CHAPTER IV

AN IMPROVEMENT OF THE FEYNMAN ACTION

After the Feynman formulation for an effective evaluation of the polaron ground state energy was published in 1955, various properties of the polaron have been studied by using the same method. Recently this problem has again assumed considerable significance for the following reasons.

First, effective masses have been measured directly by cyclotron resonance techniques in various materials with the polaron coupling constants α lying in the region $1<\alpha<4$. It is therefore of interest to obtain accurate theoretical values for the polaron contribution to the effective mass. As yet there is no rigorous way to compare the accuracy of the various polaron effective masses calculated from different methods. We can only assume that the method which gives the best ground state energy will also imply the best value of the effective mass. Consequently it is important to have a highly accurate method of calculating the polaron energy.

Secondly, experiments on the ionization energy of bound polarons require for their interpretation the theoretical difference in energy between the free-polaron ground state and the energy of the bound polaron. Since these energies are usually calculated separately, it is important to have good values for the free polaron ground state energy.

The method of improvement and the detailed evaluation of the ground state energy by the new treatment will be presented in this chapter.

IV.1 The Trial Action

According to Chapter III, the exact coulomb potential has been represented by the harmonic oscillator potential of the Feynman trial action. The schematic physical picture is shown in Fig.4. It is clear that this approximation is not sufficient to describe the deep bound state. It is thus reasonable to improve the Feynman action by choosing a more appropriate action.

Abe and Okamoto[13] (1971) have introduced the trial action in the form

$$S_1 = -\frac{1}{2}\int_0^{\beta}\left(\frac{d\underset{\sim}{r}_{el}}{dt}\right)^2 dt - \frac{c_1}{2}\iint_0^{\beta} dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_1|t-s|} - \frac{c_2}{2}\iint_0^{\beta} dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_2|t-s|} . \quad (4.1)$$

Note that the potential energy part is in almost the same form as that of Feynman(3.37), but that the former has one additional term. In this case the strength and frequencies of harmonic oscillators are varied by the four adjustable parameters C_1, C_2, ω_1, and ω_2 .

The physical meaning of the trial action S_1 is considered as that of the three coupled particle model shown in Fig.6, and the schematic physical picture which represents the new trial potential is also shown in Fig.5.

IV.2 Ground State Energy

In this section, we shall evaluate the polaron ground state energy when the trial action is given by (4.1).

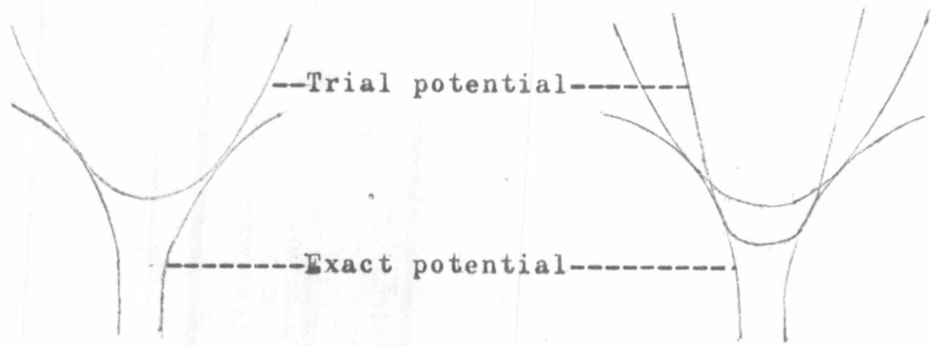

Fig. 4 The physical picture of Feynman's potential.

Fig. 5 The physical picture of Abe and Okamoto's potential.

$k_1 = M_1\omega_1^2$, $4C_1 = M_1\omega_1^3$

$k_1 = M_1\omega_1^2$, $4C_1 = M_1\omega_1^3$

$k_2 = M_2\omega_2^2$, $4C_2 = M_2\omega_2^3$

Fig. 6 The two and three coupled particle models.

The polaron action at absolute zero temperature is given in Chapter III by

$$S = -\frac{1}{2}\int_0^{\mathcal{J}}\left(\frac{d\underset{\sim}{r}}{dt}\right)^2 dt + \frac{\alpha}{2^{3/2}}\iint_0^{\mathcal{J}} dt ds \frac{e^{-|t-s|}}{|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|} , \quad (4.2)$$

and an upper bound on the ground state energy E obtained from the variational principle is

$$E_g \leq E = E_1 - \mathcal{S} . \quad (4.3)$$

Our first objective is to find out $\mathcal{S}$, which can be expressed as

$$\mathcal{S} = \frac{\langle S - S_1 \rangle}{\mathcal{J}} = A + B + C , \quad (4.4)$$

where
$$A = \frac{\alpha}{2^{3/2}} \int_0^{\mathcal{J}} ds \, e^{-|t-s|} \left\langle \frac{1}{|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|} \right\rangle , \quad (4.4a)$$

$$B = \frac{C_1}{2} \int_0^{\mathcal{J}} ds \, e^{-\omega_1|t-s|} \left\langle |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 \right\rangle , \quad (4.4b)$$

and
$$C = \frac{C_2}{2} \int_0^{\mathcal{J}} ds \, e^{-\omega_2|t-s|} \left\langle |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 \right\rangle . \quad (4.4c)$$

To determine the A term, we express $\frac{1}{|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|}$ as a Fourier transform, thus

$$A = \frac{\alpha}{2^{3/2}} \int_0^{\infty} ds \, e^{-|t-s|} \int_{-\infty}^{\infty} \frac{d^3\underset{\sim}{K}}{2\pi^2 K^2} \left\langle \exp\left[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s))\right]\right\rangle . \quad (4.5)$$

Then we need to study

$$\left\langle \exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s))]\right\rangle = \frac{\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} \exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s))]}{\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}}$$

$$= \int \mathcal{D}\underset{\sim}{r}_{el}(t) \exp\Big[-\frac{1}{2}\int \left(\frac{d\underset{\sim}{r}_{el}}{dt}\right)^2 dt - \frac{C_1}{2}\iint dt ds |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 e^{-\omega_1|t-s|} - \frac{C_2}{2}\iint dt ds |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 e^{-\omega_2|t-s|} + \int f(t)\cdot\underset{\sim}{r}_{el}(t) dt\Big], \quad (4.6)$$

where a normalization factor is dropped out and the term $i\underset{\sim}{k}\cdot(\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s))$ is converted into the time integration form by introducing

$$\underset{\sim}{f}(t) \quad = \quad i\underset{\sim}{k}\cdot(\delta(t-\tau)-\delta(t-\sigma)).$$

The path integration (4.6) can be carried out by the Gaussian integral method as described in Section III.3, then the x component of (4.6) becomes

$$\left\langle \exp[ik_x(x(\tau)-x(\sigma))]\right\rangle = \exp\Big[-\frac{1}{2}\int\Big(\frac{d\bar{x}(t)}{dt}\Big)^2 dt - \frac{c_1}{2}\iint dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2 e^{-\omega_1|t-s|}$$
$$- \frac{c_2}{2}\iint dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2 e^{-\omega_2|t-s|}$$
$$+ \int f_x(t)\,\bar{x}(t)\,dt\Big] \quad , \quad (4.7)$$

where $\bar{x}(t)$ is the classical path which minimizes the expression. By using the principle of least action, we require that the classical path $\bar{x}(t)$ satisfies the condition $\delta S=0$, where S is the action given by (4.7).

Hence

$$\delta S = 0 = -\frac{1}{2}\int 2\Big(\frac{d\bar{x}(t)}{dt}\Big)\delta\dot{\bar{x}}(t)dt - \frac{c_1}{2}\iint dt\,ds\,2[\bar{x}(t)-\bar{x}(s)]e^{-\omega_1|t-s|}\delta[\bar{x}(t)-\bar{x}(s)]$$
$$-\frac{c_2}{2}\iint dt\,ds\,2[\bar{x}(t)-\bar{x}(s)]e^{-\omega_2|t-s|}\delta[\bar{x}(t)-\bar{x}(s)] + \int f_x(t)\delta\bar{x}(t)dt$$
$$= \int\Big[\frac{d^2\bar{x}(t)}{dt^2} - 2c_1\int ds[\bar{x}(t)-\bar{x}(s)]e^{-\omega_1|t-s|} - 2c_2\int ds[\bar{x}(t)-\bar{x}(s)]e^{-\omega_2|t-s|}$$
$$+ f_x(t)\Big]\delta\bar{x}(t)dt \quad ,$$

which gives the equation of motion of the classical path

$$\frac{d^2\bar{x}(t)}{dt^2} = 2c_1\int ds[\bar{x}(t)-\bar{x}(s)]e^{-\omega_1|t-s|} + 2c_2\int ds[\bar{x}(t)-\bar{x}(s)]e^{-\omega_2|t-s|} - f_x(t). \quad (4.8)$$

Eq. (4.7) can be simplified by using the differential equation (4.8) as

$$\left\langle \exp[iK_x(x(\tau)-x(\delta))]\right\rangle = \exp\Big[-\tfrac{1}{2}\frac{d\bar{x}(t)}{dt}\cdot\bar{x}(t)\Big|_0^{\delta} + \tfrac{1}{2}\int\frac{d^2\bar{x}(t)}{dt^2}\bar{x}(t)dt - \frac{c_1}{2}\iint dtds[\bar{x}(t)-\bar{x}(s)]\times$$

$$\bar{x}(t)e^{-\omega_1|t-s|} + \frac{c_1}{2}\iint dtds[\bar{x}(t)-\bar{x}(s)]\bar{x}(s)e^{-\omega_1|t-s|}$$

$$-\frac{c_1}{2}\iint dtds[\bar{x}(t)-\bar{x}(s)]\bar{x}(t)e^{-\omega_2|t-s|}$$

$$+\frac{c_2}{2}\iint dtds[\bar{x}(t)-\bar{x}(s)]\bar{x}(s)e^{-\omega_2|t-s|}$$

$$+\int f_x(t)\bar{x}(t)dt\Big]$$

$$= \exp\left[\frac{iK_x}{2}\left(\bar{x}(\tau)-\bar{x}(\delta)\right)\right] . \qquad (4.9)$$

The last expression has been obtained by substituting the classical path $\bar{x}(t)$ at time τ and δ . Next the integro-differential equation (4.8) must be solved. To accomplish this we define

$$Y(t) = \frac{\omega_1}{2}\int_0^{\delta} e^{-\omega_1|t-s|}\bar{x}(s)\,ds , \qquad (4.10)$$

and

$$Z(t) = \frac{\omega_2}{2}\int_0^{\delta} e^{-\omega_2|t-s|}\bar{x}(s)\,ds . \qquad (4.11)$$

Then, the classical path equation of motion(4.8) can be written as

$$\frac{d^2\bar{x}(t)}{dt^2} = \frac{4c_1}{\omega_1}\left(\bar{x}(t)-Y(t)\right)+\frac{4c_2}{\omega_2}\left(\bar{x}(t)-Z(t)\right)-f_x(t) , \qquad (4.12)$$

where we have substituted $\int ds\, e^{-\omega_1|t-s|}$ and $\int ds\, e^{-\omega_2|t-s|}$ by $\frac{2}{\omega_1}$ and $\frac{2}{\omega_2}$ the validity of which will be discussed in Chapter VI.

The differential equations of the variable y(t) and z(t) can be obtained by applying the second order differentiation with respect to t to (4.10) and (4.11), thus

$$\frac{d^2Y(t)}{dt^2} = \omega_1^2\left[Y(t) - \bar{x}(t)\right] , \qquad (4.13)$$

and

$$\frac{d^2Z(t)}{dt^2} = \omega_2^2\left[Z(t) - \bar{x}(t)\right] . \qquad (4.14)$$

The equations (4.12), (4.13),and (4.14) are easily separated; the differential equation of the classical path then becomes

$$\left\{(D^2-\omega_2^2)\left[(D^2-\omega_1^2)\left(D^2-\frac{4C_1}{\omega_1}-\frac{4C_2}{\omega_2}\right)-4C_1\omega_1\right]-4C_2\omega_2(D^2-\omega_1^2)\right\}\bar{x}(t) = -(D^2-\omega_2^2)(D^2-\omega_1^2)\,f_x(t) ,$$

$$\left\{D^6-(V_1^2+V_2^2)D^4-(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2)\,D^2\right\}\bar{x}(t) = -(D^2-\omega_2^2)(D^2-\omega_1^2)\,f_x(t) . \qquad (4.15)$$

We note that the integro- differential equation (4.8) is now converted to the ordinary sixth order differential equation (4.15), which can be solved by applying Laplace transformation. To do this we first obtain

$$\begin{aligned} &p^6 f(p) - p^5\bar{x}(0) - p^4\dot{\bar{x}}(0) - p^3\ddot{\bar{x}}(0) - p^2\dddot{\bar{x}}(0) - p\,\ddddot{\bar{x}}(0) - \overset{.....}{\bar{x}}(0) \\ &-(V_1^2+V_2^2)\left[p^4 f(p) - p^3\bar{x}(0) - p^2\dot{\bar{x}}(0) - p\ddot{\bar{x}}(0) - \dddot{\bar{x}}(0)\right] \\ &+(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2)\left[p^2 f(p) - p\bar{x}(0) - \dot{\bar{x}}(0)\right] \end{aligned} = -\int_0^\infty e^{-pt}(D^2-\omega_2^2)(D^2-\omega_1^2)\,f_x(t)\,dt . \qquad (4.16)$$

Since the time interval $(0,\sigma)$ is very large we can neglect transient terms in (4.16). We thus obtain

$$\left[p^6-(V_1^2+V_2^2)p^4+(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2)p^2\right]f(p) = -ik_x\int_0^\infty e^{-pt}\left(D^4-(\omega_1^2+\omega_2^2)D^2+\omega_1^2\omega_2^2\right)\left(\delta(t-\tau)-\delta(t-\sigma)\right)dt . \qquad (4.17)$$

By using the properties of the Dirac delta function, the right side of (4.17) can be integrated. We then have

$$\left[p^6-(V_1^2+V_2^2)p^4+(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2)p^2\right]f(p) = -ik_x\left[p^4-(\omega_1^2+\omega_2^2)p^2+\omega_1^2\omega_2^2\right](e^{-p\tau}-e^{-p\sigma})$$

$$f(p) = \frac{-ik_x\left[p^4-(\omega_1^2+\omega_2^2)p^2+\omega_1^2\omega_2^2\right](e^{-p\tau}-e^{-p\sigma})}{p^6-(V_1^2+V_2^2)p^4+(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2)p^2} . \qquad (4.18)$$

The desired classical path $\bar{x}(t)$ can be directly determined by applying inverse Laplace transformation to (4.18). To do this we shall use the equality

$$L^{-1}\left[\frac{M(p)}{N(p)}\right] = \sum_{n=1}^{m} \frac{M(a_n)}{N'(a_n)} e^{a_n t} , \quad (4.19)$$

where

$$N(p) = (p-a_1)(p-a_2)\ldots\ldots(p-a_m) . \quad (4.19a)$$

The inverse Laplace transform of (4.18) is

$$\bar{x}(t) = \bar{x}(t,\tau) + \bar{x}(t,\sigma) , \quad (4.20)$$

where

$$\bar{x}(t,\tau) = L^{-1}\left\{f(p,\tau)\right\} , \quad (4.20a)$$

$$f(p,\tau) = \frac{-iK_x\left\{p^4-(\omega_1^2+\omega_2^2)p^2+\omega_1^2\omega_2^2\right\}e^{-p\tau}}{p^6-(\nu_1^2+\nu_2^2)p^4+(\nu_2^2\omega_1^2+\nu_1^2\omega_2^2-\omega_1^2\omega_2^2)} , \quad (4.20b)$$

and

$$\bar{x}(t,\sigma) = L^{-1}\left\{f(p,\sigma)\right\} , \quad (4.20c)$$

$$f(p,\sigma) = \frac{-iK_x\left\{p^4-(\omega_1^2+\omega_2^2)p^2+\omega_1^2\omega_2^2\right\}e^{-p\sigma}}{p^6-(\nu_1^2+\nu_2^2)p^4+(\nu_2^2\omega_1^2+\nu_1^2\omega_2^2-\omega_1^2\omega_2^2)} . \quad (4.20d)$$

The denominator of $f(p,\tau)$ can be separated into six factors; then we obtain

$$\bar{x}(t,\tau) = L^{-1}\left\{\frac{M(p,\tau)}{N(p)}\right\} , \quad (4.21)$$

where

$$M(p,\tau) = -iK_x\left[p^4-(\omega_1^2+\omega_2^2)p^2+\omega_1^2\omega_2^2\right]e^{-p\tau} ,$$

and

$$N(p) = (p-Q_1)(p+Q_1)(p-Q_2)(p+Q_2)(p-Q_3)(p+Q_3) .$$

By using the equality (4.19), (4.21) then becomes

$$\bar{x}(t,\tau) = -iK_x \frac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)\, H(t-\tau)\sinh Q_1(t-\tau)}{Q_1(Q_1^2-Q_2^2)(Q_1^2-Q_3^2)}$$

$$- iK_x \frac{(Q_2^2-\omega_1^2)(Q_2^2-\omega_2^2)\, H(t-\tau)\sinh Q_2(t-\tau)}{Q_2(Q_2^2-Q_1^2)(Q_2^2-Q_3^2)}$$

$$- iK_x \frac{(Q_3^2-\omega_1^2)(Q_3^2-\omega_2^2)\, H(t-\tau)\sinh Q_3(t-\tau)}{Q_3(Q_3^2-Q_1^2)(Q_3^2-Q_2^2)} \qquad (4.22)$$

Similarly, $\bar{x}(t,\sigma)$ has the same form as (4.22), and thus the classical path (4.20) can be determined. The result is

$$\bar{x}(t) = \frac{-iK_x(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{Q_1(Q_1^2-Q_2^2)(Q_1^2-Q_3^2)}\left[H(t-\tau)\sinh Q_1(t-\tau) - H(t-\sigma)\sinh Q_1(t-\sigma)\right]$$

$$- \frac{iK_x(Q_2^2-\omega_1^2)(Q_2^2-\omega_2^2)}{Q_2(Q_2^2-Q_1^2)(Q_2^2-Q_3^2)}\left[H(t-\tau)\sinh Q_2(t-\tau) - H(t-\sigma)\sinh Q_2(t-\sigma)\right]$$

$$- \frac{iK_x(Q_3^2-\omega_1^2)(Q_3^2-\omega_2^2)}{Q_3(Q_3^2-Q_1^2)(Q_3^2-Q_2^2)}\left[H(t-\tau)\sinh Q_3(t-\tau) - H(t-\sigma)\sinh Q_3(t-\sigma)\right] . \qquad (4.23)$$

Since $\bar{x}(t)$ must satisfy the boundary condition $\bar{x}(\mathcal{J}) = 0$, we have

$$\bar{x}(\mathcal{J}) = 0 = 2iK_x . \frac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{(Q_1^2-Q_2^2)(Q_1^2-Q_3^2)}\left[\cosh Q_1(\mathcal{J}-\tfrac{\tau+\sigma}{2}) . \frac{\sinh Q_1(\frac{\tau-\sigma}{2})}{Q_1}\right]$$

$$+2iK_x . \frac{(Q_1^2-\omega_1^2)(Q_2^2-\omega_2^2)}{(Q_2^2-Q_1^2)(Q_2^2-Q_3^2)}\left[\cosh Q_2(\mathcal{J}-\tfrac{\tau+\sigma}{2}) . \frac{\sinh Q_2(\frac{\tau-\sigma}{2})}{Q_2}\right]$$

$$+2iK_x . \frac{(Q_3^2-\omega_1^2)(Q_3^2-\omega_2^2)}{(Q_3^2-Q_1^2)(Q_3^2-Q_2^2)}\left[\cosh Q_3(\mathcal{J}-\tfrac{\tau+\sigma}{2}) . \frac{\sinh Q_3(\frac{\tau-\sigma}{2})}{Q_3}\right] . \qquad (4.24)$$

Since the time interval $\mathcal{J}$ is very large, we obtain the conditions

$$\sinh \frac{Q_1(\tau-\sigma)}{2} = 0 \quad \text{or} \quad \sinh Q_1|\tau-\sigma| = 1-e^{-Q_1|\tau-\sigma|}, \qquad (4.25a)$$

$$\sinh \frac{Q_2(\tau-\sigma)}{2} = 0 \quad \text{or} \quad \sinh Q_2|\tau-\sigma| = 1-e^{-Q_2|\tau-\sigma|}, \qquad (4.25b)$$

and

$$\frac{\sinh Q_3(\tau-\sigma)/2}{Q_3} = \frac{(\tau-\sigma)}{2} , \qquad (4.25c)$$

where Q_3 is zero.

By substituting (4.23) and (4.25a, b, c) into (4.9), we obtain

$$\left\langle \exp[ik_x(x(\tau)-x(\sigma))]\right\rangle = \exp\left\{-\frac{k_x^2}{2}\left[\frac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{Q_1^3\,(Q_1^2-Q_2^2)}\left[H(\tau-\sigma)\sinh Q_1(\tau-\sigma)+H(\sigma-\tau)\sinh Q_1(\sigma-\tau)\right]\right.\right.$$

$$+\frac{(Q_2^2-\omega_1^2)(Q_2^2-\omega_2^2)}{Q_2^3\,(Q_2^2-Q_1^2)}\left[H(\tau-\sigma)\sinh Q_2(\tau-\sigma)+H(\sigma-\tau)\sinh Q_2(\sigma-\tau)\right]$$

$$\left.\left.+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}\left[H(\tau-\sigma)(\tau-\sigma)-H(\sigma-\tau)(\sigma-\tau)\right]\right]\right\}$$

$$=\exp\left\{-\frac{k_x^2}{2}\left[\frac{1}{(Q_1^2-Q_2^2)}\left[\frac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{Q_1^3}(1-e^{-Q_1|\tau-\sigma|})\right.\right.\right.$$

$$\left.\left.\left.+\frac{(Q_2^2-\omega_2^2)(\omega_1^2-Q_2^2)}{Q_2^3}(1-e^{-Q_2|\tau-\sigma|})+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\right]\right]\right\}. \quad (4.26)$$

Now Q_1^2, Q_2^2 and Q_3^2 are the solutions of the cubic equation obtained from the denominator of (4.18). If we let $P^2=y$, the cubic equation is

$$y^3-(V_1^2+V_2^2)y^2+(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2)y = 0 ,$$

which may be reduced to

$$y^2-(V_1^2+V_2^2)y+(V_2^2\omega_1^2+V_1^2\omega_2^2-\omega_1^2\omega_2^2) = 0 , \quad (4.27)$$

where one of the solutions is $Q_3^2=0$.

The values of Q_1^2 and Q_2^2 are easily obtained from (4.27) as

$$V_\pm^2 = Q_{\substack{1\\2}}^2 = \frac{1}{2}\left[(V_1^2+V_2^2) \pm\left\{(V_1^2-V_2^2)^2+4(V_1^2-\omega_1^2)(V_2^2-\omega_2^2)\right\}^{\frac{1}{2}}\right]$$

$$= \frac{1}{2}\left[(V_1^2+V_2^2) \pm\left\{(V_1^2-V_2^2)^2+64\frac{C_1C_2}{\omega_1\omega_2}\right\}^{\frac{1}{2}}\right] , \quad (4.28)$$

where

$$V_1^2 = \omega_1^2+\frac{4C_1}{\omega_1} , \quad (4.29a)$$

$$V_2^2 = \omega_2^2+\frac{4C_2}{\omega_2} , \quad (4.29b)$$

and Q_1^2, Q_2^2 have been replaced by V_+^2 and V_-^2, respectively.

By using (4.26) and (4.28), we obtain

$$\left\langle \exp\left[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s))\right]\right\rangle = \exp\left\{ -\frac{K^2}{2} G|t-s| \right\}, \tag{4.30}$$

where

$$G|t-s| = \frac{1}{(V_+^2 - V_-^2)}\left[\frac{(V_+^2-\omega_1^2)(V_+^2-\omega_2^2)}{V_+^3}(1-e^{-V_+|t-s|}) + \frac{(V_-^2-\omega_2^2)(\omega_1^2-V_-^2)}{V_-^3}(1-e^{-V_-|t-s|})\right] + \frac{\omega_1^2\omega_2^2}{V_+^2V_-^2}|t-s| . \tag{4.31}$$

The result is correctly normalized since it is valid for $\underset{\sim}{K}=0$.

By using (4.28) and (4.29a,b), C_1 and C_2 can be represented by $V_\pm$, ω_1 and ω_2 as

$$\frac{4C_1}{\omega_1} = -\frac{1}{(\omega_1^2-\omega_2^2)}(V_+^2-\omega_1^2)(V_-^2-\omega_1^2) , \tag{4.32a}$$

$$\frac{4C_2}{\omega_2} = \frac{1}{(\omega_1^2-\omega_2^2)}(V_+^2-\omega_2^2)(V_-^2-\omega_2^2) , \tag{4.32b}$$

where $\omega_1 > \omega_2 > 0$ and C_1, $C_2 > 0$.

By substituting (4.30) for (4.5), the A term is determined as

$$\begin{aligned} A &= \frac{\alpha}{2^{3/2}}\int_0^\infty ds\, e^{-|t-s|}\int_{-\infty}^{\infty}\frac{dK}{2\pi^2K^2}\,4\pi K^2 \exp\left\{-\frac{K^2}{2}G|t-s|\right\} \\ &= \frac{2\alpha}{2^{3/2}\pi}\int_0^\infty ds\, e^{-|t-s|}\sqrt{\frac{2\pi}{G(t-s)}} \\ &= \frac{\alpha}{\pi^{1/2}}\int_0^\infty dy\,\frac{e^{-y}}{\sqrt{G(y)}} , \end{aligned} \tag{4.33}$$

where G is given by (4.31).

The next problem is to find the B term. To do this the value of $\langle |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2\rangle$ must be determined. First, we differentiate both sides of (4.26) with respect to K_x

$$\langle -(x(t)-x(s))^2 \exp[iK_x(x(t)-x(s))]\rangle = \left\{-G|t-s| + K_x^2 G|t-s|\right\}\exp\left\{-\frac{K_x^2}{2}G|t-s|\right\}$$

$$\langle (x(t)-x(s))^2 \rangle \quad = \quad \frac{1}{3}\langle |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 \rangle \quad = \quad G|t-s| , \tag{4.34}$$

where we have taken the limit $K_x=0$ and have assumed the medium to be isotropic.

Then the B term can be determined by substituting (4.34) into (4.4b), thus

$$B = \frac{3C_1}{2}\int_0^{\infty} ds\, e^{-\omega_1|t-s|}\left\{\frac{1}{V_+^2-V_-^2}\left[\frac{(V_+^2-\omega_1^2)(V_+^2-\omega_2^2)}{V_+^3}\,(1-e^{-V_+|t-s|})\right.\right.$$

$$\left.\left. + \frac{(V_-^2-\omega_2^2)(\omega_1^2-V_1^2)}{V_-^3}\,(1-e^{V_-|t-s|}) + \frac{\omega_1^2\omega_2^2}{V_+^2 V_-^2}\,|t-s|\right]\right\}$$

$$= \frac{3C_1}{2}\left[\frac{1}{V_+^2-V_-^2}\cdot\frac{(V_+^2-\omega_1^2)(V_+^2-\omega_2^2)}{V_+^3}\cdot\frac{2V_+}{\omega_1(V_++\omega_1)} + \frac{1}{V_+^2-V_-^2}\cdot\right.$$

$$\left.\frac{(V_-^2-\omega_2^2)(\omega_1^2-V_-^2)}{V_-^3}\cdot\frac{2V_-}{\omega_1(V_-+\omega_1)} + \frac{\omega_1^2\omega_2^2}{V_+^2V_-^2}\cdot\frac{2}{\omega_1^2}\right]$$

$$= \frac{3C_1}{\omega_1}\left[\frac{V_-V_+ + \omega_2^2}{V_+V_-\,(V_++V_-)}\right] . \tag{4.35}$$

We can obtain C in the same manner, thus

$$C = \frac{3C_2}{\omega_2}\left[\frac{V_-V_+ + \omega_1^2}{V_+V_-\,(V_++V_-)}\right] . \tag{4.36}$$

We have already determined A,Band C, and our objective in finding $\mathscr{A}$ in(4.4) is now accomplished.

Finally, we must evaluate the value of E_1. Recall the expression

$$\int \mathscr{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} \quad \sim \quad e^{-E_1 \mathcal{J}} \tag{4.37}$$

and the trial action

$$S_1 = -\frac{1}{2}\int\left(\frac{d\underset{\sim}{r}_{el}}{dt}\right)^2 dt - \frac{C_1\gamma}{2}\iint dtds\,|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 e^{-\omega_1|t-s|}$$

$$-\frac{C_2\gamma}{2}\iint dtds\,|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 e^{-\omega_2|t-s|} \quad , \qquad (4.38)$$

where we have replaced C_1 and C_2 by $C_1\gamma$ and $C_2\gamma$.

By differentiating both sides of (4.37) with respect to γ ,

we obtain

$$-\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}\left[\frac{C_1}{2}\iint dtds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_1|t-s|} + \frac{C_2}{2}\iint dtds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_2|t-s|}\right] \sim -\frac{\delta E_1}{\delta\gamma}e^{-E_1\mathcal{J}}$$

$$\frac{\frac{1}{\gamma}\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}\left[\frac{C_1}{2}\, dtds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_1|t-s|} + \frac{C_2}{2}\, dtds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_2|t-s|}\right]}{\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}} = \frac{\delta E_1}{\delta\gamma}$$

$$\frac{1}{\gamma}\left[\frac{C_1}{2}\iint dtds\, e^{-\omega_1|t-s|}\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2\rangle + \frac{C_2}{2}\iint dtds\, e^{-\omega_2|t-s|}\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|\rangle\right] = \frac{\delta E_1}{\delta\gamma}$$

$$\frac{1}{\gamma}(B+C) = \frac{\delta E_1}{\delta\gamma} .$$

$$(4.39)$$

The ground state energy E_1 can be obtained by integrating the above equation

$$E_1 = \int_0^1 \frac{d\gamma}{\gamma}(B+C) \quad , \qquad (4.40)$$

where the value of B+C can be obtained from (4.35) and (4.36) as

$$B+C = \frac{3}{4}\left\{(V_+ + V_-) - \frac{(\omega_1^2+V_+V_-)(\omega_2^2 + V_+V_-)}{V_+V_-(V_+ + V_-)}\right\} . \qquad (4.41)$$

From (4.28) and (4.29a,b), we obtain the relations

$$V_+V_- = \left[\omega_1^2\omega_2^2 + 4C_2\gamma\omega_1^2/\omega_2 + 4C_1\gamma\omega_2^2/\omega_1\right]^{\frac{1}{2}} , \qquad (4.42a)$$

and

$$V_+ + V_- = \left[\omega_1^2+\omega_2^2+4C_1\gamma/\omega_1+4C_2\gamma/\omega_2+2\sqrt{\omega_1^2\omega_2^2+4C_2\gamma\omega_1^2/\omega_2+4C_1\gamma\omega_2^2/\omega_1}\right]^{\frac{1}{2}}. \qquad (4.42b)$$

Then the integration (4.40) is carried out as

$$E_1 = \int_0^1 \frac{d\gamma}{\gamma}\frac{3}{4}\left\{(V_++V_-) - \frac{(\omega_1^2+V_+V_-)(\omega_2^2+V_+V_-)}{V_+V_-(V_++V_-)}\right\} \qquad (4.43)$$

$$= \frac{3}{2}(V_++V_- - \omega_1 - \omega_2) ,$$

where we have used (3.41), (3.42a,b) and the fact that $E_1=0$ when $\gamma=0$.

Finally, we obtain the upper bound to the ground state energy (4.3) by using (4.43) and (4.41). The result is

$$E = E_1 - A - B - C$$

$$= \frac{3}{2}(V_++V_--\omega_1-\omega_2) - \frac{3}{4}\left\{(V_++V_-) - \frac{(\omega_1^2+V_+V_-)(\omega_2^2+V_+V_-)}{V_+V_-(V_++V_-)}\right\} - A$$

$$= \frac{3}{4}\cdot\frac{1}{V_+V_-(V_++V_-)}\left[V_+V_-(V_++V_--\omega_1-\omega_2)^2 + (V_+V_- - \omega_1\omega_2)^2\right] - A , \qquad (4.44)$$

where A given by (4.33) .

In order to obtain the polaron ground state energy, the upper bound on the ground state energy expression (4.44) must be minimized numerically with respect to the four variational parameters v_+, v_- , ω_1 and ω_2 . The results of numerical calculation and some discussions of this improvement will be given in Chapter VII .