1 \cdot 2)$$

where the action S_0 corresponds to Hamiltonian H_0 and the operator $e^{i\omega \cdot X(\tau)}$ is defined by $e^{\tau H_0} e^{i\omega \cdot X} e^{-\tau H_0}$. At first, we shall derive Eq. (A.1.1).

From the meaning of path-integration, we can see that

$$\int e^{S_0(X')} (\partial^n X'(t) / \partial t^n)_{t=0} \mathfrak{D} \left(X'(t) : \begin{matrix} X_2(u) \\ X_1(0) \end{matrix} \right) = \sum_m \int d\mathbf{q} e^{-uE_m^0} \\ \times \psi_m^{0*}(\mathbf{X}_1 \mathbf{q}) \psi_m^0(\mathbf{X}_2 \mathbf{q}) \langle m | \underbrace{[H_0 \cdots [H_0, \mathbf{X}] \cdots]}_n | m \rangle,$$

where $\psi_m^0(\mathbf{X}, \mathbf{q})$ is the eigenfunction of Hamiltonian H_0 . Using this equation, we can derive Eq. (A.1.1) as follows:

$$\int e^{[S_0(X') + i\omega \cdot (X'(\tau) - X'(\sigma))]} \mathfrak{D} \left(X' : \begin{matrix} X_2(u) \\ X_1(0) \end{matrix} \right) = \int e^{[S_0(X') + i\omega \cdot (X'(\tau - \sigma) - X'(0))]} \mathfrak{D} \left(X' : \begin{matrix} X_2(u) \\ X_1(0) \end{matrix} \right), \\ = \sum_{n=0}^{\infty} \int e^{S_0(X')} \left[\frac{\partial^n}{\partial (\tau - \sigma)^n} e^{i\omega \cdot X'(\tau - \sigma)} \right]_{\tau - \sigma = 0} e^{-i\omega \cdot X'(0)} \frac{(\tau - \sigma)^n}{n!} \mathfrak{D} \left(X' : \begin{matrix} X_2(u) \\ X_1(0) \end{matrix} \right), \\ = \sum_{n=0}^{\infty} \sum_m \int d\mathbf{q} e^{-uE_m^0} \psi_m^{0*}(\mathbf{X}_1 \mathbf{q}) \psi_m^0(\mathbf{X}_2 \mathbf{q}) \\ \times \left[\frac{\partial^n}{\partial (\tau - \sigma)^n} \langle m | e^{(\tau - \sigma)H_0} e^{i\omega \cdot X} e^{-(\tau - \sigma)H_0} e^{-i\omega \cdot X} | m \rangle \right]_{\tau - \sigma = 0} \frac{(\tau - \sigma)^n}{n!} \\ = \sum_m \int d\mathbf{q} e^{-uE_m^0} \psi_m^{0*}(\mathbf{X}_1 \mathbf{q}) \psi_m^0(\mathbf{X}_2 \mathbf{q}) \langle m | e^{(\tau - \sigma)H_0} e^{i\omega \cdot X} e^{-(\tau - \sigma)H_0} e^{-i\omega \cdot X} | m \rangle, \\ = \sum_m \int d\mathbf{q} e^{-uE_m^0} \psi_m^{0*}(\mathbf{X}_1 \mathbf{q}) \psi_m^0(\mathbf{X}_2 \mathbf{q}) \langle m | e^{\tau H_0} e^{i\omega \cdot X} e^{-\tau H_0} e^{\sigma H_0} e^{-i\omega \cdot X} e^{-\sigma H_0} | m \rangle.$$

Noting that $e^{(i\omega \cdot X(0))} = \exp \left[i\omega \int_{-\infty}^u \delta(t) \mathbf{X}(t) dt \right]$ and the boundary condition $\mathbf{X}'(0) = \mathbf{X}_1$, we can see that

$$\int e^{[S_0(X') + i\omega \cdot X(\tau)]} \mathfrak{D} \left(X' : \begin{matrix} X_2(u) \\ X_1(0) \end{matrix} \right) = \lim_{\sigma \rightarrow 0} \int e^{[S_0(X') + i\omega \cdot (X(\tau) - X(\sigma))]} \mathfrak{D} \left(X' : \begin{matrix} X_2(u) \\ X_1(0) \end{matrix} \right). \tag{A.1.3}$$

This equation is also simply derived by using the superposition of action. We can derive Eq. (A.1.2) in the same way as the derivation of Eq. (A.1.1) by using Eq. (A.1.3).

Using Eqs. (A.1.1) and (A.1.2), we can easily derive the average values of Eq. (9). For example, we get

$$\langle e^{i\omega \cdot (X'(\tau) - X'(\sigma))} \rangle_{X_2, X_1; \lambda} = \left\{ \sum_{\mathbf{k}} e^{-k^2 \lambda / 2 + i\mathbf{k} \cdot (\mathbf{X}_2 - \mathbf{X}_1)} \langle \mathbf{k} | e^{i\omega \cdot X(\tau)} e^{-i\omega \cdot X(\sigma)} | \mathbf{k} \rangle \right\} \\ \div \left\{ \sum_{\mathbf{k}} e^{-k^2 \lambda / 2 + i\mathbf{k} \cdot (\mathbf{X}_2 - \mathbf{X}_1)} \right\} = \exp(i\omega \cdot (\mathbf{X}_2 - \mathbf{X}_1) (\tau - \sigma) / \lambda) \\ \times \exp \left(\frac{-\omega^2 (\tau - \sigma)}{2} \left(1 - \frac{(\tau - \sigma)}{\lambda} \right) \right).$$

In the same way as the derivation of Eqs. (A·1·1) and (A·1·2), we obtain Eq. (26). Applying Eq. (26) to the case of weak interaction, we simply get Eq. (11).

Appendix II

At first we shall derive the formulae (A·2·1) :

$$\sum_{\omega} F(\omega) \left[\int_0^{\beta+it} ds (\beta+it-s) e^{-f(\omega)s} + \int_0^{-it} ds (-it-s) e^{-f(\omega)s} \right] \simeq 2\pi t \sum_{\omega} F(\omega) \delta(f(\omega)). \tag{A·2·1}$$

We obtain, after some elementary integrations,

$$\sum_{\omega} F(\omega) \int_0^{\beta+it} ds (\beta+it-s) e^{-f(\omega)s} = \sum_{\omega} F(\omega) \left[\frac{(\beta+it)}{f(\omega)} + \frac{1}{f^2(\omega)} \right].$$

We are interested in the asymptotic form of the above equation for a large time t . Since $\exp(-if(\omega)t)$ oscillates rapidly in time, the term including this factor remains finite near the region in which $f(\omega)$ nearly equals zero. Therefore we can put $f(\omega)\beta \rightarrow 0$ in the numerical factor of the term including $\exp(-if(\omega)t)$ of this equation. Therefore, it holds

$$\begin{aligned} \sum_{\omega} F(\omega) \int_0^{\beta+it} ds (\beta+it-s) e^{-f(\omega)s} &\simeq \sum_{\omega} \left[\frac{(\beta+it)}{f(\omega)} + \frac{1-e^{-if(\omega)t}}{f^2(\omega)} \right] F(\omega) \\ &= \sum_{\omega} \left[\frac{i}{f(\omega)} \left(t + \frac{\sin f(\omega)t}{f(\omega)} \right) + \frac{(1-\cos f(\omega)t)}{f^2(\omega)} \right] F(\omega) + \sum_{\omega} \frac{\beta}{f(\omega)} F(\omega). \end{aligned} \tag{A·2·2}$$

Further, we get

$$\begin{aligned} \sum_{\omega} F(\omega) \int_0^{-it} ds (-it-s) e^{-f(\omega)s} &= \sum_{\omega} \left[-\frac{i}{f(\omega)} \left\{ t + \frac{\sin f(\omega)t}{f(\omega)} \right\} + \frac{(1-\cos f(\omega)t)}{f^2(\omega)} \right] F(\omega). \end{aligned} \tag{A·2·3}$$

From the above equations, we obtain

$$\begin{aligned} \sum_{\omega} F(\omega) \left[\int_0^{\beta+it} ds (\beta+it-s) e^{-f(\omega)s} + \int_0^{-it} ds (-it-s) e^{-f(\omega)s} \right] \\ \simeq \sum_{\omega} \frac{\beta}{f(\omega)} F(\omega) + 2 \sum_{\omega} \frac{F(\omega) [1-\cos f(\omega)t]}{[f(\omega)]^2}. \end{aligned}$$

If we employ the procedure that is the same as that used in the theory of

ordinary time dependent perturbation, to the term including $1 - \cos f(\boldsymbol{\omega})t$, this equation is transformed into

$$\sum_{\boldsymbol{\omega}} \frac{\beta F(\boldsymbol{\omega})}{f(\boldsymbol{\omega})} + 2\pi t \sum_{\boldsymbol{\omega}} F(\boldsymbol{\omega}) \delta(f(\boldsymbol{\omega})).$$

For a large time t , we obtain

$$\sum_{\boldsymbol{\omega}} F(\boldsymbol{\omega}) \left[\int_0^{\beta+it} ds (\beta+it-s) e^{-f(\boldsymbol{\omega})s} + \int_0^{-it} ds (-it-s) e^{-f(\boldsymbol{\omega})s} \right] \simeq 2\pi t \sum_{\boldsymbol{\omega}} F(\boldsymbol{\omega}) \delta(f(\boldsymbol{\omega})). \quad (\text{A}\cdot\text{2}\cdot\text{1})$$

The last two terms in Eq. (11) appearing in § 2 have the following form:

$$\sum_{\boldsymbol{\omega}} F(\boldsymbol{\omega}) \int_0^{\beta+it} e^{-f_1(\boldsymbol{\omega})s_1} ds_1 \int_0^{-it} e^{-f_2(\boldsymbol{\omega})s_2} ds_2.$$

After elementary integrations, we get

$$\begin{aligned} \sum_{\boldsymbol{\omega}} F(\boldsymbol{\omega}) \int_0^{\beta+it} e^{-f_1(\boldsymbol{\omega})s_1} ds_1 \int_0^{-it} e^{-f_2(\boldsymbol{\omega})s_2} ds_2 &= \sum_{\boldsymbol{\omega}} iF(\boldsymbol{\omega}) \left(\frac{1-f_1(\boldsymbol{\omega})\beta}{f_1(\boldsymbol{\omega})} \right) \\ &\times \int_0^t e^{if_2(\boldsymbol{\omega})z} dz + \sum_{\boldsymbol{\omega}} e^{-\beta f_1(\boldsymbol{\omega})} F(\boldsymbol{\omega}) \int_0^t e^{-if_1(\boldsymbol{\omega})z_1} dz_1 \int_0^t e^{if_2(\boldsymbol{\omega})z_2} dz_2. \end{aligned}$$

For a large time t , the right-hand side of this equation tends to

$$\begin{aligned} \sum_{\boldsymbol{\omega}} iF(\boldsymbol{\omega}) \left(\frac{1-f_1(\boldsymbol{\omega})\beta}{f_1(\boldsymbol{\omega})} \right) [\pi\delta(f_2(\boldsymbol{\omega})) + iP/f_2(\boldsymbol{\omega})] \\ + \sum_{\boldsymbol{\omega}} F(\boldsymbol{\omega}) e^{-\beta f_1(\boldsymbol{\omega})} [\pi\delta(f_1(\boldsymbol{\omega})) + iP/f_1(\boldsymbol{\omega})] [\pi\delta(f_2(\boldsymbol{\omega})) + iP/f_2(\boldsymbol{\omega})]. \end{aligned}$$

These terms can be neglected with comparison to the terms which are proportional to t , for a large time t .

References

- 1) Y. Ōsaka, Prog. Theor. Phys. **22** (1959), 437.
- 2) H. Nakano, Prog. Theor. Phys. **15** (1956), 77.
R. Kubo, Can. J. Phys. **34** (1956), 1274.
- 3) R. P. Feynman, Phys. Rev. **97** (1955), 660.
- 4) T. D. Shultz, M. I. T. Tech. Rep. (1956), No. 6; Phys. Rev. **116** (1959), 596.
- 5) A. Morita, Science Rep. Tōhoku Univ. **38** (1954), 1; **38** (1954), 158.