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# On the Feynman theory of polarons—a translation of the path integral variational method into a Hamiltonian formalism

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**Abstract.** Feynman's powerful path integral variational method is translated into the language of a Hamiltonian formalism. The lowest energy and the effective mass expressions of Feynman are exactly reproduced in a Hamiltonian language. We introduce two kinds of subsidiary vector fields, one of which is intended to approximate the true interaction and still be simple enough to be exactly solvable. The other has negative energy and will compensate the effects of the first one approximately.

## 1. Introduction

A useful dynamical approximation method for quantum field theoretical models, applicable for any coupling strength, is always highly interesting. In this respect the polaron model Hamiltonian was extensively studied in the fifties, because of its simplicity enabling one to draw some definite conclusions, but still complicated enough so as not to be exactly solvable. The lowest energy and the effective mass of polarons are well known in the weak and also strong coupling regions. But, of course, physically the most interesting and also the most difficult cases are the intermediate coupling regions. In 1954 Feynman (1955, 1972) developed a powerful variational method covering all the coupling strengths. Until recently this seemed to be the most successful approach to this problem. On the other hand, this variational method was based on a path integral and, as is well known, practically only the Gaussian type of trial functional can be evaluated in path integrals. So Feynman desired to find out how his method may be expressed in conventional notation, so as to be able to extend it for other trial functionals. About 25 years ago, we studied this problem (Yamazaki 1956) but were not able to succeed. This is a successor of our old paper, which solves the problem mentioned above.

In § 2 we define our extended model Hamiltonian for the polaron.‡ We introduce two kinds of dynamically independent vector fields  $\mathbf{A}$  and  $\mathbf{D}$ , whose interactions are governed by  $H_A$  and  $H_D$  which, up to the sign, have the same form.  $H_A$  is intended to cover, as well as possible, the real interaction  $H_I$ , while  $H_D$  is used to compensate the effects of an arbitrarily added interaction  $H_A$ , and will give the  $B$  term in (F32).

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‡ We use the same notations as Feynman (1955), and refer to his equations as (F32) etc.

The appearance of negative energy or of indefinite metric seems at first sight strange in such a problem, but in Feynman's  $(S - S_1)$ ,  $S_1$  and hence the potential belonging to this  $S_1$  has a 'wrong' sign representing a compensation. The simplest way of expressing this situation in Hamiltonian language is the use of negative energy or of ghost creation and annihilation operators.

We will use the total momentum operator, so as to be able to treat the effective mass at the same time.  $H_A$  is simple enough so that  $H_0 + H_A = H_1$  can be diagonalised exactly, which will be explicitly performed in § 3. In § 4 we evaluate  $\exp[-(H_0 + H_A + H_I + H_D)T]$  for large  $T$  and eliminate the phonon variable  $a_k$  and the negative energy field  $\mathbf{D}$ . After this elimination of the indefinite metric we can use the powerful Feynman inequality of the type  $\langle e^x \rangle \geq e^{\langle x \rangle}$  in our formalism. Then we will find out that our  $H_1$  gives  $E_1$  (F33). As a second-order perturbation due to  $H_I$  we get the  $A$  term (F31). In this way we can completely translate Feynman's results into our Hamiltonian language. Due to the extra interaction  $H_A$ , our conserved total momentum operator changes correspondingly. By taking this into account correctly, we obtain quite naturally the 'correct' expression for the effective mass. Instead of Feynman's imaginary 'velocity', we used the canonical conjugate momentum operator, and obtained at first a somewhat different expression for the effective mass, as compared with Feynman. Still we find that our final answer for the effective mass agrees completely with that of Feynman, without adding any *ad hoc* arguments. This is also a nice feature of our formalism, and gives confidence that our method is a correct translation of Feynman's path integral method.

Appendix 1 gives a formulation, which eliminates electron variables at first. Appendix 2 gives some detailed operator calculus, omitted in the text. Appendix 3 covers the relations between  $A$ ,  $B$  and  $E_1$ .

### The extended Hamiltonian $H'$

The polaron Hamiltonian is given by

$$H = H_0 + H_I \quad (1)$$

where

$$H_0 = \frac{1}{2} \mathbf{P}^2 + \int d^3k a_k^* a_k \quad (2)$$

$$H_I = i\kappa \int \frac{d^3k}{k} (a_k^* e^{-i\mathbf{k}\mathbf{x}} - a_k e^{+i\mathbf{k}\mathbf{x}}) \quad \kappa = \left( \frac{\sqrt{2}\alpha}{4\pi^2} \right)^{1/2}. \quad (3)$$

The total momentum operator  $\mathbf{P}'$  given by

$$\mathbf{P}' = \mathbf{P} + \int d^3k k a_k^* a_k \quad (4)$$

is conserved,

$$[\mathbf{P}', H] = 0. \quad (5)$$

Now we extend our Hilbert space by introducing two kinds of dynamically independent vector fields  $\mathbf{A}$ , and  $\mathbf{D}$ , whose interactions are given by

$$H_A = w(\mathbf{A}^* + (\sqrt{2C}/w)\mathbf{X})(\mathbf{A} + (\sqrt{2C}/w)\mathbf{X}) \quad (6)$$

$$H_D = -w(\mathbf{D} + (\sqrt{2C}/w)\mathbf{X})(\mathbf{D}^* + (\sqrt{2C}/w)\mathbf{X}) \quad (7)$$

$$[A_i, A_j^*] = [D_i, D_j^*] = \delta_{ij}. \quad (8)$$

Other commutators with  $A_i, A_j^*, D_i, D_j^*$  are all zero, except those given in (8). Let us consider our extended Hamiltonian

$$\begin{aligned} H' &= H + H_A + H_D \\ &= (H_0 + H_A - w\mathbf{D}\mathbf{D}^*) + H_I - \sqrt{2C}(\mathbf{X}, \mathbf{D} + \mathbf{D}^*) - (2C/w)\mathbf{X}^2 \\ &\equiv H_1 + H_I + H'_D. \end{aligned} \quad (9)$$

The negative energy fields  $\mathbf{D}, \mathbf{D}^*$  are introduced so as to compensate the effect of the arbitrary added interaction  $H_A$ ; their roles become clear in the calculation of § 4†. Our intention is to treat  $H_1$  as unperturbed and  $H_I$  as perturbation, while  $H'_D$  plays the role of a compensation. Now the total momentum which is conserved is given by

$$\mathbf{P}_1 = \mathbf{P} + \int d^3k k a_k^* a_k - (\sqrt{4C}/w)\mathbf{\Pi} \quad [\mathbf{P}_1, H_1 + H_I] = 0 \quad (10)$$

where

$$\mathbf{\Pi} = i\sqrt{\frac{1}{2}}(\mathbf{A}^* - \mathbf{A}).$$

### 3. The Hamiltonian $H_1$

The quadratic Hamiltonian

$$H_1 = \frac{1}{2}\mathbf{P}^2 + \int d^3k k a_k^* a_k + w\left(\mathbf{A}^* + \frac{\sqrt{2C}}{w}\mathbf{X}\right)\left(\mathbf{A} + \frac{\sqrt{2C}}{w}\mathbf{X}\right) - w\mathbf{D}\mathbf{D}^* \quad (11)$$

can be diagonalised by the following unitary transformation  $U$ :

$$\bar{H}_1 \equiv U^{-1}H_1U = \frac{3}{2}(v-w) + \frac{1}{2}\mathbf{P}^2 + \int d^3k k a_k^* a_k + v\mathbf{B}^*\mathbf{B} - w\mathbf{D}\mathbf{D}^* \quad (12)$$

where explicitly

$$U = \exp\{i \tan^{-1}[(4C/w^3)^{1/2}](\sqrt{w}\mathbf{X}\mathbf{\Pi} - (w)^{-1/2}\mathbf{P}\boldsymbol{\phi})\} \quad (13)$$

$$\boldsymbol{\phi} = \frac{1}{\sqrt{2}}(\mathbf{A}^* + \mathbf{A}) = \left(\frac{w}{2v}\right)^{1/2}(\mathbf{B}^* + \mathbf{B}) \quad (14)$$

$$\mathbf{\Pi} = \frac{i}{\sqrt{2}}(\mathbf{A}^* - \mathbf{A}) = i\left(\frac{v}{2w}\right)^{1/2}(\mathbf{B}^* - \mathbf{B}) \quad 4C = w(v^2 - w^2)$$

and in general

$$\begin{aligned} \bar{\mathbf{X}} &\equiv U^{-1}\mathbf{X}U = \frac{w}{v}\left(\mathbf{X} + \frac{\sqrt{4C}}{w^2}\boldsymbol{\phi}\right) & \bar{\mathbf{P}} &\equiv U^{-1}\mathbf{P}U = \frac{w}{v}\left(\mathbf{P} + \frac{\sqrt{4C}}{w}\mathbf{\Pi}\right) \\ \bar{\boldsymbol{\phi}} &\equiv U^{-1}\boldsymbol{\phi}U = \frac{w}{v}\left(\boldsymbol{\phi} - \frac{\sqrt{4C}}{w}\mathbf{X}\right) & \bar{\mathbf{\Pi}} &\equiv U^{-1}\mathbf{\Pi}U = \frac{w}{v}\left(\mathbf{\Pi} - \frac{\sqrt{4C}}{w^2}\mathbf{P}\right). \end{aligned} \quad (15)$$

† The lowest energy state  $|O_D\rangle$  of  $H_{D0} = -w\mathbf{D}\mathbf{D}^*$  is given by  $\mathbf{D}^*|O_D\rangle = 0$ , and  $(H_{D0} - n\omega)\mathbf{D}_i^+|O_D\rangle = 0$ .

By this  $U$  transformation, our total momentum  $\mathbf{P}_1$  given in (10) transforms into

$$\bar{\mathbf{P}}_1 \equiv U^{-1} \mathbf{P}_1 U = (v/w) \mathbf{P} + \int d^3k \, k a_k^* a_k \quad [\bar{\mathbf{P}}_1, \bar{H}_1] = [\bar{\mathbf{P}}_1, \bar{H}_1 + \bar{H}_I] = 0 \quad (16)$$

where

$$\bar{H}_I \equiv U^{-1} H_I U = i \kappa \int \frac{d^3k}{k} (a_k^* e^{-ik\bar{\mathbf{x}}} - a_k e^{+ik\bar{\mathbf{x}}}). \quad (17)$$

The eigenstate of total momentum  $\mathbf{P}_1$ , with the eigenvalue  $\mathbf{P}'_1$ , is given by

$$\mathbf{P}_1 |\Psi(\mathbf{P}'_1)\rangle = \mathbf{P}'_1 |\Psi(\mathbf{P}'_1)\rangle \quad |\Psi(\mathbf{P}'_1)\rangle = U |\Phi((w/v)\mathbf{P}'_1)\rangle \quad (18)$$

where  $|\Phi(\mathbf{P}')\rangle$  is defined as

$$\mathbf{P} |\Phi(\mathbf{P}')\rangle = \mathbf{P}' |\Phi(\mathbf{P}')\rangle \quad a_k |\Phi(\mathbf{P}')\rangle = 0.$$

Hence we see that the lowest eigenstate of  $H_1$  with the total momentum  $\mathbf{P}'_1$  is given by

$$H_1 |\Psi(\mathbf{P}'_1)\rangle = E_{1Y}(\mathbf{P}'_1) |\Psi(\mathbf{P}'_1)\rangle$$

where

$$E_{1Y}(\mathbf{P}'_1) = \frac{3}{2}(v-w) + \frac{1}{2}(w/v)^2 \mathbf{P}'_1{}^2 \quad |\Psi(\mathbf{P}'_1)\rangle = U |\Phi(w/v \mathbf{P}'_1)\rangle \quad (19)$$

$$a_k \left| \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \right\rangle = \mathbf{B} \left| \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \right\rangle = \mathbf{D}^* \left| \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \right\rangle = 0$$

$$\mathbf{P} \left| \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \right\rangle = \frac{w}{v} \mathbf{P}'_1 \left| \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \right\rangle.$$

By comparing  $E_{1Y}$  with Feynman's  $E_1$

$$\frac{1}{2}(v/w)^2 U^2 \leftrightarrow \frac{1}{2}(w/v)^2 \mathbf{P}'_1{}^2 \quad \frac{1}{2} m^* U^2 \leftrightarrow (2m^*)^{-1} \mathbf{P}'_1{}^2 \quad (20)$$

we see clearly that our effective mass  $m^*$  in the unperturbed  $H_1$  is  $(v/w)^2$  times the original (unit) mass of the electron.

#### 4. Elimination of $a_k$ and $D$ fields and the use of the inequality $\langle e^x \rangle \geq e^{\langle x \rangle}$

Let us calculate

$$\begin{aligned} \lim_{T \rightarrow \infty} e^{-H'T} &= \lim_{T \rightarrow \infty} \exp[-(H_1 + H_I + H'_D)T] \\ &= e^{-H_1 T} P \exp\left(-\int_0^T dt (H_I(t) + H'_D(t))\right) \quad \dagger \end{aligned} \quad (21)$$

where

$$H_I(t) = e^{H_1 t} H_I e^{-H_1 t} \quad H'_D(t) = e^{H_1 t} H'_D e^{-H_1 t}. \quad (22)$$

† From now on we omit  $\lim_{T \rightarrow \infty}$ , meaning  $T$  is always tending to  $\infty$ .  $P$  is the ordering operator defined in the last line of (21), meaning as usual that the operators in the  $\exp(\ )$  are arranged in decreasing order of  $t$  from left to right.

Now, taking the expectation value of (21) by  $|\Psi(\mathbf{P}'_1)\rangle$ , the leading term of the exponent will not be influenced, and we obtain ( $|\Psi_0\rangle$  represents the true vacuum state of  $H'$ , and  $E_0$  is its eigenvalue)

$$\begin{aligned} \langle \Psi(\mathbf{P}'_1) | e^{-H'T} | \Psi(\mathbf{P}'_1) \rangle &= e^{-E_0 T} \langle \Psi_0 | \Psi(\mathbf{P}'_1) \rangle^2 \\ &= e^{-E_1 T} \left\langle \Psi(\mathbf{P}'_1) \left| P \exp \left( - \int_0^T dt [H_I(t) + H'_D(t)] \right) \right| \Psi(\mathbf{P}'_1) \right\rangle \\ &= e^{-E_1 T} \left\langle \Phi \left( \frac{w}{v} \mathbf{P}'_1 \right) \left| P \exp \left( - \int_0^T dt [\bar{H}_I(t) + \bar{H}'_D(t)] \right) \right| \Phi \left( \frac{w}{v} \mathbf{P}'_1 \right) \right\rangle \end{aligned} \tag{23}$$

where explicitly

$$\begin{aligned} \bar{H}_I(t) &= i\kappa \int \frac{d^3k}{k} (a_k^* e^{+t - ik\bar{\mathbf{X}}(t)} - a_k e^{-t + ik\bar{\mathbf{X}}(t)}) \\ \bar{H}'_D(t) &= -\sqrt{2C} (\mathbf{D} e^{+wt} + \mathbf{D}^* e^{-wt}, \bar{\mathbf{X}}(t)) - \frac{2C}{w} \bar{\mathbf{X}}^2(t) \\ \bar{\mathbf{X}}(t) &= e^{\bar{H}_1 t} \bar{\mathbf{X}} e^{-\bar{H}_1 t}. \end{aligned} \tag{24}$$

As  $a_k^*$ ,  $a_k$  and  $\mathbf{D}$ ,  $\mathbf{D}^*$  appear only linearly in the  $P$  exponent of (23) we can eliminate these variables using the properties of  $|\Phi(w/v)\mathbf{P}'_1\rangle$  as given in (19). Performing this, we easily obtain

$$\begin{aligned} \left\langle \Phi \left( \frac{w}{v} \mathbf{P}'_1 \right) \left| P \exp \left( - \int_0^T dt [\bar{H}_I(t) + \bar{H}'_D(t)] \right) \right| \Phi \left( \frac{w}{v} \mathbf{P}'_1 \right) \right\rangle &= \left\langle \Phi \left( \frac{w}{v} \mathbf{P}'_1 \right) \left| P \exp \left[ -T \left( -\kappa^2 \int \frac{d^3k}{k^2} \int_0^T d\tau e^{-\tau} e^{i\mathbf{k}\bar{\mathbf{X}}(\tau)} e^{-i\mathbf{k}\bar{\mathbf{X}}(0)} \right. \right. \right. \right. \\ &\quad \left. \left. \left. - C \int_0^T d\tau e^{-w\tau} (\bar{\mathbf{X}}(\tau) - \bar{\mathbf{X}}(0))^2 \right) \right] \right| \Phi \left( \frac{w}{v} \mathbf{P}'_1 \right) \right\rangle. \end{aligned} \tag{25}$$

The remaining exponent is a complicated expression of the operators  $\bar{\mathbf{X}}(\tau)$  whose dependence on  $\tau$  is governed by  $\bar{H}_1$ , and ordered in ' $P$ ' order, in the sense of Feynman's ordered operator. As we have already eliminated our indefinite metric field  $\mathbf{D}$ , we can now use Feynman's inequality  $\langle e^x \rangle \geq e^{\langle x \rangle}$  and get

$$\begin{aligned} (25) &\geq \exp \left[ -T \left( -\kappa^2 \int \frac{d^3k}{k^2} \int_0^T d\tau e^{-\tau} \langle P(e^{i(\mathbf{k}\bar{\mathbf{X}}(\tau) - \bar{\mathbf{X}}(0))}) \rangle \right. \right. \\ &\quad \left. \left. - C \int_0^T d\tau e^{-w\tau} \langle P(\bar{\mathbf{X}}(\tau) - \bar{\mathbf{X}}(0))^2 \rangle \right) \right] \\ &\equiv \exp \{ -T [ -A_Y(\mathbf{P}'_1) - B_Y(\mathbf{P}'_1) ] \} \end{aligned} \tag{26}$$

where  $\langle \dots \rangle$  means to take the expectation value by the state  $|\Phi(w/v)\mathbf{P}'_1\rangle$ . The ' $P$ ' ordering in the above equations (26) is important. In appendix 2 we give the detailed

calculation for this expectation value. The results are

$$\begin{aligned}
 I &\equiv \langle P(e^{i(k, \bar{X}(\tau) - \bar{X}(0))}) \rangle \\
 &= \langle e^{ik\bar{X}(\tau)} e^{-ik\bar{X}(0)} \rangle \quad (\tau > 0) \\
 &= \exp[-(k^2/2v^2)F(\tau) + (w/v)^2 \mathbf{P}'_1 k\tau] \tag{27}
 \end{aligned}$$

where  $F(\tau)$  is defined as in (F42)

$$F(\tau) = w^2\tau + [(v^2 - w^2)/v](1 - e^{-v\tau}). \tag{28}$$

Comparing (27) with (F29) and (F41), we notice two differences. The reason why Feynman has the factor ‘i’ in front of his  $U$ , in contrast to our expression, is clear since he used an imaginary velocity, while we used the canonical conjugate ‘operator’  $\mathbf{P}$ . The second difference  $(w/v)^2$  comes just as remarked in (20), showing the effective mass  $(v/w)^2$  in the lowest approximation as in § 3. Nevertheless these differences cause no difference in the final results, as will be shown in § 5.

The evaluation of

$$\langle P(\bar{X}(\tau) - \bar{X}(0))^2 \rangle = 2\langle \bar{X}^2(0) - \bar{X}(\tau)\bar{X}(0) \rangle \quad (\tau > 0)$$

can be done as done by Feynman, by expanding both sides of (27) with respect to  $k$  up to order  $k^2$ . Therefore we have

$$\langle P(\bar{X}(\tau) - \bar{X}(0))^2 \rangle = [3F(\tau)/v^2] - [(w/u)^2 \mathbf{P}'_1]^2 \tau^2. \tag{29}$$

Inserting (27) and (29) into (26), we obtain ( $T = \infty$ )

$$\begin{aligned}
 A_Y(\mathbf{P}'_1) &= \frac{\alpha}{\sqrt{2}} \int_0^\infty d\tau \int \frac{d^3k}{2\pi^2 k^2} e^{-\tau} \exp\left(-\frac{k^2}{2v^2}F(\tau) + \left(\frac{w}{v}\right)^2 \mathbf{P}'_1 k\tau\right) \\
 B_Y(\mathbf{P}'_1) &= \frac{3C}{vw} - \frac{4C}{w^3} \frac{\mathbf{P}'_1{}^2}{2(v/w)^4}. \tag{30}
 \end{aligned}$$

The energy value becomes now

$$E_Y(\mathbf{P}'_1) = E_{1Y}(\mathbf{P}'_1) - A_Y(\mathbf{P}'_1) - B_Y(\mathbf{P}'_1). \tag{31}$$

### 5. Summary and discussion

If we expand formula (31) in powers of  $\mathbf{P}'_1$ , up to order  $\mathbf{P}'_1{}^2$ , we get finally

$$E(\mathbf{P}'_1) = \frac{3}{2}(v - w) + \frac{1}{2}\mathbf{P}'_1{}^2 (w/v)^2 - A - \frac{1}{2}A' \mathbf{P}'_1{}^2 (w/v)^4 - 3C/vw + (4C/w^3)\frac{1}{2}\mathbf{P}'_1{}^2 (w/v)^4 \tag{32}$$

where

$$A = \pi^{-1} \alpha v \int_0^\infty d\tau e^{-\tau} [F(\tau)]^{-1/2}. \tag{33}$$

This coincides with (F31), while

$$A' \equiv \frac{\alpha v^3}{3\sqrt{\pi}} \int_0^\infty d\tau e^{-\tau} [F(\tau)]^{-3/2} \tag{34}$$

so we get

$$E(\mathbf{P}'_1) = \frac{3}{4v} (v - w)^2 - A + \frac{\mathbf{P}'_1{}^2}{2} \left(\frac{w}{v}\right)^2 \left[ 1 - \left(\frac{w}{v}\right)^2 A' + \frac{4C}{w^3} \left(\frac{w}{v}\right)^2 \right]. \tag{35}$$

The ground state energy is exactly the same as given by Feynman. Concerning the effective mass  $m^*$ , we remark that the second and third terms in the square brackets of (35) are small corrections compared with the main term. (They are numerically really small as can be seen from the numerical work of Schultz (1959).) Hence, our effective mass expression, obtained by regarding the last term of (35) as  $\mathbf{P}'_1{}^2/2m^*$ , is given by

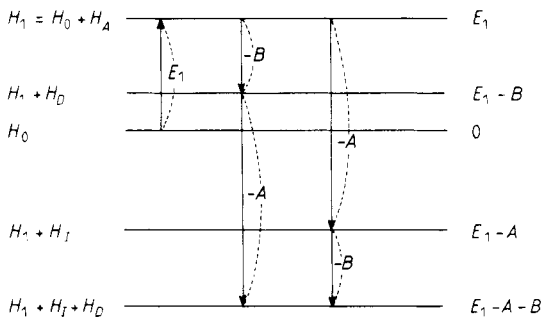
$$m^* = \left(\frac{v}{w}\right)^2 \left[ 1 + \left(\frac{w}{v}\right)^2 A' - \frac{4C}{w^3} \left(\frac{w}{v}\right)^2 \right] = \left(\frac{v}{w}\right)^2 \left[ 1 - \frac{v^2 - w^2}{v^2} + \left(\frac{w}{v}\right)^2 A' \right] = 1 + A'. \tag{36}$$

This is also precisely the same result as obtained by Feynman (F45).

In this derivation concerning the effective mass calculation, we need no *ad hoc* reasoning to avoid the imaginary velocity etc, and everything is consistent.

We have not yet proved that our  $E(\mathbf{P}'_1)$  given above is the upper bound for the true  $E_0$ , since we have used our extended Hamiltonian. Concerning this point, we can say the following. Firstly, if we drop  $H_D$  and only add  $H_A$ , we will get  $E_1 - A$ , which is certainly an upper bound, since  $H_A$  is positive definite and  $E_1(0)$  is positive as it should be. Secondly, the calculation of the  $A$  term is independent of the presence of  $H_D$ , and is determined only by  $H_1$  and  $H_I^\dagger$ . On the other hand, the calculation of the  $B$  terms is independent of  $\alpha$  or  $H_I$ , and is determined only by  $H_1$  and  $H_D^\dagger$ .  $B$  is positive and represents the compensation of  $H_A$  due to  $H_D$ , but it is not an overcompensation, as  $E_1(0) - B_V(0) = (3/4v)(v - w)^2$  is still positive.  $H_{D0}$  have only positive eigenvalues as remarked already in the footnote of p 3677. The situation can be summarised as shown in figure 1. The above mentioned facts seem already to show that our  $E_1 - B - A$  gives an upper bound, as was proved by Feynman.

The above argument that  $E_1 - A - B$  is an upper bound is still a plausibility argument and not a proof. Anyway, we think we can at least translate what Feynman had done so nicely with the path integral variational method into the language of the usual Hamiltonian formalism, which was the purpose of the present paper.



**Figure 1.** The lowest energy eigenvalues for different combinations of interaction Hamiltonian. The absolute scale has no meaning. It is different for each value of  $\alpha$ .

<sup>†</sup> These are, of course concerned with the formal expressions of  $A$  and  $B$ . At the final stage of varying the parameters  $v$  and  $w$ , they correlate with each other.



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**Appendix 1. The method of first eliminating electron variables**

In Feynman’s theory, the phonon variables are first eliminated, and the remaining electron variables are treated by the path integral method, while those given above were the translation into Hamiltonian language of this method. On the other hand, it is well known that by a unitary transformation  $V$

$$\begin{aligned} \tilde{H} &\equiv V^{-1}(H_0 + H_I)V \\ &= \frac{1}{2} \left( \mathbf{P} - \int d^3k \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}} \right)^2 + \int d^3k a_{\mathbf{k}}^* a_{\mathbf{k}} + i\kappa \int \frac{d^3k}{k} (a_{\mathbf{k}}^* - a_{\mathbf{k}}) \end{aligned} \tag{A1.1}$$

$$\tilde{\mathbf{P}} \equiv V^{-1} \mathbf{P} V = V^{-1} \left( \mathbf{P} + \int d^3k \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}} \right) V = \mathbf{P}$$

where

$$V = \exp \left( -1 \int d^3k \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}} \mathbf{X} \right),$$

we could first eliminate the variable  $\mathbf{X}$  from the total Hamiltonian. The remaining  $\mathbf{P}$  represents a (conserved) total momentum. If we could find a minimum eigenvalue of (A1.1) for given  $\mathbf{P}$ , we would get a more certain bound for the effective mass than that given above.

We have in our case

$$\tilde{H}_A = V^{-1} H_A V = H_A \quad \tilde{H}'_D = V^{-1} H'_D V = H'_D \tag{A1.2}$$

$$\tilde{\mathbf{P}}_1 = V^{-1} \mathbf{P}_1 V = \mathbf{P} - (\sqrt{4C}/w) \mathbf{\Pi} \tag{A1.3}$$

$$\begin{aligned} \tilde{H}' &= V^{-1}(H_0 + H_I + H_A + H_D)V \\ &= \tilde{H} + w \left( \mathbf{A}^* + \frac{\sqrt{2C}}{w} \mathbf{X} \right) \left( \mathbf{A} + \frac{\sqrt{2C}}{w} \mathbf{X} \right) - w \left( \mathbf{D} + \frac{\sqrt{2C}}{w} \mathbf{X} \right) \left( \mathbf{D}^* + \frac{\sqrt{2C}}{w} \mathbf{X} \right) \\ \tilde{H}' &\equiv U^{-1} V^{-1} (H_0 + H_I + H_A + H_D) V U \\ &= \frac{3}{2}(v - w) + \int d^3k a_{\mathbf{k}}^* a_{\mathbf{k}} + \frac{1}{2} \mathbf{P}^2 + \frac{1}{2} \left( \int d^3k \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}} \right)^2 \\ &\quad - \frac{w}{v} \left( \mathbf{P} + \frac{\sqrt{4C}}{w} \mathbf{\Pi} \right) \int d^3k \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}} + v \mathbf{B}^* \mathbf{B} - w \mathbf{D} \mathbf{D}^* \\ &\quad + i\kappa \int \frac{d^3k}{k} (a_{\mathbf{k}}^* - a_{\mathbf{k}}) - \sqrt{2C} (\mathbf{D} + \mathbf{D}^*, \bar{\mathbf{X}}) - \frac{2C}{w} \bar{\mathbf{X}}^2 \end{aligned} \tag{A1.4}$$

with

$$\tilde{\mathbf{P}}_1 \equiv U^{-1} V^{-1} \mathbf{P}, \quad VU = (v/w) \mathbf{P} \quad (\text{A1.5})$$

and  $\bar{\mathbf{X}}$  as given by (15). In this case our  $\tilde{\mathbf{H}}_1$ , given by the sum of the first and second lines of (A1.4), is not yet diagonal, as it still contains the  $\Pi = i(v/2w)^{1/2}(\mathbf{B}^* - \mathbf{B})$ . So let us further transform  $\tilde{\mathbf{H}}_1$  by  $W$  defined by

$$W = \exp\left[i\left(\frac{2C}{v^3 w}\right)^{1/2} \int d^3 k \mathbf{k} a_k^* a_k, \mathbf{B} + \mathbf{B}^*\right] = \exp\left(i\frac{(4C)^{1/2}}{vw} \int d^3 k \mathbf{k} a_k^* a_k \phi\right) \quad (\text{A1.6})$$

with the result

$$\bar{\mathbf{H}}_1 \equiv W^{-1} \tilde{\mathbf{H}}_1 W$$

$$\begin{aligned} &= \frac{3}{2}(v-w) + \int d^3 k a_k^* a_k + v\mathbf{B}^* \mathbf{B} - w\mathbf{D}\mathbf{D}^* + \frac{1}{2}\left(\mathbf{P} - \frac{w}{v} \int d^3 k \mathbf{k} a_k^* a_k\right)^2 \quad (\text{A1.7}) \\ &= \frac{3}{2}(v-w) + \int d^3 k a_k^* a_k + v\mathbf{B}^* \mathbf{B} - w\mathbf{D}\mathbf{D}^* + \frac{1}{2}(v/w)^{-2} \left(\tilde{\mathbf{P}}_1 - \int d^3 k \mathbf{k} a_k^* a_k\right)^2. \end{aligned}$$

The last line is expressed by using the total momentum  $\tilde{\mathbf{P}}_1$ . We see quite naturally that in this lowest approximation the effective mass is given by  $(v/w)^2$ . Using

$$\begin{aligned} \bar{\mathbf{H}}_I &\equiv W^{-1} \tilde{\mathbf{H}}_I W = i\kappa \int \frac{d^3 k}{k} \left[ a_k^* \exp\left(-i\frac{\sqrt{4C}}{vw}(\mathbf{k}\phi)\right) - a_k \exp\left(+i\frac{\sqrt{4C}}{vw}(\mathbf{k}\phi)\right) \right] \\ \bar{\mathbf{H}}_D &\equiv W^{-1} \tilde{\mathbf{H}}_D W = -\sqrt{2C}(\bar{\mathbf{X}}, \mathbf{D} + \mathbf{D}^*) - (2C/w)\bar{\mathbf{X}}^2 \end{aligned} \quad (\text{A1.8})$$

we can eliminate  $\mathbf{X}$  from  $\bar{\mathbf{H}}_1$  and  $\bar{\mathbf{H}}_I$ , and give the same  $E_{1Y}(\mathbf{P}'_1)$  and also  $A_Y(\mathbf{P}'_1)$  as will be shown in appendix 2.  $\bar{\mathbf{H}}_D$  still contains  $\bar{\mathbf{X}}$ , so we cannot yet completely eliminate the electron variables so as to be able to express everything by  $a_k, a_k^*, \mathbf{B}, \mathbf{B}^*$ , only. For the calculation of  $\bar{\mathbf{H}}_D$ , with respect to the terms leading to  $B_Y(\mathbf{P}'_1)$  we must still take into account the non-commutativity of  $\tilde{\mathbf{P}}_1$  and  $\bar{\mathbf{X}}$ .

## Appendix 2. Operator calculus leading to (27)

$$\begin{aligned} I &= \left\langle \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \left| e^{i\mathbf{k}\bar{\mathbf{X}}(\tau)} e^{-i\mathbf{k}\bar{\mathbf{X}}(0)} \right| \Phi\left(\frac{w}{v} \mathbf{P}'_1\right) \right\rangle \\ &= \left\langle e^{\bar{\mathbf{H}}_1 \tau} e^{i\mathbf{k}\bar{\mathbf{X}}} e^{-\bar{\mathbf{H}}_1 \tau} e^{-i\mathbf{k}\bar{\mathbf{X}}} \right\rangle \\ &= \left\langle e^{i\mathbf{k}\bar{\mathbf{X}}} \exp[-(\bar{\mathbf{H}}_1 - E_{1Y}(\mathbf{P}'_1))\tau] e^{-i\mathbf{k}\bar{\mathbf{X}}} \right\rangle \\ &= \left\langle \exp\left[i\mathbf{k} \frac{w}{v} \left(\mathbf{X} + \frac{\sqrt{4C}}{w^2} \phi\right)\right] \exp\left\{-\left[\frac{1}{2}\mathbf{P}^2 - \frac{1}{2}\left(\frac{w}{v} \mathbf{P}'_1\right)^2 + v\mathbf{B}^* \mathbf{B}\right]\tau\right\} \right. \\ &\quad \left. \times \exp\left[-i\mathbf{k} \frac{w}{v} \left(\mathbf{X} + \frac{\sqrt{4C}}{w^2} \phi\right)\right] \right\rangle \\ &= \left\langle \exp\left(i\frac{w}{v}(\mathbf{k}\mathbf{X})\right) \exp\left\{-\frac{1}{2}\left[\mathbf{P}^2 - \left(\frac{w}{v} \mathbf{P}'_1\right)^2\right]\tau\right\} \exp\left(-i\frac{w}{v}(\mathbf{k}\mathbf{X})\right) \right\rangle \\ &\quad \times \left\langle \exp\left(i\frac{\sqrt{4C}}{vw}(\mathbf{k}\phi)\right) \exp(-v\mathbf{B}^* \mathbf{B}\tau) \exp\left(-i\frac{\sqrt{4C}}{vw}(\mathbf{k}\phi)\right) \right\rangle \quad (\text{A2.1}) \end{aligned}$$

$$\begin{aligned}
&= \left\langle \exp \left\{ -\frac{1}{2} \left[ \left( \mathbf{P} - \frac{w}{v} \mathbf{k} \right)^2 - \left( \frac{w}{v} \mathbf{P}'_1 \right)^2 \right] \tau \right\} \right\rangle \left\langle \exp \left[ i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k}, \mathbf{B} + \mathbf{B}^*) \right] \right. \\
&\quad \left. \times \exp(-v\mathbf{B}^* \mathbf{B} \tau) \exp \left[ -i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k}, \mathbf{B} + \mathbf{B}^*) \right] \right\rangle \\
&= \exp \left\{ -\frac{1}{2} \left[ \left( \frac{w}{v} \mathbf{P}'_1 - \frac{w}{v} \mathbf{k} \right)^2 - \left( \frac{w}{v} \mathbf{P}'_1 \right)^2 \right] \tau \right\} \exp \left( -\frac{2C}{wv^3} k^2 \right) \\
&\quad \times \left\langle \exp \left[ i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k} \mathbf{B}) \right] \exp(-v\mathbf{B}^* \mathbf{B} \tau) \exp \left[ -i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k} \mathbf{B}^*) \right] \right\rangle \\
&= \exp \left[ -\frac{1}{2} \left( \frac{w}{v} \right)^2 (k^2 - 2\mathbf{k} \mathbf{P}'_1) \tau \right] \exp \left( -\frac{2C}{wv^3} k^2 \right) \\
&\quad \times \left\langle \exp \left[ i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k} \mathbf{B}) \right] \exp \left[ -i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k} \mathbf{B}^*) e^{-v\tau} \right] \right\rangle \\
&= \exp \left[ -\frac{1}{2} \left( \frac{w}{v} \right)^2 (k^2 - 2\mathbf{k} \mathbf{P}'_1) \tau \right] \exp \left( -\frac{2C}{wv^3} k^2 (1 - e^{-v\tau}) \right) \\
&= \exp \left[ -\frac{k^2}{2v^2} \left( w^2 \tau + \frac{v^2 - w^2}{v} (1 - e^{-v\tau}) \right) + \left( \frac{w}{v} \right)^2 \mathbf{k} \mathbf{P}'_1 \tau \right].
\end{aligned}$$

This is our equation (27) and leads to  $A_Y(\mathbf{P}'_1)$  and  $B_Y(\mathbf{P}'_1)$ . Now we want to show the calculation leading to  $A_Y(\mathbf{P}'_1)$  by the formalism given in appendix 1.

$$\begin{aligned}
I' &= \left\langle a_k \exp \left( i \frac{\sqrt{4C}}{vw} (\mathbf{k} \boldsymbol{\phi}) \right) \exp \{ -[\bar{H}_1 - E_{1Y}(\mathbf{P}'_1)] \tau \} \exp \left( -i \frac{\sqrt{4C}}{vw} (\mathbf{k} \boldsymbol{\phi}) \right) a_k^* \right\rangle \\
&= \left\langle \exp \left[ i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k}, \mathbf{B} + \mathbf{B}^*) \right] \right. \\
&\quad \times \exp \left\{ -\left[ \frac{1}{2} \left( \mathbf{P} - \frac{w}{v} \mathbf{k} \right)^2 - \frac{1}{2} \left( \frac{w}{v} \mathbf{P}'_1 \right)^2 + 1 + v\mathbf{B}^* \mathbf{B} \right] \tau \right\} \\
&\quad \left. \times \exp \left[ -i(2C/wv^3)^{1/2} (\mathbf{k}, \mathbf{B} + \mathbf{B}^*) \right] \right\rangle \\
&= e^{-\tau} \exp \left[ -\frac{1}{2} \left( \frac{w}{v} \right)^2 (k^2 - 2\mathbf{P}'_1 \mathbf{k}) \right] \left\langle \exp \left[ i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k}, \mathbf{B} + \mathbf{B}^*) \right] \right. \\
&\quad \left. \times \exp(-v\mathbf{B}^* \mathbf{B} \tau) \exp \left[ -i \left( \frac{2C}{wv^3} \right)^{1/2} (\mathbf{k}, \mathbf{B} + \mathbf{B}^*) \right] \right\rangle. \tag{A2.2}
\end{aligned}$$

The rest is the same as in (A2.1) and gives

$$I' = e^{-\tau} \exp \left[ -\frac{k^2}{2v^2} F(\tau) + \left( \frac{w}{v} \right)^2 \mathbf{k} \mathbf{P}'_1 \tau \right]. \tag{A2.3}$$

The  $e^{-\tau}$  term comes from  $\int d^3k a_k^* a_k$  contained in  $\bar{H}_1$ . This term was already taken in the other formulation, namely in (24), where we had used

$$a_k(t) = e^{\bar{H}_1 t} a_k e^{-\bar{H}_1 t} = a_k e^{-t}. \tag{A2.4}$$

This  $e^{-t}$  appears in (26) in the form  $e^{-\tau}$ . So we can obtain in both formulations the same correct expression for  $A_Y$ , and hence  $B_Y$ .

The calculation in this appendix clearly shows that the dynamics of Feynman's variable  $X_\tau$ , which obeys his action  $S_1$ , is completely governed by our  $H_1$  in the Hamiltonian formalism.

### Appendix 3. The relation between $E_1$ , $A$ and $B$

We have derived our  $A$ ,  $B$ ,  $E_1$  in the text, but they are related to each other just as in Feynman, in spite of a somewhat different appearance in the signs and coefficients in  $P_1'^2/2$  and  $U^2/2$ .

$$\begin{aligned}
 E_{1Y}(P_1') &= \frac{3}{2}(v-w) + \frac{1}{2} \left(\frac{w}{v}\right)^2 P_1'^2 & E_{1F}(U) &= \frac{3}{2}(v-w) + \frac{1}{2} \left(\frac{v}{w}\right)^2 U^2 \\
 A_Y(P_1') &= A - A' \left(\frac{w}{v}\right)^4 \frac{P_1'^2}{2} & A_F(U) &= A + A' \frac{U^2}{2} \\
 B_Y(P_1') &= \frac{3C}{vw} - \frac{4C}{w^3} \left(\frac{w}{v}\right)^4 \frac{P_1'^2}{2} & B_F(U) &= \frac{3C}{vw} + \frac{4C}{w^3} \frac{U^2}{2}.
 \end{aligned}
 \tag{A3.1}$$

The relations between  $A_Y$  and  $B_Y$ ,  $A_F$  and  $B_F$  are the same, because they are derived in the same way. Feynman derived his  $E_{1F}$  by integrating

$$C \, dE_{1F}/dC = B_F. \tag{A3.2}$$

On the other hand we have not used this equation. We derived  $E_{1Y}$  and  $B_Y$  separately. Still we can easily derive the corresponding equation

$$C \, dE_{1Y}/dC = B_Y \tag{A3.3}$$

by differentiating  $E_{1Y}$  by  $C$  and assuming that only  $v$  depends on  $C$ . We get also the 'correct' sign in front of  $P_1'^2/2$  in  $B_Y$ . This looks at first a little bit strange, because our correspondence

$$(w/v)^2 P_1' \leftrightarrow U \tag{A3.4}$$

seems to mean that if  $U$  is independent of  $C$ , then  $P_1'$  should depend on  $C$  through  $v$ . But this is not the case, because everything is consistent if we use only  $P_1'$  by assuming that this is independent of  $C$ . We should only take care that, in the case of the calculation, the above correspondence (A3.4) is not mixed up. The relation (A3.3) seems to show that our formulation, as it stands, is consistent and satisfactory.

### References

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