

## Slow Electrons in a Polar Crystal

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A variational principle is developed for the lowest energy of a system described by a path integral. It is applied to the problem of the interaction of an electron with a polarizable lattice, as idealized by Fröhlich. The motion of the electron, after the phonons of the lattice field are eliminated, is described as a path integral. The variational method applied to this gives an energy for all values of the coupling constant. It is at least as accurate as previously known results. The effective mass of the electron is also calculated, but the accuracy here is difficult to judge.

**A**N electron in an ionic crystal polarizes the lattice in its neighborhood. This interaction changes the energy of the electron. Furthermore, when the electron moves the polarization state must move with it. An electron moving with its accompanying distortion of the lattice has sometimes been called a polaron. It has an effective mass higher than that of the electron. We wish to compute the energy and effective mass of such an electron. A summary giving the present state of this problem has been given by Fröhlich.<sup>1</sup> He makes simplifying assumptions, such that the crystal lattice acts much like a dielectric medium, and that all the important phonon waves have the same frequency. We will not discuss the validity of these assumptions here, but will consider the problem described by Fröhlich as simply a mathematical problem. Aside from its intrinsic interest, the problem is a much simplified analog of those which occur in the conventional meson theory when perturbation theory is inadequate. The method we shall use to solve the polaron problem is new, but the pseudoscalar symmetric meson field problems involve so many further complications that it cannot be directly applied there without further development.

We shall show how the variational technique which is so successful in ordinary quantum mechanics can be extended to integrals over trajectories.

### STATEMENT OF THE PROBLEM

With Fröhlich's assumptions, the problem is reduced to that of finding the properties of the following Hamiltonian:

$$H = \frac{1}{2} \mathbf{P}^2 + \sum_{\mathbf{K}} a_{\mathbf{K}}^+ a_{\mathbf{K}} + i(\sqrt{2}\pi\alpha/V)^{\frac{1}{2}} \sum_{\mathbf{K}} \frac{1}{K} \times [a_{\mathbf{K}}^+ \exp(-i\mathbf{K} \cdot \mathbf{X}) - a_{\mathbf{K}} \exp(i\mathbf{K} \cdot \mathbf{X})]. \quad (1)$$

Here  $\mathbf{X}$  is the vector position of the electron,  $\mathbf{P}$  its conjugate momentum,  $a_{\mathbf{K}}^+$ ,  $a_{\mathbf{K}}$  the creation and annihilation operators of a phonon (of momentum  $\mathbf{K}$ ). The frequency of a phonon is taken to be independent of  $\mathbf{K}$ . Our units are such that  $\hbar$ , this frequency, and the

electron mass are unity. The quantity  $\alpha$  acts as a coupling constant, which may be large or small. In conventional units it is given by

$$\alpha = \frac{1}{2} \left( \frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon} \right) \frac{e^2}{\hbar\omega} \left( \frac{2m\omega}{\hbar} \right)^{\frac{1}{2}},$$

where  $\epsilon$ ,  $\epsilon_{\infty}$  are the static and high frequency dielectric constant, respectively. In a typical case, such as NaCl,  $\alpha$  may be about 5. The wave function of the system satisfies ( $\hbar=1$ )

$$i\partial\psi/\partial t = H\psi, \quad (2)$$

so that if  $\varphi_n$  and  $E_n$  are the eigenfunctions and eigenvalues of  $H$ ,

$$H\varphi_n = E_n\varphi_n, \quad (3)$$

then any solution of (2) is of the form

$$\psi = \sum_n C_n \varphi_n e^{-iE_n t}.$$

Now we can cast (1) and (2) into the Lagrangian form of quantum mechanics and then eliminate the field oscillators (specializing to the case that all phonons are virtual). Doing this in exact analogy to quantum electrodynamics,<sup>2</sup> we find that we must study the sum over all trajectories  $\mathbf{X}(t)$  of  $\exp(iS')$ , where

$$S' = \frac{1}{2} \int \left( \frac{d\mathbf{X}}{dt} \right)^2 dt + 2^{-\frac{1}{2}} \alpha i \int \int | \mathbf{X}_t - \mathbf{X}_s |^{-1} e^{-i|t-s|} dt ds. \quad (4)$$

This sum will depend on the initial and final conditions and on the time interval  $T$ . Since it is a solution of the Schrödinger Eq. (2), considered as a function of  $T$  it will contain frequencies  $E_n$ , the lowest of which we seek. It is difficult to isolate the lowest frequency, however.

For that reason, consider the mathematical problem of solving

$$\partial\psi/\partial t = -H\psi, \quad (5)$$

without question as to the meaning of  $t$ . This has the same eigenvalues and eigenfunctions as (3), but a

<sup>1</sup> H. Fröhlich, *Advances in Physics* 3, 325 (1954). References to other work is given here.

<sup>2</sup> R. P. Feynman, *Phys. Rev.* 80, 440 (1950).

solution will have the form

$$\psi = \sum_n C_n e^{-E_n t} \varphi_n.$$

For large  $t$  any solution therefore asymptotically dies out exponentially, the last exponent surviving being that of the lowest  $E$ , say  $E_0$ .

An equation such as (5) can be converted to a path integral just as easily as (2) is, and the integral over the oscillator coordinates can again be done in an analogous way. The Lagrangian form corresponding to (5) turns out to be

$$K = \int \exp S \mathcal{D} \mathbf{X}(t), \tag{6}$$

with

$$S = -\frac{1}{2} \int \left( \frac{d\mathbf{X}}{dt} \right)^2 dt + 2^{-\frac{1}{2}} \alpha \int \int |\mathbf{X}_t - \mathbf{X}_s|^{-1} e^{-|t-s|} dt ds. \tag{7}$$

This is just as one might expect from replacing  $t$  in (4) by  $-it$ . Now, since  $K$  is a solution of (5), its asymptotic form for a large  $t$  interval, 0 to  $T$  is

$$K \sim e^{-E_0 T} \tag{8}$$

as  $T \rightarrow \infty$ . Therefore, we must estimate the path integral (6) for large  $T$ .

VARIATIONAL PRINCIPLE

The method we shall use is a type of variational method. Choose any  $S_1$  which is simple and purports to be some sort of approximation to  $S$ . Then write

$$\int \exp S \mathcal{D} \mathbf{X}(t) = \int \exp(S - S_1) \exp S_1 \mathcal{D} \mathbf{X}(t). \tag{9}$$

Now this last expression can be looked upon as the average of  $\exp(S - S_1)$ , the average being taken with positive weight  $\exp S_1$ . But for any set of real quantities  $f$  the average of  $\exp f$  exceeds the exponential of the average,

$$\langle \exp f \rangle \geq \exp \langle f \rangle. \tag{10}$$

Hence if in (9) we replace  $S - S_1$  by its average,

$$\langle S - S_1 \rangle = \int (S - S_1) \exp S_1 \mathcal{D} \mathbf{X}(t) / \int \exp S_1 \mathcal{D} \mathbf{X}(t), \tag{11}$$

we will underestimate the value of (9). Therefore, if  $E$  is computed from

$$\int \exp \langle (S - S_1) \rangle \exp S_1 \mathcal{D} \mathbf{X}(t) \sim \exp -ET, \tag{12}$$

then we know that  $E$  exceeds the true  $E_0$ ,

$$E \geq E_0. \tag{13}$$

If there are any free parameters in  $S_1$  we can choose as the "best" values those which minimize  $E$ .

Since  $\langle S - S_1 \rangle$  defined in (11) is proportional to  $T$ , let us write

$$\langle S - S_1 \rangle = sT. \tag{14}$$

Furthermore, the factor  $\exp \langle S - S_1 \rangle$  in (12) is constant, of course, and may be taken outside the integral. Finally, suppose the lowest energy  $E_1$  for the action  $S_1$  is known,

$$\int \exp S_1 \mathcal{D} \mathbf{X}(t) \sim \exp(-E_1 T), \tag{15}$$

then we have

$$E = E_1 - s \tag{16}$$

from (12), with  $s$  given by (11) and (14). (In the case that  $S$  and  $S_1$  are both simple actions [of the form of (18) below] this can readily be shown to be equivalent to the usual variational principle.)

POSSIBLE TRIAL ACTIONS

Some of the methods which have been applied to this problem, so far, correspond to various choices for  $S_1$ . The perturbation method corresponds to  $S_1 = -\frac{1}{2} \int (d\mathbf{X}/dt)^2 dt$  and gives

$$E = -\alpha. \tag{17}$$

We see immediately that the perturbation result is an upper limit to  $E_0$ , a result proven only with much greater effort by more usual methods, by Gurari<sup>3</sup> and Lee and Pines.<sup>4</sup> Another suggestion is

$$S_1 = -\frac{1}{2} \int (d\mathbf{X}/dt)^2 dt + \int V(\mathbf{X}_t) dt, \tag{18}$$

where  $V$  is a potential to be chosen. If a Coulomb potential is chosen,  $V(R) = Z/R$ , and the parameter  $Z$  varied, one finds

$$E = -(25/256)\alpha^2 = -0.098\alpha^2$$

asymptotically for the case that  $\alpha$  is very large. For large  $\alpha$  this corresponds to Landau's method<sup>1</sup> with a trial function of the form  $e^{-\beta r}$ . If a harmonic potential  $V(R) = kR^2$  is used (corresponding to a Gaussian trial function in Landau's method) the value is somewhat improved:

$$E = -(1/3\pi)\alpha^2 = -0.106\alpha^2. \tag{19}$$

If  $\alpha$  is not so large, the form (18) can still be used in (16). The evaluation of  $s$  requires knowledge of the eigenfunctions and eigenvalues for the potential  $V$ .

<sup>3</sup> M. Gurari, Phil. Mag. 44, 329 (1953).

<sup>4</sup> T. Lee and D. Pines, Phys. Rev. 88, 960 (1952). Lee, Low, and Pines, Phys. Rev. 90, 297 (1953).

The result is somewhat difficult to evaluate for the Coulomb potential, but fairly simple for the harmonic case [see (34) below]. However, it is readily shown that for any  $\alpha$  less than about 6 no choice of  $V$  can improve the result (17) for  $V=0$ . Fröhlich has asked for a method which works uniformly over the entire range of  $\alpha$ . He points out that the artificial binding to a special origin, which (18) implies, is a disadvantage. It is this which presumably makes any potential  $V$  give a poorer result than  $V=0$  for small  $\alpha$ .

To remedy this, I thought a good idea would be to use for  $S_1$  the action for a particle bound by a potential  $V(\mathbf{X}-\mathbf{Y})$  to another particle of coordinate  $\mathbf{Y}$ . This latter could have finite mass, so no permanent origin would be assumed. Of course the action for such a system would contain both  $\mathbf{X}(t)$  and  $\mathbf{Y}(t)$ . But the variables  $\mathbf{Y}(t)$  could be integrated out, at least in principle, leaving an effective  $S_1$  depending only on  $\mathbf{X}$ . At first I tried a Coulomb interaction for  $V(\mathbf{X}-\mathbf{Y})$  but it was rather complicated. The technique may be useful in more difficult problems. But here we have already seen that an harmonic binding should be as good, if not better. Further, an extra particle bound harmonically has its variables  $\mathbf{Y}(t)$  appearing quadratically in the action. It may therefore be easily eliminated explicitly. The result we know from studies of similar problems in electrodynamics. We are, in this way, led to consider the choice

$$S_1 = -\frac{1}{2} \int \left( \frac{d\mathbf{X}}{dt} \right)^2 dt - \frac{1}{2} C \int \int [\mathbf{X}_t - \mathbf{X}_s]^2 \times \exp(-w|t-s|) dt ds, \quad (20)$$

where  $C$  and  $w$  are parameters, to be chosen later to minimize  $E$ .

#### EVALUATION OF THE ENERGY

Since  $S_1$  contains  $\mathbf{X}$  only quadratically, all the necessary path integrals are easily done.<sup>5</sup> Because the method may not be familiar we outline it briefly here. Define the symbol  $\langle \rangle$  as

$$\langle F \rangle = \int F \exp S_1 \mathcal{D}\mathbf{X}(t) / \int \exp S_1 \mathcal{D}\mathbf{X}(t).$$

Then comparison of  $S_1$  and  $S$  shows that

$$s = \frac{1}{T} \langle S - S_1 \rangle = 2^{-3} \alpha \int \langle |\mathbf{X}_t - \mathbf{X}_s|^{-1} \rangle e^{-|t-s|} ds + \frac{1}{2} C \int \langle (\mathbf{X}_t - \mathbf{X}_s)^2 \rangle e^{-w|t-s|} ds = A + B. \quad (21)$$

<sup>5</sup> R. P. Feynman, Phys. Rev. 84, 108 (1951), Appendix C.

We concentrate first on the first term  $A$  of (21). In it we may express  $|\mathbf{X}_t - \mathbf{X}_s|^{-1}$  by a Fourier transform,

$$|\mathbf{X}_t - \mathbf{X}_s|^{-1} = \int d^3\mathbf{K} \exp[i\mathbf{K} \cdot (\mathbf{X}_t - \mathbf{X}_s)] (2\pi^2 K^2)^{-1}. \quad (23)$$

For this reason we need to study

$$\langle \exp[i\mathbf{K} \cdot (\mathbf{X}_\tau - \mathbf{X}_\sigma)] \rangle = \int \exp S_1 \exp[i\mathbf{K} \cdot (\mathbf{X}_\tau - \mathbf{X}_\sigma)] \mathcal{D}\mathbf{X}(t) / \int \exp S_1 \mathcal{D}\mathbf{X}(t). \quad (23)$$

The integral in the numerator is of the form

$$I = \int \exp \left[ -\frac{1}{2} \int \left( \frac{d\mathbf{X}}{dt} \right)^2 dt - \frac{1}{2} C \int \int (\mathbf{X}_t - \mathbf{X}_s)^2 \times e^{-w|t-s|} dt ds + \int \mathbf{f}(t) \cdot \mathbf{X}(t) dt \right] \mathcal{D}\mathbf{X}(t), \quad (24)$$

where specifically

$$\mathbf{f}(t) = i\mathbf{K}\delta(t-\tau) - i\mathbf{K}\delta(t-\sigma). \quad (25)$$

Now we shall find (24) insofar as it depends on  $\mathbf{f}$  or  $\mathbf{K}$  aside from a normalization factor which drops out in (23). Incidentally let us notice that the three rectangular components separate in (24) and we need only consider a scalar case. The method of integration is to substitute  $X(t) = X'(t) + Y(t)$ , where  $X'(t)$  is that special function for which the exponent is maximum. The variable of integration is now  $Y(t)$ . Since the exponent is quadratic in  $X(t)$  and  $X'$  renders it an extremum, it can contain  $Y(t)$  only quadratically. Evidently  $Y$  then separates off as a factor not containing  $f$ , which may be integrated to give an unimportant constant (depends on  $T$  only). Therefore within such a constant

$$I = \exp \left[ -\frac{1}{2} \int \dot{X}'^2 dt - \frac{1}{2} C \int \int (X'_t - X'_s)^2 \times e^{-w|t-s|} dt ds + \int f(t) X'_t dt \right], \quad (26)$$

where  $X'$  is that function which minimizes the expression [subject for convenience, to  $X'(0) = X'(T) = 0$  if the time interval is 0 to  $T$ ]. The variation problem gives the integral equation

$$d^2 X'(t)/dt^2 = 2C \int (X'_t - X'_s) e^{-w|t-s|} ds - f(t). \quad (27)$$

Using (27), (26) can be simplified to

$$I = \exp \left[ \frac{1}{2} \int f(t) X'(t) dt \right]. \quad (28)$$

We need merely solve (27) and substitute into (28). To do this we define

$$Z(t) = \frac{w}{2} \int e^{-w|t-s|} X_s' ds,$$

so that

$$d^2Z(t)/dt^2 = w^2[Z(t) - X'(t)],$$

while (27) is

$$d^2X'(t)/dt^2 = \frac{4C}{w} [X'(t) - Z(t)] - f(t).$$

The equations are readily separated and solved. The solution for  $X'(t)$  substituted into (28) gives, for the case (25),

$$I = \langle \exp[i\mathbf{K} \cdot (\mathbf{X}_r - \mathbf{X}_\sigma)] \rangle = \exp \left[ -\frac{2CK^2}{v^3w} (1 - e^{-v|\tau-\sigma|}) - \frac{w^2}{2v^2} K^2 |\tau - \sigma| \right], \quad (29)$$

where we have made the substitution

$$v^2 = w^2 + (4C/w). \quad (30)$$

The result is correctly normalized since it is valid for  $\mathbf{K}=0$ . The integral on  $K$  in (22) is a simple Gaussian, so that substitution into  $A$  gives

$$A = \pi^{-\frac{1}{2}} \alpha v \int_0^\infty \left[ w^2 \tau + \frac{v^2 - w^2}{v} (1 - e^{-v\tau}) \right]^{-\frac{1}{2}} e^{-\tau} d\tau. \quad (31)$$

To find  $B$  we need  $\langle (\mathbf{X}_r - \mathbf{X}_\sigma)^2 \rangle$ . This can be obtained by expanding both sides of (29) with respect to  $\mathbf{K}$  up to order  $K^2$ . Therefore

$$\frac{1}{3} \langle (\mathbf{X}_r - \mathbf{X}_\sigma)^2 \rangle = \frac{4C}{v^3w} (1 - e^{-|\tau-\sigma|}) + \frac{w^2}{v^2} |\tau - \sigma|.$$

The integral in  $B$  is now easily performed and the expression simplifies to

$$B = 3C/vw. \quad (32)$$

Finally we need  $E_1$ , the energy belonging to our action  $S_1$ . This is most easily obtained by differentiating both sides of (15) with respect to  $C$ . One finds immediately

$$CdE_1/dC = B,$$

so that, in view of (32) and (30), integration gives

$$E_1 = \frac{3}{2}(v-w),$$

since  $E_1=0$  for  $C=0$ . Since  $E_1 - B = (3/4v)(v-w)^2$  we obtain finally for our energy expression:

$$E = \frac{3}{4v}(v-w)^2 - A, \quad (33)$$

with  $A$  given in (31). The quantities  $v, w$  can be considered as two parameters which may be varied separately to obtain a minimum.

The integral in  $A$  unfortunately cannot be performed in closed form, so that a complete determination of  $E$  requires numerical integration. It is, however, possible to obtain approximate expressions in various limiting cases. The case of large  $\alpha$  corresponds to large  $v$ . The choice  $w=0$  leads to an integral

$$A = \pi^{-\frac{1}{2}} \alpha v^{\frac{1}{2}} \int_0^\infty e^{-\tau} d\tau [1 - e^{-v\tau}]^{-\frac{1}{2}} = \frac{\alpha \Gamma(1/v)}{v^{\frac{1}{2}} \Gamma(\frac{1}{2} + 1/v)}, \quad (34)$$

and  $E_1 = 3v/4$ . It corresponds to the use of a fixed harmonic binding potential in (18). For large  $v$ ,  $e^{-v\tau}$  can be neglected, so that  $A = \pi^{-\frac{1}{2}} \alpha v^{\frac{1}{2}}$ . This corresponds to using a Gaussian trial function in Landau's method. For  $\alpha$  less than 5.8 and  $w=0$ , (33) does not give a minimum unless  $v=0$ , so that the  $w=0$  case does not give a single expression for all ranges of  $\alpha$ . In spite of this disadvantage the result with (34) is relatively simple and fairly accurate. For  $\alpha > 6$ , only fairly large  $v$  are important, and the asymptotic formula (good to 1 percent for  $v > 4$ ),

$$A = \alpha(v/\pi)^{\frac{1}{2}} [1 + (2 \ln 2)/v],$$

is convenient. Fröhlich, however, considers the discontinuity at  $\alpha=6$  as a serious disadvantage, which it is the purpose of this paper to avoid. This we do by choosing  $w$  different from zero.

Let us study (33), just for small  $\alpha$ , in case  $w$  is not zero. The minimum will occur for  $v$  near  $w$ . Therefore write  $v = (1 + \epsilon)w$ , consider  $\epsilon$  small, and expand the root in (31). This gives

$$A = \alpha(v/w) \left[ 1 - \epsilon \int_0^\infty \tau^{-\frac{1}{2}} e^{-\tau} (1 - e^{-w\tau}) d\tau / w\pi^{\frac{1}{2}} + \dots \right].$$

The integral is

$$2w^{-1} [(1+w)^{\frac{1}{2}} - 1] = P. \quad (35)$$

The problem (33) then corresponds, in this order, to minimizing

$$E = \frac{3}{4}w\epsilon^2 - \alpha - \alpha\epsilon(1-P).$$

That is,

$$\epsilon = 2\alpha(1-P)/3w,$$

which is valid for small  $\alpha$  only, as  $\epsilon$  was assumed small. The resulting energy is

$$E = -\alpha - \alpha^2(1-P)^2/3w.$$

Our method therefore gives a correction even for small  $\alpha$ . It is least for  $w=3$ , in which case it gives

$$E = -\alpha - \alpha^2/81 = -\alpha - 1.23(\alpha/10)^2. \quad (36)$$

It is not sensitive to the choice of  $w$ . For example, for  $w=1$  the 1.23 falls only to 0.98. The method of Lee and Pines<sup>6</sup> gives exactly this result (36) to this order. The perturbation expansion has been carried to

<sup>6</sup> T. Lee and D. Pines, Phys. Rev. **92**, 883 (1953).

second order by Haga<sup>7</sup> who shows that the exact coefficient of the  $(\alpha/10)^2$  term should be 1.26, so that our variational method is remarkably accurate for small  $\alpha$ .

The opposite extreme of large  $\alpha$  corresponds to large  $v$ , and, as we shall see,  $w$  near 1. Since  $v \gg w$  the integral (31) reduces in the first approximation to (34), which we can use in its asymptotic form. The next approximation in  $w$  can be obtained by expanding the radical in (31), considering  $w/v \ll 1$ . Furthermore,  $e^{-v\tau}$  is negligible. In this way we get

$$E = \frac{3}{4v}(v-w)^2 - \alpha(v/\pi)^{\frac{1}{2}} \left( 1 + \frac{2 \ln 2}{v} - \frac{w^2}{2v} \right). \quad (37)$$

This is minimum, within our approximation of large  $v$ , when  $w=1$ , and  $v = (4\alpha^2/9\pi) - (4 \ln 2 - 1)$ :

$$E = -\alpha^2/3\pi - 3 \ln 2 - \frac{3}{4} = -0.106\alpha^2 - 2.83. \quad (38)$$

The approximations do not keep  $E$  as an upper limit as, unfortunately, the further terms, of order  $1/\alpha^2$  are probably positive.

For further numerical work it is probably sufficiently accurate to take  $w=1$  for all  $\alpha$ , rather than do the extra work needed to minimize this extra variable. This value of  $w$  means that the trial  $S_1$  has the same time exponential in the interaction term as does  $S$ . For small  $\alpha$ , that is,  $v$  near 1, the integral can be expanded in a power series in  $(v-1)$ . The resulting energy is ( $w=1$ ):

$$E = -\alpha - 0.98(\alpha/10)^2 - 0.60(\alpha/10)^3 - 0.14(\alpha/10)^4 \dots \quad (39)$$

The two expressions (38), (39) fit fairly well near  $\alpha=5$ . For practical purposes it may suffice to use (39) below  $\alpha=5$  and (38) above. If more accuracy than 3 percent is needed near  $\alpha=5$  numerical integration of  $A$  must be performed. The value of  $v$  which gives (39) is

$$v = 1 + 1.14(\alpha/10) + 1.35(\alpha/10)^2 + 1.88(\alpha/10)^3.$$

This may help to choose an appropriate  $v$ . For  $w=3$  the results are

$$E = -\alpha - 1.23(\alpha/10)^2 - 0.64(\alpha/10)^3 \dots, \\ v = 3 + 2.22(\alpha/10) + 1.97(\alpha/10)^2 \dots.$$

**EFFECTIVE MASS**

Another quantity of interest is the effective mass. If the particle moves with a mean group velocity  $V$ , its energy should be greater. For small  $V$  the energy goes as  $V^2$ , and writing it as  $mV^2/2$ , we call  $m$  the effective mass. Since there is an operator analogous to the momentum which commutes with the Hamiltonian, it would be expected that there is a variational principle which minimizes the energy for each momentum. That is, we ought to be able to extend our method to yield

<sup>7</sup> E. Haga, Progr. Theoret. Phys. (Japan) 11, 449 (1954).

an upper limit to the energy for each value of  $V$ , or better, of momentum  $Q$ . We have not found the expected extension.

If we limit ourselves just to finding the effective mass for low velocities, however, we may proceed in this manner: For a free particle of mass  $m$  whose initial coordinate is 0 and final coordinate is  $\mathbf{X}_T$  the sum on trajectories is

$$\exp(-mX_T^2/2T). \quad (40)$$

Hence we can study the effective mass for our system by studying the asymptotic form of (6) in the case  $\mathbf{X}_T \neq 0$ . The asymptotic form should vary for small  $\mathbf{X}_T$  as  $\exp(-E_0T - mX_T^2/2T)$ , its dependence on  $\mathbf{X}_T$  determining  $m$ . This only requires that (27) be solved for the boundary conditions  $\mathbf{X}'=0$  at  $t=0$  and  $\mathbf{X}'=\mathbf{X}_T$  at  $t=T$ . There are some confusing complications at the end points so it is easier to proceed as follows. We will put  $\mathbf{X}_T = \mathbf{U}T$  so that the propagation (40) is  $\exp(-\frac{1}{2}mU^2T)$ . [Note that  $\mathbf{U}$  is not a physical velocity because  $t$  is an artificial parameter in Eq. (5), and is not the time.] That is, we seek the total energy and equate it to  $E_0 + \frac{1}{2}mU^2$ . But if we substitute  $\mathbf{X}' = \mathbf{X}'' + \mathbf{U}t$  into (27), we see that it is a solution if  $\mathbf{X}''$  is. This  $\mathbf{X}''$  goes from 0 at  $t=0$  to 0 at  $t=T$ , and is therefore our previous solution. Such a substitution into (26) means that the term involving  $\mathbf{f}$  adds a term  $\exp(\int t \mathbf{U} \cdot \mathbf{f} dt)$  so that this is the factor by which  $I$  is multiplied, aside from normalization. For the  $\mathbf{f}$  given in (25) this is  $\exp[i\mathbf{K} \cdot \mathbf{U}(\tau - \sigma)]$  so that we now have

$$\langle \exp[i\mathbf{K} \cdot (\mathbf{X}_\tau - \mathbf{X}_\sigma)] \rangle = \exp \left[ -\frac{K^2}{2v^2} F(|\tau - \sigma|) + i\mathbf{K} \cdot \mathbf{U}(\tau - \sigma) \right], \quad (41)$$

where

$$F(\tau) = w^2\tau + \frac{v^2 - w^2}{v}(1 - e^{-v\tau}). \quad (42)$$

Substitution into (22) and (21) gives for  $A$  the value

$$A(\mathbf{U}) = 2^{-\frac{1}{2}}\alpha \int_0^\infty \int_0^\infty (2\pi^2 K^2)^{-1} e^{-\tau} \times \exp \left[ -\frac{K^2}{2v^2} F(\tau) + i\mathbf{K} \cdot \mathbf{U}\tau \right] d^3\mathbf{K} d\tau. \quad (43)$$

Second differentiation of (41) with respect to  $\mathbf{K}$  shows that

$$\langle (\mathbf{X}_t - \mathbf{X}_s)^2 \rangle = 3F(t-s)v^{-2} + U^2(t-s)^2,$$

so that one obtains for  $B$  the value

$$B = \frac{3C}{vw} + \frac{2C}{w^3} U^2.$$

We again find  $E_1$  from  $dE_1/dC = B/C$  and  $E_1 = \frac{1}{2}U^2$  for  $C=0$ . Thus

$$E_1 = \frac{3}{2}(v-w) + \frac{1}{2}U^2(1 + 4Cw^{-3}),$$

and our final expression is

$$E = \frac{1}{2}U^2 + (3/4v)(v-w)^2 - A(\mathbf{U}). \tag{44}$$

We next expand  $A(\mathbf{U})$  to order  $U^2$  and write the kinetic energy as  $mU^2/2$  to find, finally,

$$m = 1 + \frac{1}{3}\pi^{-\frac{1}{2}}\alpha v^3 \int_0^\infty [F(\tau)]^{-\frac{1}{2}} e^{-\tau} \tau^2 d\tau. \tag{45}$$

The values of the parameters to use in (45) are those which were previously found to minimize  $E$  when  $\mathbf{U}=0$ .

For small  $\alpha$  this gives

$$m = 1 + \frac{1}{8}\alpha + 0.025\alpha^2 + \dots \tag{46}$$

for  $w=3$ , while for  $w=1$  the 0.025 becomes 0.023. For large  $\alpha$  it becomes

$$m = 16\alpha^4/81\pi^4 = 202(\alpha/10)^4. \tag{47}$$

Our energy values, coming from a minimum principle, are much more accurate than the mass values, whose precision, especially for large  $\alpha$ , is hard to judge. Since (46) and (47) do not match well, intermediate values of  $\alpha$  require numerical integration of (45).

Lee and Pines<sup>6</sup> have worked with a different type of variational principle. It seems to be nearly as good as ours for  $\alpha$  less than about 5, but is poor for larger  $\alpha$  (for example, at  $\alpha=15$ , Lee and Pines find  $E_0 < -17.6$ , while we find  $E_0 < -26.8$ ). This appears to contradict their statement that their method is exact for large  $\alpha$ . They are referring to a different problem, however, in which the upper momenta are cut off. This means that in  $S$  in (7) the function  $|\mathbf{X}_t - \mathbf{X}_s|^{-1}$  is replaced by some other function  $V(|\mathbf{X}_t - \mathbf{X}_s|)$  which differs for small  $|\mathbf{X}_t - \mathbf{X}_s|$ . It is evident, for large  $\alpha$ , that the best trajectory will be the one that wanders only slightly and the energy will be  $2^{-\frac{1}{2}}\alpha V(0)$  in the limit. Their method gives this result in the limit, as ours would also. For the case where  $V$  is singular, so  $V(0)$  does not exist their method is not exact, and it is inaccurate for

for intermediate values of  $\alpha$  even if  $V(0)$  exists, if  $V$  has steep walls.

The method is readily extended to cases in which the photon frequencies are not constant, and the coupling is not just proportional to  $K^{-1}$ . The same trial action  $S_1$  can be used, but the integral for  $A$  becomes more complicated. For the Hamiltonian

$$H = \frac{1}{2}P^2 + \sum_K \omega_K a_{K^+} a_K + V^{-\frac{1}{2}} \sum_K [C_{K^*} a_{K^+} \exp(-i\mathbf{K} \cdot \mathbf{X}) + C_{K} a_K \exp(+i\mathbf{K} \cdot \mathbf{X})],$$

Eq. (33) still holds; the only change is that the integral for  $A$  becomes

$$A = \int \int_0^\infty \exp\left[-\omega_K \tau - \frac{K^2}{2v^2} F(\tau)\right] |C_K|^2 d\tau d^3\mathbf{K} (2\pi)^{-3},$$

where  $F(\tau)$  is given in (42).

An attempt has been made to apply this method to meson problems. The case of scalar nucleons interacting by scalar mesons seems tractable, but the greater complexity of the more realistic problems shows the need for further development.

We are limited in our choice of  $S_1$  to quadratic functionals, for those are the only ones we can evaluate directly as path integrals. It would be desirable to find out how this method may be expressed in conventional notation, for a wider class of trial functionals might thereby become available.

I am indebted to H. Fröhlich for bringing the problem to my attention, and for his comments on it, and to G. Speisman for emphasizing the importance of the general inequality (10).

*Note added in proof.*—Professor Fröhlich and Professor Pines have kindly informed me that S. I. Pekar [Zhur. Eksptl. i Teort. Fiz. **19**, 796 (1949)] has calculated the limiting values of energy and mass for large  $\alpha$ , by an adiabatic approximation. The energy is  $-0.1088\alpha^2$  and the mass is  $232(\alpha/10)^4$ . Therefore our variational method gives an error of only 3 percent in the energy and 15 percent in the mass for large  $\alpha$ , and presumably smaller errors for smaller  $\alpha$ .