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A Second Order Correction to Feynman's Path Integral Calculation of the Polaron Self-Energy.

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INTEGRAL CALCULATION OF THE POLARON SELF-
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A SECOND ORDER CORRECTION TO FEYNMAN'S PATH
INTEGRAL CALCULATION OF THE POLARON SELF-ENERGY

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
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in

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ABSTRACT

The second order term of a series expansion for the exact Feynman path integral expression for the polaron self-energy is calculated. For all values of the polaron coupling constant, the result yields a correction of less than two percent to Feynman's variational approximation of the polaron self-energy.

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CHAPTER 1

INTRODUCTION

The polaron problem is the study of the motion of a single electron introduced into the otherwise empty conduction band of a semi-conductive ionic crystal. The usual initial approach to the description of the motion of a conduction electron is the Bloch approximation¹ which assumes that the lattice ions are rigidly attached to their lattice sites. In this approximation, the electron moves under the influence of a spatially periodic static potential having the periodicity of the lattice with the result² that the electron, when moving slowly, moves as a free particle of mass, m , called the Bloch mass. However for an ionic crystal this approximation is inadequate, because the lattice ions are unshielded charges and are therefore sensitive to the presence of the conduction electron. Thus the conduction electron induces an appreciable displacement of the lattice ions from the static configuration assumed by the Bloch approximation. Then, in turn, the electron experiences, in addition to the static electric field accounted for in the Bloch approximation, the incremental electric field resulting from the displacement of the lattice ions from their lattice sites.

Fröhlich's³ Hamiltonian, derived in Appendix A, for describing this system involves several idealizations. The wave vector of the electron is presumed to be small compared to the reciprocal lattice spacings. According to this assumption, the electronic wave function will vary only slightly over the distance of many lattice spacings. Therefore the electron is regarded as moving under the influence of a continuous macroscopic polarization field, namely the average dipole moment per unit volume arising from the displacement of the ions from their lattice sites. As discussed in the derivation in Appendix A, the electron interacts predominately with the long wavelength longitudinal optical modes of the lattice. Finally the simplifying assumption is made that these modes all have a common frequency, ω . Therefore Fröhlich's Hamiltonian describes an idealized system consisting of the electron of Bloch mass, m , interacting with the macroscopic polarization field resulting from the long wavelength longitudinal optical modes of the crystal all of which are assumed to have a single frequency, ω . Fröhlich's Hamiltonian is given by

$$H(\alpha) = \frac{1}{2}P^2 + \sum_{\vec{v}} \frac{1}{v^2} (p_{\vec{v}}^2 + q_{\vec{v}}^2 - 1) + [8\sqrt{2}\pi\alpha/S]^{\frac{1}{2}} \cdot \sum_{\vec{v}} |\vec{v}|^{-1} q_{\vec{v}} \begin{cases} \cos(\vec{v} \cdot \vec{x}) \\ \sin(\vec{v} \cdot \vec{x}) \end{cases}, \quad (1)$$

where the cosine is used if $v_x > 0$, or if $v_x = 0$ and $v_y > 0$,

or if $v_x=0$, $v_y=0$, and $v_z \geq 0$ (otherwise the sine term is to be used), where $\tilde{x}$ and $\tilde{p}$ are the electron coordinate and momentum, and where $q_{\tilde{v}}$ and $p_{\tilde{v}}$ are polarization field oscillator coordinates and their corresponding conjugate momenta. The parameter α is a dimensionless coupling constant characteristic of the crystal ($\alpha \sim 1-4$ for alkali halides⁴) and S is the normalization volume. The limit $S \rightarrow \infty$ is to be taken with

$$\lim_{S \rightarrow \infty} \Sigma_{\tilde{v}} = S(2\pi)^{-3} \int d^3 \tilde{v}. \quad (2)$$

A natural system of units is employed in which $\hbar=\omega=m=1$.

The name "polaron" has been given to the entity consisting of the Bloch conduction electron together with its accompanying nonradiative polarization field. Accordingly, Fröhlich defines the polaron self-energy, $E_0(\alpha)$, as the least eigenvalue of $H(\alpha)$.

The polaron problem has been of long standing interest not just because it is pertinent to solid state physics, but also because it serves as a relatively uncomplicated prototype field-theoretical problem involving the interaction of a particle with its self-produced field. Because of this extended interest, the coupling constant, α , is regarded as an independent parameter. It is one of the aims of the research on the polaron problem to develop calculational methods which are accurate for all values of α , with the hope that such

methods may be used in dealing with the more complicated self-energy problems which arise in the theory of strong interactions.

The principal investigations of the polaron self-energy are described in a review paper by Allcock.⁵ For small values of coupling constant, α , the interaction term can be treated as perturbative with respect to the remainder of the Hamiltonian. The result is

$$E_0(\alpha) = -\alpha - a_c \alpha^2 + O^3(\alpha) \approx -\alpha - .01592 \alpha^2 + O^3(\alpha), \quad (3)$$

where

$$a_c = \ln(1 + 3\sqrt{2}/4) - 1/\sqrt{2}. \quad (4)$$

A weak coupling variational technique by Lee, Low, and Pines⁶ gives $(-\alpha)$ as an overestimate for all values of α . For large coupling, there are both underestimates⁷ and overestimates⁸⁻¹⁰ which establish that, for asymptotically large α , the self-energy is proportional to $-\alpha^2$.

Feynman¹¹ has developed a variational upper bound approximation to the polaron self-energy which yields the correct result to first order in α for weak coupling, agrees with the earlier upper bound approximations for strong coupling, and provides a smooth transitional behavior for intermediate coupling. Feynman's approach

is to obtain an exact explicit path integral expression for the self-energy and then to overestimate the result in a form which contains only a single ordinary integral which has to be done numerically.¹² This overestimate involves two variational parameters which are chosen to minimize the self-energy expression.

In this paper, an infinite series expansion for Feynman's exact self-energy expression is developed in such a way that Feynman's variational approximation for the self-energy is the sum of the zeroth and first order terms. It is the purpose of this work to calculate the second order term and thereby to obtain a refined evaluation of the polaron self-energy.

CHAPTER 2

EXACT EXPRESSION FOR THE POLARON SELF-ENERGY

To obtain Feynman's exact expression for the self-energy in terms of a Feynman path integral, one may begin by expressing the solution to the time dependent Schrödinger equation for the polaron Hamiltonian, given in Eq. (1), in the form

$$\Psi(\underline{x}, \underline{q}, t_f) = \int d^3 \underline{x}' \int d\underline{q}' K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', t_i=0) \cdot \Psi(\underline{x}', \underline{q}', t_i=0), \quad (5)$$

where the symbol, $\underline{q}$, represents the set of all polarization field oscillator coordinates, $\Psi(\underline{x}', \underline{q}', t_i=0)$ is the wavefunction at $t_i=0$, and $\Psi(\underline{x}, \underline{q}, t_f)$ is the solution at any later time, t_f . The function $K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', 0)$ is the kernel for the time development of the solution to the Schrödinger equation. The kernel is determined by the requirements

$$H(\alpha)K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', 0) = i\partial_{t_f} K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', 0) \quad (6)$$

and

$$\lim_{t_f \rightarrow 0^+} K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', 0) = \delta(\underline{x} - \underline{x}') \prod_{\underline{v}} \delta(\underline{q}_{\underline{v}} - \underline{q}'_{\underline{v}}). \quad (7)$$

It is well known that if $\psi_n(\underline{x}, \underline{q})$ represents a complete orthonormal set of eigenfunctions of the Hamiltonian operator with corresponding eigenvalues $E_n(\alpha)$, then

$$K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', 0) = \sum_n \psi_n(\underline{x}, \underline{q}) \psi_n^*(\underline{x}', \underline{q}') e^{-iE_n(\alpha)t_f}. \quad (8)$$

The kernel, K , can be alternatively expressed as a Feynman path integral:

$$K(\underline{x}, \underline{q}, t_f; \underline{x}', \underline{q}', 0) = \int_{\underline{x}', 0}^{\underline{x}, t_f} D\underline{x}(t) \int_{\underline{q}', 0}^{\underline{q}, t_f} D\underline{q}(t) e^{iS}, \quad (9)$$

where

$$S = \int_0^{t_f} L(\underline{x}, \dot{\underline{x}}, \underline{q}, \dot{\underline{q}}, t) dt, \quad (10)$$

where L is the polaron Lagrangian (obtained from Eq. (1) in the usual manner) given by

$$L(\underline{x}, \dot{\underline{x}}, \underline{q}, \dot{\underline{q}}, t) = \frac{1}{2} \dot{\underline{x}}^2 + \frac{1}{2} \sum_{\underline{v}} (\dot{\underline{q}}_{\underline{v}}^2 - \underline{q}_{\underline{v}}^2 + 1) - [8\sqrt{2}\pi\alpha/S]^{\frac{1}{2}} \cdot \sum_{\underline{v}} |\underline{v}|^{-1} \underline{q}_{\underline{v}} \begin{cases} \cos(\underline{v} \cdot \underline{x}) \\ \sin(\underline{v} \cdot \underline{x}) \end{cases}. \quad (11)$$

The notation

$$\int_{z_0, 0}^{z_f, t_f} f[z(t)] Dz(t) \quad (12)$$

denotes a single-fold Feynman path integral over paths, $z(t)$, satisfying the boundary conditions $z(0)=z_0$ and $z(t_f)=z_f$. This Feynman path integral is defined by the following set of operations: The interval $[0, t_f]$ is divided into N subintervals, each of length $\epsilon = t_f/N$.

Then

$$\int_{z_0, 0}^{z_f, t_f} f[z(t)] Dz(t) = \lim_{N \rightarrow \infty} \left[\frac{2\pi i t_f}{N} \right]^{\frac{1}{2}N} \int_{-\infty}^{+\infty} dz_1 \int_{-\infty}^{+\infty} dz_2 \cdots \int_{-\infty}^{+\infty} dz_{N-1} f[z(t)], \quad (13)$$

where

$$z(t) = \begin{cases} z_0 + \frac{z_1 - z_0}{\epsilon} [t - 0] & \text{for } 0 \leq t \leq \epsilon \\ z_1 + \frac{z_2 - z_1}{\epsilon} [t - \epsilon] & \text{for } \epsilon \leq t \leq 2\epsilon \\ \vdots & \\ z_{N-1} + \frac{z_N - z_{N-1}}{\epsilon} [t - (N-1)\epsilon] & \text{for } N\epsilon - \epsilon \leq t \leq N\epsilon. \end{cases} \quad (14)$$

In Eq. (9), the symbol, $D_{\tilde{x}}(t)$, denotes path integration over each of the three rectangular components of $\tilde{x}$, the integration over each component being performed in the manner just described.

The verification that Eq. (9) does represent the kernel for the time development of the solution to the Schrödinger equation requires showing that the path integral given by Eq. (9) satisfies Eqs. (6) and (7). This result is established by direct substitution of Eq. (9) into Eqs. (6) and (7) and by making use of the definition of derivative and path integral to perform the indicated operations.

A convenient exact expression for the polaron self-energy may be obtained in terms of K , namely

$$E_0(\alpha) = \lim_{T \rightarrow \infty} \{-T^{-1} \ln[G_{00}(-iT)]\}, \quad (15)$$

where, according to Eq. (8),

$$G_{00}(t_f) \equiv \prod_{\tilde{v}} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dq_{\tilde{v}} dq'_{\tilde{v}} \phi_0^*(q_{\tilde{v}}) \phi_0(q'_{\tilde{v}}) K(0, q, t_f; 0, q', 0) \quad (16)$$

$$= \sum_n a_n^*(0) a_n(0) e^{-iE_n(\alpha)t_f}, \quad (17)$$

wherein $\phi_0(q)$ represents the simple harmonic oscillator ground state function and

$$a_n(0) = \prod_{\tilde{v}} \int_{-\infty}^{+\infty} dq_{\tilde{v}} \psi_n(0, q) \phi_0^*(q_{\tilde{v}}). \quad (18)$$

The validity of Eq. (15) is apparent from Eq. (17), and its utility is that Eqs. (15) and (16) constitute a significantly simplifiable explicit procedure for calculating $E_0(\alpha)$. Simplification of Eq. (16) may be achieved by substituting into Eq. (16) the path integral expression for K given by Eqs. (9)-(11), by employing Eq. (13), and by actually performing all of the resultant integrations over oscillator coordinates. All of the integrals are of the standard type of an exponential of a quadratic form. (Path integrals of exponential functions of quadratic forms in coordinates and their time derivatives may be performed analytically.¹³⁾)

The result is

$$G_{00}(t_f) = \int_{0,0}^{0,t_f} e^{iS_{D\tilde{x}}(t)}, \quad (19)$$

where

$$S = \int_0^{t_f} \frac{1}{2} [d\tilde{x}(t)/dt]^2 dt + \alpha 8^{-1/2} \int_0^{t_f} \int_0^{t_f} e^{-i|t-s|} |\tilde{x}(t) - \tilde{x}(s)|^{-1} dt ds. \quad (20)$$

Substitution of Eq. (19) with (20) into Eq. (15) yields, upon the simple change, $-it \rightarrow t$, of integration variable,

$$E_0(\alpha) = -\lim_{T \rightarrow \infty} \{T^{-1} \ln[\int_{0,0}^{0,T} e^{-S_{D\tilde{x}}(t)}]\}, \quad (21)$$

where

$$S = \int_0^T \frac{1}{2} [d\tilde{x}(\tau)/d\tau]^2 d\tau - \alpha 8^{-1/2} \int_0^T \int_0^T e^{-|\tau-\sigma|} |\tilde{x}(\tau) - \tilde{x}(\sigma)|^{-1} d\tau d\sigma. \quad (22)$$

Equation (21) with (22) is Feynman's exact, explicit expression for the polaron self-energy. The first integrand of S may be regarded as the kinetic energy of a particle and the second as a time dependent Coulombic interaction of the particle at time τ with itself at time σ . The exponential reduces the interaction with a time constant of 1 ($1/\omega$ in ordinary units).

CHAPTER 3

FEYNMAN'S VARIATIONAL PRINCIPLE

Feynman has developed a variational principle¹¹ for obtaining an overestimate to the exact self-energy. The derivation of this principle involves the following definition of the path average of a function $f[\underline{x}(t)]$ of path:

$$\langle f[\underline{x}(t)] \rangle \equiv \frac{\int_{\underline{0},0}^{\underline{0},T} f[\underline{x}(t)] e^{-S'[\underline{x}(t)]} D\underline{x}(t)}{\int_{\underline{0},0}^{\underline{0},T} e^{-S'[\underline{x}(t)]} D\underline{x}(t)}, \quad (23)$$

where S' proports to approximate S and is chosen so that the path integral in the denominator can be performed. Comparison of Eq. (23) with Eq. (21) reveals that the denominator of Eq. (23) defines an approximate self-energy, $E'_0(\alpha)$, namely

$$E'_0(\alpha) = -\lim_{T \rightarrow \infty} \{T^{-1} \ln[\int_{\underline{0},0}^{\underline{0},T} e^{-S'[\underline{x}(t)]} D\underline{x}(t)]\}. \quad (24)$$

By adding and subtracting S' in the exponential in Eq. (21) and by using Eqs. (23) and (24), one can

write the exact self-energy expression, as given by Eq. (21), in the form,

$$E_0(\alpha) = E'_0(\alpha) + \lim_{T \rightarrow \infty} \{-T^{-1} \ln \langle e^{-\Delta S} \rangle\}, \quad (25)$$

where

$$\Delta S = S - S'. \quad (26)$$

Feynman's variational principle is based on the general property of real valued linear averaging functions that

$$\langle e^x \rangle \geq e^{\langle x \rangle}. \quad (27)$$

This result follows from the inequality

$$e^x \geq y(x), \quad (28)$$

where $y(x)$ is the tangent to e^x at the point $\langle x \rangle$. Since

$$y(x) = e^{\langle x \rangle} (x - \langle x \rangle) + e^{\langle x \rangle}, \quad (29)$$

then averaging both sides of Eq. (28) yields the desired inequality, Eq. (27). Use of Eq. (27) with Eq. (25) gives

$$E_0(\alpha) \leq E_F \equiv E'_0(\alpha) + \lim_{T \rightarrow \infty} \{T^{-1} \langle \Delta S \rangle\}, \quad (30)$$

where $E'_0(\alpha)$ is given by Eq. (24) and where $\langle \Delta S \rangle$ is to be evaluated in accordance with Eq. (23).

For S' , Feynman uses

$$S' = \int_0^T \frac{1}{2} [\dot{x}(\tau)]^2 d\tau + \frac{1}{2} C \int_0^T \int_0^T e^{-w|\tau-\sigma|} [x(\tau) - x(\sigma)]^2 d\tau d\sigma, \quad (31)$$

wherein C and w are variational parameters chosen to minimize the variational overestimate, E_F , in Eq. (30).

This choice for S' to approximate S replaces the Coulombic interaction of S with a simple harmonic interaction of adjustable strength, C , and replaces the unit time constant in S with an adjustable time constant $1/w$.

CHAPTER 4

CALCULATION OF THE POLARON SELF-ENERGY

A series expansion can be obtained for Feynman's exact self-energy expression by expanding the right side of Eq. (25) in powers of ΔS . The result is that

$$E_O(\alpha) = E_F + \Delta E_2 + O^3(\Delta S), \quad (32)$$

where E_F is Feynman's variational result given by Eq. (30) and where

$$\Delta E_2 = -\lim_{T \rightarrow \infty} \{ (2T)^{-1} \langle (\Delta S - \langle \Delta S \rangle)^2 \rangle \}, \quad (33)$$

wherein the angle brackets denote the path average defined by Eq. (23). For the purpose of reduction, Feynman's self-energy, given by Eq. (30), and the second order correction term, given by Eq. (33), may be written as

$$E_F = E_O'(\alpha) - \lim_{T \rightarrow \infty} B - \lim_{T \rightarrow \infty} A \quad (34)$$

and

$$\Delta E_2 = -\frac{1}{2} \lim_{T \rightarrow \infty} \frac{\langle V^2[\underline{x}(t)] \rangle - T^2 A^2}{T} - C \left[\frac{\partial}{\partial C} \right]_{T, \alpha, w} (2A+B) + B, \quad (35)$$

where $E'_0(\alpha)$ is specified by Eq. (24) with Eq. (31),

$$V[\underline{x}(t)] = -\alpha 8^{-\frac{1}{2}} \int_0^T \int_0^T e^{-|\tau-\sigma|} |\underline{x}(\tau) - \underline{x}(\sigma)|^{-1} d\tau d\sigma, \quad (36)$$

$$A = -\langle V[\underline{x}(t)] \rangle / T, \quad (37)$$

and

$$B = \frac{1}{2} C T^{-1} \int_0^T \int_0^T e^{-w|\tau-\sigma|} \langle [\underline{x}(\tau) - \underline{x}(\sigma)]^2 \rangle d\tau d\sigma. \quad (38)$$

In order to evaluate $\langle V^2[\underline{x}(t)] \rangle$, A , and B , it is convenient to introduce the generating function

$$W[\underline{f}(t)] \equiv \langle \exp \left\{ \int_0^T \underline{f}(t) \cdot \underline{x}(t) dt \right\} \rangle. \quad (39)$$

Then

$$A = \alpha 8^{-\frac{1}{2}} T^{-1} \int_0^T \int_0^T \int e^{-|\tau-\sigma|} (2\pi^2 k^2)^{-1} W[\underline{f}_{\underline{k}}(t)] d^3 \underline{k} d\tau d\sigma, \quad (40)$$

$$B = \frac{1}{2} C T^{-1} \int_0^T \int_0^T e^{-W|\tau-\sigma|} \{-\nabla_{\tilde{k}}^2 W[f_{\tilde{k}}(t)]\}_{\tilde{k}=0} d\tau d\sigma, \quad (41)$$

and

$$\begin{aligned} \langle V^2[\tilde{x}(t)] \rangle &= \alpha^2 8^{-1} T^2 \int_0^T \int_0^T \int_0^T \int_0^T \int \int e^{-|\tau-\sigma|} e^{-|\tau'-\sigma'|} \\ &\quad \cdot (2\pi^2 k^2)^{-1} (2\pi^2 k'^2)^{-1} W[f_{\tilde{k},\tilde{k}'}(t)] \\ &\quad \cdot d^3 \tilde{k} d^3 \tilde{k}' d\tau d\sigma d\tau' d\sigma', \end{aligned} \quad (42)$$

where

$$f_{\tilde{k}}(t) = i\tilde{k}[\delta(t-\tau) - \delta(t-\sigma)] \quad (43)$$

and

$$f_{\tilde{k},\tilde{k}'}(t) = i\tilde{k}[\delta(t-\tau) - \delta(t-\sigma)] + i\tilde{k}'[\delta(t-\tau') - \delta(t-\sigma')]. \quad (44)$$

A workable form for W is needed in order to simplify Eqs. (40)-(42). Combining Eq. (39) with Eq. (23) gives

$$W[\underline{f}(t)] = \frac{\int_{0,0}^{0,T} \exp\{\int_0^T \underline{f}(t) \cdot \underline{x}(t) dt - S'\} D\underline{x}(t)}{\int_{0,0}^{0,T} e^{-S'} D\underline{x}(t)}, \quad (45)$$

where S' , given by Eq. (31), is repeated here for ease of reference:

$$S' = \int_0^T \frac{1}{2} [\underline{dx}(t)/dt]^2 dt + \frac{1}{2} C \int_0^T \int_0^T e^{-w|\tau-\sigma|} [\underline{x}(\tau) - \underline{x}(\sigma)]^2 d\tau d\sigma. \quad (46)$$

The desired simplification can be accomplished by changing the path integration variable $\underline{x}(t)$ in the numerator of Eq. (45) to a new variable $\underline{y}(t) = \underline{x}(t) - \underline{x}'(t)$, where $\underline{x}'(t)$ is that path for which the exponent in the numerator of Eq. (45) is extremal and for which $\underline{x}'(0) = \underline{x}'(T) = 0$. The resultant numerator contains the denominator as a factor, with the immediate outcome that

$$W[\underline{f}(t)] = \exp\left\{-\int_0^T \frac{1}{2} [\underline{dx}'(t)/dt]^2 dt - \frac{1}{2} C \int_0^T \int_0^T e^{-w|t-\sigma|} \cdot [\underline{x}'(t) - \underline{x}'(\sigma)]^2 dt d\sigma + \int_0^T \underline{f}(t) \cdot \underline{x}'(t) dt\right\}.$$

To find $\underline{x}(t)$, such that the exponent of the numerator of Eq. (45) is extremal, one may set to zero the functional derivative of that exponent with respect to each rectangular component, $x_i(t)$, of $\underline{x}(t)$. The equation for the extremizing path, $\underline{x}'(t)$, obtained in this manner is

$$d^2 \underline{x}'_i(t)/dt^2 = 2C \int_0^T e^{-w|t-\sigma|} [\underline{x}'_i(t) - \underline{x}'_i(\sigma)] d\sigma - f_i(t), \quad (48)$$

where $f_i(t)$ is the i th rectangular component of $\underline{f}(t)$. Equations (47) and (48) may be combined to yield

$$W[\underline{f}(t)] = \exp\left\{\frac{1}{2} \int_0^T \underline{x}'(t) \cdot \underline{f}(t) dt\right\}. \quad (49)$$

The solution for $\underline{x}'(t)$ of Eq. (48), subject to the boundary conditions $\underline{x}'(0) = \underline{x}'(T) = 0$, is obtained in Appendix B. The result is that (apart from transient terms which are appreciable only near $t=0$ and $t=T$ and which, in the required limit $T \rightarrow \infty$, will be irrelevant to the desired evaluation of Eqs. (40)-(42))

$$\underline{x}'(t) = -(2v^2)^{-1} \int_0^T F(|t-t'|) \underline{f}(t') dt', \quad (50)$$

where, in the limit $T \rightarrow \infty$,

$$F(t) = (v^2 - w^2)v^{-1}[1 - e^{-vt}] + w^2t, \quad (51)$$

wherein

$$v = [w^2 + (4C/w)]^{\frac{1}{2}}. \quad (52)$$

In obtaining this result, use has been made of the property of $\tilde{f}_{\tilde{k}}(t)$ and $\tilde{f}_{\tilde{k},\tilde{k}'}(t)$ that the integral over t of $\tilde{f}_{\tilde{k}}(t)$ from $t=0$ to $t=T$ vanishes. Once Eqs. (49)-(52) with Eqs. (43) and (44) are used in Eqs. (40)-(42), then the $\tilde{k}$ -integrations in A and $\langle V^2[\tilde{x},(t)] \rangle$ can be performed, and both of the integrations for B can be done. The results are given below in a form useful for evaluating E_F and ΔE_2 as given by Eqs. (34) and (35):

$$A = \alpha v (2\sqrt{\pi}T)^{-1} \int_0^T \int_0^T e^{-|\tau-\sigma|} F^{-\frac{1}{2}}(|\tau-\sigma|) d\tau d\sigma, \quad (53)$$

$$\lim_{T \rightarrow \infty} B = 3C(wv)^{-1}, \quad (54)$$

and

$$\begin{aligned} \frac{\langle V^2[\tilde{x}(t)] \rangle - T^2 A^2}{T} &= \alpha^2 v^2 (4\pi T)^{-1} \int_0^T \int_0^T \int_0^T \int_0^T e^{-|\tau-\sigma|} \\ &\quad \cdot e^{-|\tau'-\sigma'|} [F(|\tau-\sigma|) F(|\tau'-\sigma'|)]^{-\frac{1}{2}} \\ &\quad \cdot (Q^{-1} \arcsin(Q) - 1) d\tau d\sigma d\tau' d\sigma', \end{aligned} \quad (55)$$

where

$$Q = \frac{\{F(|\tau-\tau'|) - F(|\tau-\sigma'|) - F(|\sigma-\tau'|) + F(|\sigma-\sigma'|)\}}{2[F(|\tau-\sigma|)F(|\tau'-\sigma'|)]^{\frac{1}{2}}}. \quad (56)$$

The quantity, $E'_O(\alpha)$, occurring in Eq. (34) can be obtained by differentiating both sides of Eq. (24) with respect to the parameter C , with w held constant, and by using Eqs. (31) and (38) to get

$$C \frac{\partial}{\partial C} \Big|_W E'_O(\alpha) = \lim_{T \rightarrow \infty} B = 3C(wv)^{-1}, \quad (57)$$

wherein Eq. (54) has been employed. Use of Eq. (52) and the boundary condition that $C=0$ corresponds to the free particle case, $E'_O(0)=0$, gives

$$E'_O(\alpha) = 3(v-w)/2. \quad (58)$$

In Appendix C, reductions are made of Eqs. (53), (55), and (56). If the results are substituted, along with Eqs. (54) and (58), into Eqs. (34) and (35), then expressions can be obtained for Feynman's variational approximation, E_F , and the second order correction term, ΔE_2 , in the following summary form:

$$E_F = 3(v-w)^2 (4v)^{-1} - 2\alpha v \pi^{-\frac{1}{2}} \int_0^{\infty} \rho \exp(-\rho^2) F^{-\frac{1}{2}}(\rho^2) d\rho$$

(59)

and

$$\begin{aligned} \Delta E_2 = & -4\alpha^2 v^2 \pi^{-1} I + \alpha v^{-1} (v^2 - w^2) \pi^{-\frac{1}{2}} \int_0^{\infty} \rho \exp(-\rho^2) \\ & \cdot F^{-\frac{1}{2}}(\rho^2) d\rho - (3/16) (v^2 - w^2)^2 v^{-3} - \frac{1}{2} \alpha (v^2 - w^2) \pi^{-\frac{1}{2}} \\ & \cdot \int_0^{\infty} \rho \exp(-\rho^2) F^{-3/2}(\rho^2) \{ (1 + w^2 v^{-2}) [1 - \exp(-v \rho^2)] \\ & + (v^2 - w^2) v^{-1} \rho^2 \exp(-v \rho^2) \} d\rho, \end{aligned} \quad (60)$$

where

$$\begin{aligned} I = & \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} [\rho_1 \exp(-\rho_1^2) F^{-\frac{1}{2}}(\rho_1^2)] [\rho_2 \exp(-\rho_2^2) \cdot F^{-\frac{1}{2}}(\rho_2^2)] \\ & \cdot [Q^{-1} \arcsin(Q) - 1] d\rho_1 d\rho_2 d\rho_3, \end{aligned} \quad (61)$$

with

$$Q = \begin{cases} Q_1 & \text{for } \rho_3 - \rho_2^2 + \rho_1^2 \geq 0 \text{ and } \rho_3 - \rho_2^2 \geq 0 \\ Q_2 & \text{for } \rho_3 - \rho_2^2 + \rho_1^2 \geq 0 \text{ and } \rho_3 - \rho_2^2 < 0 \\ Q_3 & \text{for } \rho_3 - \rho_2^2 + \rho_1^2 < 0 \text{ and } \rho_3 - \rho_2^2 < 0, \end{cases} \quad (62)$$

wherein

$$Q_1 = \frac{1}{2} F^{-\frac{1}{2}}(\rho_1^2) F^{-\frac{1}{2}}(\rho_2^2) (v^2 - w^2) v^{-1} \exp(-v\rho_3) \\ \cdot [1 - \exp(-v\rho_1^2)] [\exp(v\rho_2^2) - 1], \quad (63)$$

$$Q_2 = \frac{1}{2} F^{-\frac{1}{2}}(\rho_1^2) F^{-\frac{1}{2}}(\rho_2^2) \mathbb{I} (v^2 - w^2) v^{-1} \{ \exp[-v(\rho_2^2 - \rho_3)] \\ - \exp(-v\rho_3) [1 + \exp[-v(\rho_1^2 - \rho_2^2)] - \exp(-v\rho_1^2)] \} \\ - 2w^2 (\rho_2^2 - \rho_3) \mathbb{I}, \quad (64)$$

and

$$Q_3 = -\frac{1}{2} F^{-\frac{1}{2}}(\rho_1^2) F^{-\frac{1}{2}}(\rho_2^2) \mathbb{I} (v^2 - w^2) v^{-1} \{ \exp(-v\rho_3) \\ \cdot [1 - \exp(-v\rho_1^2)] + \exp[-v(\rho_2^2 - \rho_3)] [\exp(v\rho_1^2) - 1] \} \\ + 2w^2 \rho_1^2 \mathbb{I}. \quad (65)$$

CHAPTER 5

RESULTS

Although the integrals in Eqs. (59)-(61) must be evaluated numerically, weak and strong coupling expansions can be obtained for them. The weak coupling results, obtained in Appendix D, are that

$$E_F = -\alpha - (1/81)\alpha^2 + O^3(\alpha) \approx -\alpha - .01235\alpha^2 + O^3(\alpha), \quad (66)$$

and that the corrected energy, E_C , is given by

$$E_C \equiv E_F + \Delta E_2 = -\alpha - a_C \alpha^2 + O^3(\alpha) \approx -\alpha - .01592\alpha^2 + O^3(\alpha), \quad (67)$$

where

$$a_C = \ln(1 + 3\sqrt{2}/4) - 1/\sqrt{2}. \quad (68)$$

This corrected energy expression, E_C , is identical with the result of the fourth order perturbation expansion, which is exact to second order in α . The strong coupling results, obtained in Appendix E, are that

$$E_F = -(3\pi)^{-1} \alpha^{2+0^0}(\alpha) \approx -.1061 \alpha^{2+0^0}(\alpha) \quad (69)$$

and that the corrected energy is

$$E_C = -b_C \alpha^{2+0^0}(\alpha) \approx -.1078 \alpha^{2+0^0}(\alpha), \quad (70)$$

where

$$b_C = (4\pi)^{-1} + 2\pi^{-1} \sum_{n=1}^{\infty} \{ (2n)! / [2^{4n} (n!)^2 n(2n+1)] \}. \quad (71)$$

This refinement amounts to only a 1.6 percent correction to Feynman's strong coupling result for the self-energy.

For intermediate values of α , computer programs were written to calculate the integrals in Feynman's variational expression, given by Eq. (59), and in the second order correction term, given by Eqs. (60)-(65). The numerical calculations are discussed in Appendix F. The optimal values obtained for the variational parameters, v and w , differ slightly from those reported by Schultz¹² and are given in Table I accurately to four significant digits. For the values of v and w reported in Table I, Feynman's self-energy, its second order correction, the corrected value, and the percentage correction were calculated and are all given in Table I accurately to within an uncertainty of at most ± 1 in the least significant digit reported.

TABLE I

α	v	w	E_F	ΔE_2	E_C	%correction to E_F
1	3.110	2.871	-1.01	-.0035	-1.02	.35
3	3.421	2.560	-3.13	-.031	-3.16	1.0
5	4.034	2.140	-5.44	-.083	-5.52	1.5
7	5.810	1.604	-8.11	-.13	-8.24	1.6
9	9.850	1.282	-11.5	-.17	-11.7	1.4
11	15.41	1.162	-15.7	-.22	-15.9	1.4
15	30.08	1.076	-26.7	-.39	-27.1	1.5

In conclusion, the second order correction term represents less than a two percent correction to Feynman's variational answer for all values of α . This conclusion is suggestive that further corrections to the self-energy would be rather insignificant.

APPENDIX A

DERIVATION OF THE POLARON HAMILTONIAN

Consider the motion of a single conduction electron of mass M_{el} introduced into a semi-conductive ionic crystal lattice which is otherwise free from conduction electrons. If only electrostatic interactions are considered, the total energy of the electron, located at $\tilde{x}$, is

$$E = p_{el}^2 / (2M_{el}) + V_{total}(\tilde{x}), \quad (A1)$$

where p_{el} is the momentum of the electron and $V_{total}(\tilde{x})$ is the potential energy of the electron due to all the ions of the lattice. If $V_B(\tilde{x})$ represents the value $V_{total}(\tilde{x})$ would have if all the ions were at rest at their lattice sites, then Eq. (A1) can be written as

$$E = p_{el}^2 / (2M_{el}) + V_B(\tilde{x}) + \Delta V(\tilde{x}), \quad (A2)$$

where

$$\Delta V(\tilde{x}) = V_{total}(\tilde{x}) - V_B(\tilde{x}). \quad (A3)$$

The Bloch approximation,¹ that all the ions are rigidly attached to their lattice sites, implies that $\Delta V(\underline{x})=0$. The result of this approximation is that, measured from the bottom of the conduction band,

$$E \equiv E_{\underline{k}} = (\hbar \underline{k})^2 / (2m), \quad (\text{A4})$$

where m is a constant called the Bloch mass and where $\underline{k}$ is the wave vector of the electron. Equation (A4) is valid only for wave vector, $\underline{k}$, small relative to the reciprocal lattice spacings.

In developing a Hamiltonian operator for this system, Fröhlich³ postulates that the result, Eq. (A4), of the Bloch approximation can be improved upon by simply adding onto Eq. (A4) the term $\Delta V(\underline{x})$, which is neglected in the beginning of the Bloch treatment. Then

$$E_{\underline{k}} = (\hbar \underline{k})^2 / (2m) + \Delta V(\underline{x}), \quad (\text{A5})$$

where $\Delta V(\underline{x})$ is given by Eq. (A3). The contribution of the i th lattice site to the difference, $\Delta V(\underline{x})$, is just the difference between the energy of the electron due to the i th ion when displaced from its lattice site and the energy of the electron due to the i th ion when fixed at its lattice site. For ion displacements small compared to the lattice spacings, this contribution has the

form of the product of the electronic charge, e , and the electrostatic potential due to an electric dipole at the i th lattice site.

The conduction electron will deform the ions in addition to displacing them from their lattice sites. However, the relaxation time for this ionic deformation is short compared to that of the displacement field so that, for a slowly moving electron, the deformation field relaxes much more quickly toward the spherically symmetrical configuration it would have if the electron were at rest. Since a spherically symmetrical field cannot exert a force on the electron, the effect upon the electron of the deformation field is negligible compared to that of the displacement field.

Since k is required to be small relative to the reciprocal lattice spacing, the wave function for the Bloch electron will vary slowly over the distance of many lattice spacings. Therefore the medium can be regarded as continuous, with the result that the electric field due to the lattice can be described by a macroscopic continuous polarization field, $\vec{P}_{\text{total}}(\vec{r})$.

According to the definition of the electric displacement, $\vec{D}(\vec{r})$, the polarization field is related to the total electric field intensity, $\vec{E}(\vec{r})$, by

$$\vec{E}(\vec{r}) = \vec{D}(\vec{r}) - 4\pi\vec{P}_{\text{total}}(\vec{r}). \quad (\text{A6})$$

Therefore, $[-4\pi\tilde{P}_{\text{total}}(\tilde{r})]$ is the contribution made by the medium to the total electric field intensity. Since the polarization field, $\tilde{P}(\tilde{x})$, due to ionic displacement accounts for the major force acting on the Bloch electron, the equation of motion of the electron is

$$m\ddot{\tilde{x}} = e[-4\pi\tilde{P}(\tilde{x})]. \quad (\text{A7})$$

Since the charge of the electron is the only free charge present, then the electric displacement can arise only from the electron. Therefore

$$\tilde{D}(\tilde{r}) = -\partial_{\tilde{r}} e/|\tilde{r}-\tilde{x}|, \quad (\text{A8})$$

and the potential energy, E_I , of interaction between the electron and the electric field, $[-4\pi\tilde{P}(\tilde{r})]$, due to polarization is given by

$$\begin{aligned} E_I &= (4\pi)^{-1} \int \tilde{D}(\tilde{r}) \cdot [-4\pi\tilde{P}(\tilde{r})] d^3\tilde{r} \\ &= -\int \tilde{D}(\tilde{r}) \cdot \tilde{P}(\tilde{r}) d^3\tilde{r}. \end{aligned} \quad (\text{A9})$$

It is useful to make the observation that there is no contribution to E_I from the transverse part, $\tilde{P}_t(\tilde{r})$, of the polarization field. This result is easily shown by substituting the right side of Eq. (A8) into Eq. (A9)

and performing the resultant integration for the transverse part, $\tilde{P}_t(\underline{r})$, of $\tilde{P}(\underline{r})$ by writing it as the sum of two integrals, one of which is converted into a surface integral which vanishes and the other of which contains the divergence of a transverse vector field which always vanishes.

The electron therefore interacts only with the polarization field resulting from the longitudinal modes of the lattice of which there are generally two kinds, the acoustical-like modes and the optical-like modes. For an acoustical mode of a given wavelength, all the ions within the region between two successive nodal planes are displaced in the same direction. Therefore, since adjacent ions are oppositely charged, the resulting adjacent dipoles within such a region cancel extensively and are neglected. For an optical mode, the ions between successive nodal planes are displaced in opposite directions and therefore produce adjacent dipole moments which add constructively. The resultant polarization is relatively large, especially for the long wavelength optical modes.

The conclusion of this discussion of modes is that only the longitudinal optical modes, and of them especially those of long wavelength, significantly interact with the electron. This is a simplifying result because these modes have a vibrational frequency, ω , which is

approximately constant. Consequently, in the absence of interaction with the electron, the polarization field, $\underline{\underline{P}}(\underline{\underline{r}})$, resulting from the long wavelength longitudinal optical modes would obey the equation of motion,

$$\ddot{\underline{\underline{P}}}(\underline{\underline{r}}) + \omega^2 \underline{\underline{P}}(\underline{\underline{r}}) = 0. \quad (\text{A10})$$

This equation of motion can be derived from the Lagrangian

$$L_0(\underline{\underline{P}}, \dot{\underline{\underline{P}}}) = \frac{1}{2}\mu \int [\dot{\underline{\underline{P}}}^2(\underline{\underline{r}}) - \omega^2 \underline{\underline{P}}^2(\underline{\underline{r}})] d^3 \underline{\underline{r}}, \quad (\text{A11})$$

where μ is an undetermined constant. According to Eq. (A9), if a given electric displacement field, $\underline{\underline{D}}(\underline{\underline{r}})$, is present, then the Lagrangian would be

$$L(\underline{\underline{P}}, \dot{\underline{\underline{P}}}) = L_0(\underline{\underline{P}}, \dot{\underline{\underline{P}}}) + \int \underline{\underline{P}}(\underline{\underline{r}}) \cdot \underline{\underline{D}}(\underline{\underline{r}}) d^3 \underline{\underline{r}}. \quad (\text{A12})$$

The equation of motion resulting from (A12) would be

$$\ddot{\underline{\underline{P}}}(\underline{\underline{r}}) + \omega^2 \underline{\underline{P}}(\underline{\underline{r}}) = \mu^{-1} \underline{\underline{D}}(\underline{\underline{r}}). \quad (\text{A13})$$

The associated constant, μ , can now be determined in terms of empirical constants associated with the ionic medium as follows: The total polarization field, $\underline{\underline{P}}_{\text{total}}$, can be written as

$$\underline{\underline{P}}_{\text{total}} = \underline{\underline{P}} + \underline{\underline{P}}', \quad (\text{A14})$$

where $\tilde{P}$ represents the field due to ionic displacement and $\tilde{P}'$ is the field due to deformation of the ions.

If a static electric field is applied to the medium, then by definition of the static dielectric constant, ϵ ,

$$4\pi\tilde{P}_{\text{total}} = [1 - (1/\epsilon)]\tilde{D}_S, \quad (\text{A15})$$

where $\tilde{D}_S$ is the static electric displacement field. It is known empirically that the natural frequency, ω , of the long wavelength longitudinal optical modes is in the infrared region and that the natural frequency, ω' , of $\tilde{P}'$ is in the ultraviolet region. If an alternating field whose frequency lies in the visible region is applied to the medium, the field due to the displacement of ions will be negligible because the ions simply cannot follow the applied field. However, the ionic deformation can easily follow this field in the same way it would for a static applied field. Therefore, in a static applied field,

$$4\pi\tilde{P}' = [1 - (1/\epsilon_\infty)]\tilde{D}_S, \quad (\text{A16})$$

where ϵ_∞ is the dielectric constant measured in the visible region. Subtraction of Eq. (A16) from (A15) gives

$$4\pi\tilde{P} = [(1/\epsilon_\infty) - (1/\epsilon)]\tilde{D}_S. \quad (\text{A17})$$

Comparison of this result with Eq. (A13) for the static case $\underline{D} = \underline{D}_s$ and $\underline{P} = 0$ yields

$$\frac{1}{\mu} = \frac{\omega^2}{4\pi} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon} \right). \quad (\text{A18})$$

The total Lagrangian, L , for the electron, the long wavelength longitudinal optical modes, and the interaction between them can be obtained by combining the kinetic energy of the electron with Eq. (A12) to get

$$\begin{aligned} L(\underline{x}, \dot{\underline{x}}, \underline{P}, \dot{\underline{P}}) = & \frac{1}{2} m \dot{\underline{x}}^2 + \frac{1}{2} \mu \int [\dot{\underline{P}}^2(\underline{r}) - \omega^2 \underline{P}^2(\underline{r})] d^3 \underline{r} \\ & + \int \underline{P}(\underline{r}) \cdot \underline{D}(\underline{r}) d^3 \underline{r}, \end{aligned} \quad (\text{A19})$$

where $\underline{P}$ is the polarization field due to the long wavelength longitudinal optical modes of frequency ω , which has been assumed to be constant, $\underline{x}$ is the electron coordinate, m is the Bloch mass, μ is given by Eq. (A18), and $\underline{D}(\underline{r})$ is given by Eq. (A8).

Subject to periodic boundary conditions, the (longitudinal) polarization field, $\underline{P}(\underline{r})$, can be expressed as

$$\underline{P}(\underline{r}, t) = [2(\mu S)^{-1}]^{\frac{1}{2}} \sum_{\underline{v}} (\underline{v}/|\underline{v}|) q_{\underline{v}}(t) \begin{cases} \cos(\underline{v} \cdot \underline{r}) \\ \sin(\underline{v} \cdot \underline{r}) \end{cases}, \quad (\text{A20})$$

where each rectangular component, v_i , of $\underline{v}$ can assume the values

$$v_i = n \frac{2\pi}{\sqrt{S}}, \quad (A21)$$

wherein $n=0, \pm 1, \pm 2, \dots$ and S is the normalization volume. In Eq. (A20) the cosine term is to be used if $v_x > 0$, or if $v_x = 0$ and $v_y > 0$, or if $v_x = 0$, $v_y = 0$, and $v_z > 0$. Otherwise the sine term is to be used. Substituting Eq. (A20) into Eq. (A19) and performing the integration over $\underline{r}$, one has

$$L = \frac{1}{2} m \dot{\underline{x}}^2 + \frac{1}{2} \sum_{\underline{v}} (\dot{q}_{\underline{v}}^2 - \omega^2 q_{\underline{v}}^2) - [8\sqrt{2}\pi\alpha/S]^{\frac{1}{2}} \cdot \sum_{\underline{v}} |\underline{v}|^{-1} q_{\underline{v}} \begin{cases} \cos(\underline{v} \cdot \underline{x}) \\ \sin(\underline{v} \cdot \underline{x}) \end{cases}, \quad (A22)$$

where

$$\alpha = \frac{e^2}{2} \frac{1}{\hbar\omega} \cdot \frac{2m\omega}{\hbar} \left(\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon} \right) \quad (A23)$$

is a dimensionless constant, called the polaron coupling constant. The Hamiltonian is obtained by the usual prescription,

$$H = p_{el} \dot{\underline{x}} + \sum_{\underline{v}} p_{\underline{v}} \dot{q}_{\underline{v}} - L,$$

where

$$p_{el} = \frac{\partial L}{\partial \dot{\underline{x}}} = m \dot{\underline{x}} \quad (A24)$$

and

$$p_{\vec{v}} = \frac{\partial L}{\partial \dot{q}_{\vec{v}}} = \dot{q}_{\vec{v}}. \quad (\text{A25})$$

The result is

$$H = \frac{1}{2} p_{el}^2 + \sum_{\vec{v}} \frac{1}{2} (p_{\vec{v}}^2 + q_{\vec{v}}^2) + [8\sqrt{2}\pi\alpha/S]^{\frac{1}{2}} \cdot \sum_{\vec{v}} |\vec{v}|^{-1} q_{\vec{v}} \begin{cases} \cos(\vec{v} \cdot \vec{x}) \\ \sin(\vec{v} \cdot \vec{x}) \end{cases}. \quad (\text{A26})$$

The classical Hamiltonian can be made into the quantum mechanical Hamiltonian operator by interpreting $\vec{x}$, p_{el} , $q_{\vec{v}}$, $p_{\vec{v}}$ as operators subject to the usual commutation relation for position operators and conjugate momentum operators. The result is given below in a system of units in which $m=\omega=\hbar=1$:

$$H = \frac{1}{2} p_{el}^2 + \sum_{\vec{v}} \frac{1}{2} (p_{\vec{v}}^2 + q_{\vec{v}}^2 - 1) + [8\sqrt{2}\pi\alpha/S]^{\frac{1}{2}} \cdot \sum_{\vec{v}} |\vec{v}|^{-1} q_{\vec{v}} \begin{cases} \cos(\vec{v} \cdot \vec{x}) \\ \sin(\vec{v} \cdot \vec{x}) \end{cases}. \quad (\text{A27})$$

As indicated by the "-1" in the second term of Eq. (A27), the energy eigenvalues of H are measured relative to the zero point energy of the polarization field.

To avoid complication which would arise in a description of the motion of the electron in a finite crystal, the limit $S \rightarrow \infty$ is to be taken with

$$\lim_{S \rightarrow \infty} \Sigma_{\tilde{v}} = (2\pi)^{-3} S \int d^3 \tilde{v}. \quad (\text{A28})$$

APPENDIX B

SOLUTION FOR THE PATH OF LEAST ENERGY

The equations

$$\ddot{x}(t) = 2C \int_0^T [x(t) - x(s)] e^{-w|t-s|} ds - f(t) \quad (B1)$$

and

$$x(0) = x(T) = 0, \quad (B2)$$

where C , w , and T are positive constants such that $T \gg w^{-1}$ and where $f(t)$ is any function for which

$$\int_0^T f(t) dt = 0, \quad (B3)$$

are to be solved for $x(t)$ only for values of t such that

$$w^{-1} \ll t \ll T - w^{-1}. \quad (B4)$$

By the Fourier integral transform identity, the functions $x(t)$ and $f(t)$, regarded as vanishing outside the interval $[0, T]$, may be expressed as

$$x(t) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} y(\omega) e^{-i\omega t} d\omega \quad (B5)$$

and

$$f(t) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} g(\omega) e^{-i\omega t} d\omega, \quad (B6)$$

where

$$y(\omega) = (2\pi)^{-\frac{1}{2}} \int_0^T x(t) e^{i\omega t} dt \quad (B7)$$

and

$$g(\omega) = (2\pi)^{-\frac{1}{2}} \int_0^T f(t) e^{i\omega t} dt. \quad (B8)$$

Substitution of Eqs. (B5) and (B6) into Eq. (B1) gives

$$\begin{aligned} \ddot{x}(t) &= -(2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} y(\omega) \omega^2 e^{-i\omega t} d\omega \\ &= +(2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} y(\omega) \omega^2 (v^2 - \omega^2) (\omega^2 + \omega^2)^{-1} e^{-i\omega t} d\omega \\ &\quad - (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} g(\omega) e^{-i\omega t} d\omega \\ &\quad - \frac{(2C)}{(2\pi)^{\frac{1}{2}}} e^{-\omega t} \int_{-\infty}^{+\infty} y(\omega) \left\{ \frac{e^{-i\omega t}}{\omega} - \frac{1}{(\omega - i\omega)} \right\} d\omega \\ &\quad - \frac{(2C)}{(2\pi)^{\frac{1}{2}}} e^{-\omega(T-t)} \int_{-\infty}^{+\infty} y(\omega) \left\{ \frac{e^{-i\omega t}}{\omega} - \frac{e^{-i\omega T}}{(\omega + i\omega)} \right\} d\omega, \end{aligned} \quad (B9)$$

where

$$v \equiv [w^2 + (4C/w)]^{1/2}. \quad (B10)$$

The last two terms of Eq. (B9) are transient terms, which may be neglected in view of the extreme inequality (B4). Equation (B9) is then equivalent to the requirement that

$$\omega^2 (\omega^2 + v^2) y(\omega) = (\omega^2 + w^2) g(\omega). \quad (B11)$$

In view of Eqs. (B3) and (B8), $g(0)=0$. Therefore, Eq. (B11) is satisfied for $\omega=0$. For $\omega \neq 0$, Eq. (B11) may be solved for $y(\omega)$. Substitution of this result into Eq. (B5) and use of Eq. (B8) gives

$$\begin{aligned} x(t) = \lim_{\epsilon \rightarrow 0} \{ & \int_0^T f(t') dt' (2\pi)^{-1} [\left(\int_{-\infty}^{-\epsilon} + \int_{+\epsilon}^{+\infty} \right) (w^2 + \omega^2) \\ & \cdot \omega^{-2} (v^2 + \omega^2)^{-1} e^{i\omega(t'-t)} d\omega] \\ & + (2\pi)^{-1/2} \int_{-\epsilon}^{+\epsilon} y(\omega) e^{-i\omega t} d\omega \} \end{aligned} \quad (B12)$$

$$\begin{aligned} = \lim_{\epsilon \rightarrow 0} \{ & \int_0^T f(t') dt' (2\pi)^{-1} [(2\pi i) (v^2 - w^2) (2iv^3)^{-1} \\ & \cdot e^{-v|t-t'|} + 2w^2 (\epsilon v^2)^{-1} - w^2 v^{-2} |t-t'| \pi] \\ & + (2\epsilon) (2\pi)^{-1} \int_0^T x(t) dt \} \end{aligned} \quad (B13)$$

$$\begin{aligned} = - (2v^2)^{-1} \int_0^T f(t') F(|t-t'|) dt', \end{aligned} \quad (B14)$$

where

$$F(t) = (v^2 - w^2)v^{-1}[1 - e^{-vt}] + w^2t. \quad (B15)$$

Equation (B14) with Eq. (B15) constitutes the desired result. In obtaining Eq. (B13), use was made of Eq. (B7) and the method of contour integration. Equation (B3) was used in getting Eq. (B14).

APPENDIX C

MATHEMATICAL REDUCTIONS

It is desired to reduce the integrals contained in Eqs. (53) and (55). Consider first the right side of Eq. (53), which can be written as

$$A = \alpha v (2\sqrt{\pi}T)^{-1} \left\{ 2 \int_0^T d\tau \int_0^\tau d\sigma e^{-(\tau-\sigma)} F^{-\frac{1}{2}}(\tau-\sigma) \right\}, \quad (C1)$$

where $F(t)$ is given by

$$F(t) = (v^2 - w^2)v^{-1} [1 - e^{-vt}] + w^2 t. \quad (C2)$$

To write Eq. (53) in the form of Eq. (C1), use has been made of the invariance of the integrand in Eq. (53) with respect to interchange of τ and σ . Upon making the change of variable, $y = \tau - \sigma$ and $x = \tau$, one has

$$A = \alpha v (2\sqrt{\pi}T)^{-1} \left\{ 2 \int_0^T dx \int_0^x e^{-y} F^{-\frac{1}{2}}(y) dy \right\}. \quad (C3)$$

Since the integrand of Eq. (C3) is independent of x , it is convenient to perform the integration over x first. The result is

$$A = \alpha v \pi^{-\frac{1}{2}} \int_0^T e^{-Y} F^{-\frac{1}{2}}(Y) dY - \alpha v \pi^{-\frac{1}{2}} T^{-1} \int_0^T Y e^{-Y} F^{-\frac{1}{2}}(Y) dY. \quad (C4)$$

The expression, A, is to be used only in Eq. (35). In that equation, only the limiting expression for A as $T \rightarrow \infty$ is employed. That limiting expression is

$$\lim_{T \rightarrow \infty} A = \alpha v \pi^{-\frac{1}{2}} \int_0^{\infty} e^{-Y} F^{-\frac{1}{2}}(Y) dY, \quad (C5)$$

where use has been made of the fact that the integral in the second term of Eq. (C4) is finite in the limit $T \rightarrow \infty$. Upon substituting Eq. (C2) into Eq. (C5), one can see that the integrand of Eq. (C5) approaches $+\infty$ as $y \rightarrow 0$. To remove this feature, which is undesirable for the purpose of numerical integration, the change of variable $y = \rho^2$ is made. The result, which is just the negative of the second term of Eq. (59), is given below:

$$\lim_{T \rightarrow \infty} A = +2\alpha v \pi^{-1} \int_0^{\infty} \rho e^{-\rho^2} F^{-\frac{1}{2}}(\rho^2) d\rho. \quad (C6)$$

The right side of Eq. (55) can be written as

$$\begin{aligned}
R \equiv \frac{\langle V^2 \rangle - T^2 A^2}{T} &= (\alpha v)^2 (\pi T)^{-1} \int_0^T d\tau \int_0^\tau d\sigma \int_0^T d\tau' \int_0^{\tau'} d\sigma' \\
&\cdot e^{-(\tau-\sigma)} e^{-(\tau'-\sigma')} [F(\tau-\sigma) F(\tau'-\sigma')]^{-\frac{1}{2}} \\
&\cdot (Q^{-1} \arcsin(Q) - 1), \tag{C7}
\end{aligned}$$

where

$$Q = \frac{F(|\tau-\tau'|) - F(|\tau-\sigma'|) - F(|\sigma-\tau'|) + F(|\sigma-\sigma'|)}{2[F(\tau-\sigma) F(\tau'-\sigma')]^{\frac{1}{2}}} . \tag{C8}$$

In terms of new integration variables,

$$\begin{aligned}
x &= \tau' - \tau \\
y &= \tau - \sigma \\
z &= \tau' - \sigma' \\
\tau &= \tau, \tag{C9}
\end{aligned}$$

one has

$$R = (\alpha v)^2 (\pi T)^{-1} \int_0^T d\tau \int_0^\tau dy \int_0^{x+\tau} dz \int_{-\tau}^{T-\tau} dx G(x, y, z), \tag{C10}$$

where

$$G(x, y, z) \equiv e^{-y} e^{-z} [F(y) F(z)]^{-\frac{1}{2}} (Q^{-1} \arcsin(Q) - 1) \tag{C11}$$

with

$$Q = \frac{F(|x|) - F(|x-z|) - F(|x+y|) + F(|x+y-z|)}{2[F(y)F(z)]^{\frac{1}{2}}} .$$

(C12)

Since the integrand of Eq. (C10) is independent of τ , it is useful to perform the integration over τ first, for the purpose of which it is necessary to make the required exchanges of integration limits in Eq. (C10). The result of this tedious, but straightforward, process is that R is expressed as the sum of six integrals, each of which has the general form

$$(\alpha v)^2 \pi^{-1} \int dx \int dy \int dz G(x,y,z) \{1 - T^{-1} g(x,y,z)\},$$

(C13)

where the function, $g(x,y,z)$ is independent of T . Since R is used only in Eq. (35), there is need only for the limiting expression for R as $T \rightarrow \infty$. In each of the six integrals, the integral corresponding to the term $G(x,y,z)g(x,y,z)$ in Eq. (C13) is finite in the limit $T \rightarrow \infty$. The resulting expression of R in the limit $T \rightarrow \infty$ is

$$\begin{aligned}
\lim_{T \rightarrow \infty} R = (\alpha v^2) \pi^{-1} \lim_{T \rightarrow \infty} \{ & \int_0^T dy \int_0^y dz \int_0^{T-y} dx \\
& + \int_0^T dz \int_0^z dy \int_{y-z}^{T-y} dx + \int_0^T dy \int_0^y dz \int_{z-y}^0 dx \\
& + \int_0^T dz \int_0^z dy \int_0^{z-y} dx + \int_0^T dy \int_0^y dz \int_{z-y}^{z-t} dx \\
& + \int_0^T dz \int_0^z dy \int_{z-T}^0 dx \} G(x,y,z). \tag{C14}
\end{aligned}$$

The symmetry property $G(-x,z,y) = G(x,y,z)$ can be employed to combine these six integrals into a single 3-fold integral over x,y,z in which each of x,y , and z ranges from 0 to T . Thus

$$\lim_{T \rightarrow \infty} R = 2(\alpha v)^2 \pi^{-1} \int_0^\infty dx \int_0^\infty dy \int_0^\infty dz G(x,y,z), \tag{C15}$$

where $G(x,y,z)$ is given by Eq. (C11) with Eq. (C12). The bothersome feature of Eq. (C15), that the integrand approaches $+\infty$ as either $y \rightarrow 0$ or $z \rightarrow 0$, is removed by making the change of integration variables, $y = \rho_1^2$ and $z = \rho_2^2$ (for ease of reading, $x = \rho_3$ is also defined). The result is just the first term of Eq. (60) with Eqs. (61)-(65).

APPENDIX D

WEAK COUPLING EXPANSION

Feynman's variational self-energy expression, E_F , as given by Eq. (59) and the second order correction term, ΔE_2 , as given by Eq. (60) with Eqs. (61)-(65) are to be expressed as a power series in the coupling constant, α , for the case of small α .

Comparison of S in Eq. (22), in terms of which Feynman's exact self-energy expression is given, and S' in Eq. (31), in terms of which the approximate self-energy expression, $E'_0(\alpha)$ in Eq. (30) is given, suggests that for small α , w be considered zeroth order in α and that C be taken as first order in α as a starting point for the required expansions. Then by Eq. (52), v can be expressed in terms of w by the relation

$$v = (1 + \eta\alpha + O^2(\alpha))w, \quad (D1)$$

where η is zeroth order in α .

First the expansion is obtained for Feynman's variational self-energy expression, which is given by

$$E_F = 3(v-w)^2(4v)^{-1} - 2\alpha v\pi^{-\frac{1}{2}} \int_0^\infty \rho e^{-\rho^2} F^{-\frac{1}{2}}(\rho^2) d\rho, \quad (D2)$$

where

$$F(\rho^2) = (v^2 - w^2)v^{-1}[1 - e^{-v\rho^2}] + w^2\rho^2. \quad (D3)$$

Using Eq. (D1), one can expand the integrand of Eq. (D2) as a series in ascending orders of α . The resulting integration is then performed term by term to get

$$\int_0^\infty \rho e^{-\frac{1}{2}F(\rho^2)} d\rho = \pi^{\frac{1}{2}}(2w)^{-1} \{1 - 2w^{-1}\eta\alpha[(w+1)^{\frac{1}{2}} - 1]\} + O^2(\alpha). \quad (D4)$$

Substituting Eq. (D4) into Eq. (D2) and using Eq. (D1) to express the rest of Eq. (D2) as a series in orders of α , one can then minimize the resulting expression with respect to w and η . The outcome, which confirms the initial assumptions concerning the α dependence of v, w , and η , is given below:

$$\eta = (2/27) + O^1(\alpha), \quad (D5)$$

$$w = 3 + O^1(\alpha), \quad (D6)$$

$$v = 3 + (2/9)\alpha + O^2(\alpha), \quad (D7)$$

by Eq. (D1), and

$$E_F = -\alpha - (1/81)\alpha^2 + O^3(\alpha). \quad (D8)$$

To obtain the second order correction term, ΔE_2 , it is sufficient to employ Eqs. (D6) and (D7) to express Eqs. (60)-(65) as a power series in α . The resulting integrations are performed term by term with the outcome,

$$\Delta E_2 = -\alpha^2[a_c - (1/81)] + O^3(\alpha), \quad (D9)$$

where

$$a_c = \ln(1+3\sqrt{2}/4) - 1/\sqrt{2}. \quad (D10)$$

APPENDIX E

STRONG COUPLING EXPANSION

Feynman's variational self-energy expression, E_F , as given by Eq. (59) and the second order correction term, ΔE_2 , as given by Eq. (60) with Eqs. (61)-(65) are to be expressed as a power series in the coupling constant, α , for the case of large α .

Comparison of S in Eq. (22), in terms of which Feynman's exact self-energy expression is given, and S' in Eq. (31), in terms of which the approximate self-energy expression $E'_0(\alpha)$ in Eq. (30) is given, suggests that for large α , w be considered zeroth order in α and that C (and hence, by Eq. (52), v) be taken large with respect to w as a starting point for the required expansion.

First the expansion is obtained for Feynman's variational self-energy expression, which can be written in the form below by making the change of integration variable $\rho=y^2$ in Eq. (59):

$$E_F = 3(v-w)^2(4v)^{-1} - \alpha v \pi^{-\frac{1}{2}} \int_0^{\infty} e^{-\rho} F^{-\frac{1}{2}}(\rho) d\rho, \quad (E1)$$

where

$$F(\rho) = (v^2 - w^2)v^{-1}[1 - e^{-v\rho}] + w^2\rho. \quad (E2)$$

The integrand of Eq. (E1) can be expressed as an infinite sum of terms, in each of which the v -dependence has the form of a power of $v^{\frac{1}{2}}$ multiplied by a power of the quantity, $(1 - e^{-v\rho})^{\frac{1}{2}}$. Expanding the latter factor as a power series in $e^{-v\rho}$, one obtains an integral which is easy to evaluate term by term. The result is

$$\int_0^\infty e^{-\rho} F^{-\frac{1}{2}}(\rho) d\rho = v^{-\frac{1}{2}} + [2\ln 2 - \frac{1}{2}w^2]v^{-3/2} + O^{-5/2}(v). \quad (E3)$$

It is found that employing only the first two terms of this result is sufficient for applying the variational principle to determine w to leading order in α and v to leading and next to leading order in α . The outcome, in which the initial assumptions concerning the α dependence of w and v are confirmed, is given below:

$$w = 1 + O^{-2}(\alpha), \quad (E4)$$

$$v = 4(9\pi)^{-1}\alpha^2 - (4\ln 2 - 1) + O^{-2}(\alpha), \quad (E5)$$

and

$$E_F = -(3\pi)^{-1}\alpha^2 - (3\ln 2 + 3/4) + O^{-2}(\alpha). \quad (E6)$$

Having obtained, from the variational principle, the values of w and v which minimize Feynman's variational self-energy expression, then one can proceed to obtain the strong coupling expansion for the second order correction term, which is Eq. (60) with Eqs. (61)-(65). For this purpose, it is useful to make the change of integration variables, $\rho_1 = y^2$ and $\rho_2 = z^2$, and to employ the same technique used for the single integrals, namely expansion in powers of $v^{\frac{1}{2}}$, $e^{-v\rho_1}$, and $e^{-v\rho_2}$. Obtaining the final result is a lengthy process in view of the complexity of the second order correction term. The outcome is

$$\Delta E_2 = -(3\pi)^{-1} \left[\sum_{n=1}^{\infty} 6 \{ (2n)! / [2^{4n} (n!)^2 n(2n+1)] \} \right. \\ \left. - (1/4) \right] \alpha^2 + O^0(\alpha), \quad (E7)$$

where the complicated sum originates from the expansion of the arcsin term in Eq. (61).

APPENDIX F

NUMERICAL CALCULATIONS

For intermediate values of the coupling constant, α , Feynman's variational self-energy expression, E_F , as given by Eq. (59) and the second order correction term, ΔE_2 , as given by Eq. (60) with Eqs. (61)-(65) were evaluated numerically using the Louisiana State University Computer Research Center IBM 360/65 computer. This machine employs approximately sixteen decimal digits of accuracy in the double precision mode, which was used for all numerical calculations.

For the purpose of performing the two single integrals, the trapezoidal Romberg quadrature method as programmed in the IBM Scientific Subroutine Package was modified to obtain accuracy to within a specifiable relative error rather than absolute error. This subroutine adjusts the integration grid automatically and in such a way that each refinement samples the integrand at points evenly distributed over the integration range. With each grid refinement the difference between the present and immediately preceeding approximation to the integral is calculated. If this difference does not decrease with successive refinements, then the integration is terminated and a "round off error" message is generated to indicate

the possibility that the integrand was not calculated to the precision necessary to obtain the integral to the required accuracy.

The upper limits used for the (improper) single integrals were obtained by requiring that an analytical overestimate to the contribution from the upper limit to infinity be less than a specified fraction of the already accumulated contribution.

The three-fold integral was performed by successive applications of the modified Romberg subroutine used for the single integrals. It was found that for fixed values of ρ_1 and ρ_2 and for a sufficiently large value of ρ_3 , the integrand merged with a truncated series expansion of the integrand. Since the series could be integrated analytically, the integration over ρ_3 was performed first by integrating numerically from zero to the value, ρ_3' , of ρ_3 for which the series could be used and then employing the analytic series result from ρ_3' to infinity. For ρ_3 integrated out, a method was needed for truncating the $\rho_1\rho_2$ integration, for which the region of integration is the first quadrant of the $\rho_1\rho_2$ plane. After integrating over a finite square with sides on the ρ_1 and ρ_2 axes, an analytic overestimate to the contribution from the region outside the square is required to be less than a specified fraction of the already accumulated contribution, as a condition for truncation.

For all numerical calculations, every occurrence of

subtractions which might result in a loss of significance in the final result was circumvented by employing an alternative expression for the difference for which subtraction error did not occur.

The three-fold integral was performed repetitively for a maximum fractional error of $1/100$ and $1/1000$. Agreement was found beyond the fourth significant figure. The single-fold integrals were done subject to the much more restrictive fractional error of $1/10^{14}$. This high accuracy was needed to obtain the optimizing values of the variational parameters, v and w , to four significant digits of accuracy for use in evaluating the second order correction term. This process required accurate knowledge of the eleventh and twelfth significant digits of Feynman's variational self-energy expression. The resulting v and w values differ by about two figures in the third significant digit from the three significant digits reported for v and w by Schultz.¹² In view of this discrepancy considerable care was exercised in checking the single integral in Feynman's variational self-energy expression. The program was tested with similar integrands whose integrals could be performed analytically and was found to give the correct result to far more than the needed twelve significant digits. Even the integrands were spot checked by hand calculations to 25 significant digits, and again the accuracy of the calculations was confirmed.

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VITA

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