Functional Equations for Path Integrals

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We consider the density matrices that arise in the statistical mechanics of the electron–phonon systems. In the path integral representation the phonon coordinates can be eliminated. This leads to an action that depends on pairs of points on a path, that depends explicitly on time differences, and that contains the phonon occupation numbers. The integral is reduced to a standard form by scaling to the thermal length. We use the technique of integration by parts and add specially chosen generating functionals to the action. We set down functional derivative equations for the source-dependent density matrix and for the mass operator. This allows us to develop a series of approximations for the operator in terms of exact propagators. The crudest approximation is a coherent potential approximation applicable at a general temperature.

KEY WORDS: Path integral; electron–phonon interaction; functional equations.

1. INTRODUCTION

Our concern is with electron–phonon problems, where the interaction is linear in the coordinates describing the phonons. We use the Feynman path integral representation of the amplitudes. It is possible to eliminate the phonon degrees of freedom. The reduced electron propagator contains an action that depends on the path positions at two times $x(u)$ and $x(u')$. It also depends explicitly on the time difference $|u - u'|$, a feature that stems from the inertial lag of the ions from which the phonons are constructed. The effective action depends on the state of the phonons, and the simplest case is the ground state to ground state phonon amplitude. There is also a "Euclidean" form of this expression in which one replaces the time by

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$\beta = it$, and obtains the corresponding multitime Wiener integral. Here β is not a physical inverse temperature. We will continue to speak of a "time" β and an "action" in the Wiener integral case.

Wiener integrals of this type also occur when one considers the equilibrium statistical mechanics of the electron phonon system at a finite physical inverse temperature β. Starting from the path integral representation of the density matrix of the system as a whole, one can again integrate over the phonon paths. The result is the reduced electron density matrix. It has an action with the same multitime type of dependence on the electron paths. There is, however, an additional β dependence arising from the thermal occupation numbers of the phonons, including separate emission and adsorption terms.

This is well known and has been explained in detail in the books of Feynman and Hibbs[1] and Feynman.[2] There are a number of advantages in using a representation where the phonon coordinates have been exactly eliminated. If the original Lagrangian has a coupling constant g, the expansion of the reduced density matrix goes in powers of g^2. In addition the thermal occupation numbers of the phonons appear directly, and correctly, in every order of the expansion. Furthermore, there is a variety of ideas and techniques that are specific to the path integral representation and are non-Hamiltonian in nature. One of these ideas is the use of nontrivial trial actions to define an unperturbed problem. Examples are the mean path action and the quadratic action used by Feynman in his polaron theory. A second idea is the semiclassical approximation scheme[3] that results from expanding about classical paths in the parameter space. Another, closely related method is the theory of the asymptotic expansions of Wiener integrals.[4-6] Techniques are also available to find successively more accurate lower and upper bounds to Wiener integrals. We have summarized and extended some of these techniques in a series of recent papers.[7]

On the other hand there are some cases where the direct use of the path integral is awkward. For example, one is frequently interested in the complex wave number and energy-dependent mass operator $\tilde{\Sigma}(k \mid s)$ in order to display the spectral properties of the system and to compute dispersion and damping of excitations. One can compute the mass operator by "hand cranking." This involves expanding the exponential and computing the spatial Fourier and temporal Laplace transforms. One can then match the series to the equation that defines the mass operator. This gives $\tilde{\Sigma}(k \mid s)$ as a series in g^2 in terms of the bare propagators. To do better, one has to sum infinite classes of diagrams.

There are other situations in which the direct use of the path integral is

awkward. For example, even in simple potential theory with delta function, shell, or hard core potentials, the evaluation of the integral involves tours de force (cf. the work of E. Lieb,[8] where, however, interesting results are derived). It is much easier to retreat to the Schrödinger equation or the Bloch equation for the density matrix, using Feynman–Kac equivalence. One then works with standard eigenfunction methods. This equivalence is easily proved from the starting point of the path integral, by using an integration by parts technique. This immediately yields the integral equation form of the Bloch equation. In the potential problem the mass operator is simply the local, energy-independent potential itself. When the starting point is the phonon-eliminated Wiener integral for the reduced electron density matrix, the integration by parts technique allows one to write down an infinite hierarchy for correlation functions. This hierarchy is the analog of the Bloch equation of the potential problem. Successive truncations of the equations of the hierarchy allow one to avoid the "hand cranking" of the simple expansion. One automatically obtains expressions for the mass operator. It is easy to find the coupling constant expansion and some limited nonperturbative extensions. However, these results are in terms of the bare propagators.

An elegant way of deriving this hierarchy is to add a generating action to the original action. The Bloch equation is replaced by a functional derivative equation. This corresponds to the standard Schwinger approach[9] to quantum field theory. However, in order to use this approach on the phonon-eliminated action, one must invent nonstandard generating actions. This is the focus of the present paper. It is then easy to find a functional equation for the source-dependent mass operator and to find a new hierarchy that involves exact propagators.

The phonon-eliminated action has mainly been used to calculate the path integral from the space-time viewpoint. Examples are cumulant expansions,[10] trial action theories, etc., as mentioned above. The connection with field theory methods, e.g., vertex functions, mass operators, and so forth, has not been examined carefully. To be sure, field theory has been extensively applied to the original coupled field Lagrangian, but this does not make real use of the advantage of the phonon-eliminated action.

There is very early work by Puff and Whitfield[11] on a Green's function formulation starting with the equations of motion for the coupled fields. They eliminate low-order phonon Green's functions and then make truncations. However, this was not carried very far. There is also interesting more recent work by Peeters and Devreese[12] on equation of motion techniques, where again one can eliminate phonon degrees of freedom. There is also a very recent paper by Kholodenko and Freed[13] on the

direct approach to the mass generator in terms of bare propagators. We feel that the generating function theory for the phonon eliminated action that we present here is a more powerful and systematic approach in the same direction.

To make clearer what we mean, we summarize our recently published work[14] on a closely related problem. This is the multiple scattering of an electron by a system of scatterers with random, uncorrelated positions. Edwards and Gulyaev[15] showed that the averaging over site positions in the path integral leads to a multitime action for the electron Green's function. In the limit of weak dense scatterers, this becomes a simpler two-time functional, without explicit time dependence. The relation is that of a Poisson to a Gaussian process.

This problem had already been studied by Edwards[16] and also by Klauder,[17] using field theoretic ideas, but not path integrals. They introduced mass operators, summed classes of diagrams, and developed coherent potential approximations. There has been considerable development along these field theoretical lines, especially in the Gaussian limit. In particular Tatarski,[18] Furutsu,[19] and Chow[20] used the method of functional derivatives to formulate the theory and extend it to compute higher correlations.

The novel aspect of our work was to start from the Edwards–Gulyaev path integral for the Poisson process. We introduced a generating action that was specific to the Poisson process, and was different from the standard generator. It produced the bare atomic scattering matrices directly. In this way it was possible to treat strong scattering exactly, without infinite summations, as had been necessary in the Edwards and the Klauder work. From this point on, the standard field theory machinery was set in motion. A density expansion was obtained for the mass operator, both in terms of bare and exact propagators, and in terms of bare and medium scattering matrices. The functional derivative method was used to derive a new hierarchy, and it was shown that nonperturbative truncations were natural.

This work utilized one of the strong points of the path integral representation, namely, the ability to do the site averaging exactly *ab initio*. We built a bridge to field theoretic approaches that are most succinctly expressed in equations for functional derivatives. The bridge used a specifically adapted nonstandard generator.

We do a similar thing here for the electron–phonon problems. The phonon-eliminated actions are simpler than the Edwards–Gulyaev (Poisson) action in that they depend on only pairs of path points. But they are more complicated in another way, namely, that there is explicit time

dependence. This again requires us to invent suitable generating actions, and we find that this can be done in several ways.

In Section 2 we introduce the actions that will be analyzed, and reduce the path integrals to a standard form by scaling to the thermal de Broglie length. A new "time" parameter is then introduced. We discuss why this procedure is necessary for actions that contain thermal weighting factors.

In Section 3 we describe the method of obtaining functional derivative equations for the path integrals. The initial case that is treated is the time-independent, nonthermal, Gaussian random potential action. Then the stardard generating functional is appropriate and the functional equation is already known. It, however, allows us to introduce the integration by parts technique that is used in everything that follows. Next we discuss the time-dependent, but ground-state polaron problem, i.e., electron-optical phonon interaction. There are at least two nonstandard generators, and one of them is analyzed in detail. We then proceed to write down a generator and a functional equation for the polaron with thermally averaged phonons. Finally we do the same thing for the general, thermal, single branch, electron–phonon action.

In Section 4, the functional equation for the Laplace transform $I(s)$ of the source-dependent path integral $\hat{I}(t)$ is studied. The focus is on a set of correlation functions which are defined as the functional derivatives of $I(s)$ evaluated in the limit of vanishing source strength. The correlation functions are linked in an infinite hierarchy of equations that involve the free electron density matrix or "bare propagator." The hierarchy can be used to derive the temperature-dependent mass operator for the general electron–phonon problem as a series in the coupling constant. It can also be truncated to find closed operator equations for the lowest-order correlation function. We show that this equation can be solved to a better approximation than straightforward iteration by introducing "screened" propagators. The screening is equivalent to including an infinite class of diagrams.

In Section 5, we derive the functional derivative equations for the source-dependent mass operator Σ_J. We consider a set of correlation functions which are the values of the functional derivatives evaluated in the limit of vanishing source strength. The correlation functions are linked in an infinite hierarchy of equations, each of which involves the exact density matrix or "propagator." In all of the cases there is natural sequence of approximations. The crudest one is a generalized "coherent potential" approximation involving a self-consistent equation for the mass operator. It applies to the density matrix at arbitrary temperatures.

The next approximation results in a linear operator equation for the first correlation function. It yields a mass operator that is accurate to the

second power of the interaction and is in terms of the exact propagators. The equation can be solved exactly when the spatial interaction is a one-dimensional delta function. The result is equivalent to the sum of an infinite class of diagrams involving exact propagators.

In Section 6 we briefly describe the theory based on a second type of generating functional. It is actually simpler to derive the bare propagator theory with the resulting functional equation. However, the functional equation for the source-dependent mass operator is more complicated. It appears easier to develop the exact propagator expansions with the first generating functional.

2. REDUCTION TO A STANDARD FORM

For the Gaussian random potential problem, the averaged action is ($\hbar = m = 1$)

$$\langle R_1 | \hat{r}(\beta) | R_2 \rangle = \int_{R_2}^{R_1} D_\beta x \exp\left[A'(\beta) \right]$$

$$A' = \frac{1}{2} \int_0^\beta \int_0^\beta f\left[x(u) - x(u') \right] du\, du' \tag{2.1}$$

$$D_\beta x = \mathscr{D}_\beta\, x \exp\left[-\frac{1}{2} \int_0^\beta \left(\frac{dx}{du} \right)^2 du \right]$$

The covariance function $f(x)$ is characterized by a strength and a length. The path integral depends only on $R = R_1 - R_2$, in virtue of the translation invariance of A'.

From $\hat{r}(\beta)$ we obtain the spectral density and density of states per unit volume by inverse Laplace transforms. Thus,

$$n(k \mid E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\, e^{\beta E} \int dR\, e^{ikR} \langle R | \tilde{r}(\beta) | 0 \rangle \tag{2.2}$$

$$n(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\, e^{\beta E} \langle 0 | \hat{r}(\beta) | 0 \rangle \tag{2.3}$$

We will concentrate on finding $\langle R | \hat{r}(\beta) | 0 \rangle$.

One can scale the path integral in units of the thermal de Broglie wavelength $\sqrt{\beta}$. Thus introduce

$$y(u) = x(u)/\sqrt{\beta}, \qquad v = u/\beta, \qquad \zeta = R/\sqrt{\beta} \tag{2.4}$$

and rename the dummy variables y and v as x and u. Then

$$\langle R | \hat{r}(\beta) | 0 \rangle = (1/\beta)^{d/2} \langle \zeta | \hat{\rho}(1) | 0 \rangle \tag{2.5}$$

Here

$$\langle \zeta | \hat{\rho}(t) | 0 \rangle = \int_0^\zeta D_1 x \exp\left[A(t) \right] \tag{2.6}$$

$$A(t) = \frac{1}{2} \int_0^t \int_0^t W\left[x(u) - x(u') \right] du\, du' \tag{2.7}$$

We call the integral that results from making the shift of the upper limit of β to unity by de Broglie scaling, the standard form. We will study $A(t)$ for general t, and set $t = 1$ at the end of the analysis. For the Gaussian random potential problem β is not a physical inverse temperature. We first compute the time-averaged Green's function and interpret β as i times the time.

For the thermodynamic polaron problem one starts the density matrix for the combined electron–phonon system at an inverse temperature β. After integrating over the optical phonon coordinates, one finds the two time action $A'(\beta)$:

$$A'(\beta) = \frac{1}{2} g_0^2 \int_0^\beta \int_0^\beta \frac{1}{|x(u) - x(u')|} \frac{e^{-\omega_0|u-u'|} + e^{-\omega_0\beta}e^{+\omega_0|u-u'|}}{1 - e^{-\omega_0\beta}} du\, du' \tag{2.8}$$

Here g_0^2 is a coupling constant, and ω_0 is the angular frequency of the optical mode.

After scaling to the thermal length, we study

$$A(t) = \frac{1}{2} \int_0^t \int_0^t \int W\left[x(u) - x(u') \,|\, \alpha \right] e^{-\alpha\omega|u-u'|} du\, du'\, d\alpha \tag{2.9}$$

Here

$$W(x \,|\, \alpha) = W(x \,|\, 1)\delta(\alpha - 1) + W(x \,|\, -1)\delta(\alpha + 1)$$

$$W(x \,|\, 1) = \frac{g^2}{|x|} (1 - e^{-\omega})^{-1}$$

$$W(x \,|\, -1) = W(x \,|\, 1)e^{-\omega} \tag{2.10}$$

$$\omega = \beta\omega_0, \qquad g^2 = g_0^2 \beta^{3/2}$$

For the general, single-branch, thermal phonon problem, with a spectrum $\omega_0(k)$, after eliminating the phonon coordinates, one is left with an action $A'(\beta)$:

$$A'(\beta) = \frac{1}{2} \int dk\, \tilde{f}(k) e^{ik \cdot [x(u) - x(u')]} \frac{e^{-\omega_0(k)|u-u'|} + e^{-\beta\omega_0(k)}e^{+\omega_0(k)|u-u'|}}{1 - e^{-\beta\omega_0(k)}} \tag{2.11}$$

It suffices to study the scaled form

$$A(t) = \frac{1}{2} \int \int dk \, d\alpha \, \tilde{W}(k \mid \alpha) \int_0^t \int_0^t e^{ik[x(\omega) - x(u')]} e^{-\alpha\omega(k)|u - u'|} \, du \, du' \quad (2.12)$$

Here

$$\tilde{W}(k \mid \alpha) = \tilde{W}(k \mid 1)\delta(\alpha - 1) + \tilde{W}(k \mid -1)\delta(\alpha + 1)$$

$$\omega(k) = \beta\omega_0\left(k/\sqrt{\beta}\right)$$

$$\tilde{W}(k \mid 1) = \beta^{(2-d/2)}\tilde{f}\left(\frac{k}{\sqrt{\beta}}\right)\left[1 - e^{-\omega(k)}\right]^{-1} \quad (2.13)$$

$$\tilde{W}(k \mid -1) = \tilde{W}(k \mid 1)e^{-\omega(k)}$$

We now explain why scaling to the thermal length is important. Associated with $\langle \zeta | \hat{\rho}(t) | 0 \rangle$ is the Laplace transform

$$\langle \zeta | \rho(s) | 0 \rangle = \int_0^\infty dt \, e^{-st} \langle \zeta | \hat{\rho}(t) | 0 \rangle \quad (2.14)$$

with the inverse

$$\langle \zeta | \hat{\rho}(t) | 0 \rangle = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, e^{st} \langle \zeta | \rho(s) | 0 \rangle \quad (2.15)$$

We will also use the spatial Fourier transform pair

$$\tilde{\rho}(k \mid s) = \int d\zeta \, e^{ik\zeta} \langle \zeta | \rho(s) | 0 \rangle$$

$$\langle \zeta | \rho(s) | 0 \rangle = \frac{1}{(2\pi)^d} \int dk \, e^{-ik\zeta} \tilde{\rho}(k \mid s) \quad (2.16)$$

$\tilde{\rho}(k \mid s)$ will be computed in terms of a mass operator $\tilde{\Sigma}(k \mid s)$, defined as

$$\tilde{\Sigma}(k \mid s) = \tilde{\rho}_0^{-1}(k \mid s) - \tilde{\rho}^{-1}(k \mid s)$$

$$\tilde{\rho}_0^{-1}(k \mid s) = s + k^2/2 \quad (2.17)$$

$\tilde{\Sigma}(k \mid s)$ is the main object of our analysis. One has

$$\langle \zeta | \hat{\rho}(t) | 0 \rangle = \int dk \, \frac{e^{-ik\zeta}}{(2\pi)^d} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, e^{st} \left[s + \frac{k^2}{2} - \tilde{\Sigma}(k \mid s) \right]^{-1} \quad (2.18)$$

On the other hand, the expression for the original $\langle R \,|\, \hat{r}(\beta)|0\rangle$ is

$$\beta^{d/2}\langle R|\hat{r}(\beta)|0\rangle$$

$$= \frac{1}{(2\pi)^d} \int dk\, e^{-ikR} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds\, e^{s\beta}\left[s + \frac{k^2}{2} - \tilde{S}(k\,|\,s)\right]^{-1} \quad (2.19)$$

where

$$\tilde{S}(k\,|\,s) = \frac{1}{\beta}\, \tilde{\Sigma}\!\left(k\sqrt{\beta}\,\,|\,s\beta\right) \qquad (2.20)$$

The quantity $\tilde{S}(k\,|\,s)$ will be β dependent when there has been thermal averaging of the phonons. It is independent of β for ground-state problems and for the Gaussian random potential problem (a zero-frequency phonon problem).

The main point is best illustrated by writing down the coherent potential approximation, which is the simplest nontrivial approximation. In Section 5 we will derive the expression

$$\tilde{\Sigma}(k\,|\,s) = \int\int dk_1\, d\alpha_1 \left[s + \alpha_1\omega(k_1) + \frac{(k+k_1)^2}{2} - \tilde{\Sigma}(k+k_1\,|\,s)\right]^{-1}$$

$$\times \tilde{W}(k_1\,|\,\alpha_1) \qquad (2.21)$$

From this it follows that

$$\tilde{S}(k\,|\,s) = \left(1 - e^{-\beta\omega_0(k)}\right)^{-1} \int dk_1\, \tilde{f}(k_1)$$

$$\times \left\{\left[s + \frac{(k+k_1)^2}{2} - \tilde{S}(k+k_1\,|\,s) + \omega_0(k_1)\right]^{-1}\right.$$

$$\left. + e^{-\beta\omega_0(k)}\left[s + \frac{(k+k_1)^2}{2} - \tilde{S}(k+k_1\,|\,s) - \omega_0(k_1)\right]^{-1}\right\}$$

$$(2.22)$$

In this last expression, everything is explicitly expressed in terms of the parameters of the original action $A'(\beta)$. We see that the β dependence of $\tilde{S}(k\,|\,s)$ comes from the thermal weights. The techniques to be employed in later sections, viz., integration by parts and introduction of suitable generat-

ing functions, can be used with $A'(\beta)$ when there are no thermal weighting factors. It is not necessary to scale to the thermal length. On the other hand, these techniques run into difficulties when $A'(\beta)$ involves β-dependent thermal weights. This is the reason for first scaling to $A(1)$, where β occurs as a parameter. Then t is introduced as a "time" evolution generator and the techniques apply.

3. CONSTRUCTION OF THE FUNCTION EQUATIONS

3.1. Gaussian Random Potential Action

We start with the simplest case, i.e., the time-dependent action that results when the potential acting on a particle is averaged over a Gaussian distribution. For this case Eq. (2.7) can be rewritten as

$$A(T) = \int \int dz \, dy_1 \, W(z - y_1) \int_0^T du \int_0^u du' \, \delta(x(u) - z) \delta(x(u') - y_1) \quad (3.1)$$

Integration by parts on the time variable allows one to write

$$\langle \zeta | \hat{\rho}(T) - \hat{\rho}_0(T) | \zeta' \rangle = \int_{\zeta'}^{\zeta} D_T x \int_0^T dt \, \frac{\partial A(t)}{\partial t} \, e^{A(t)} \quad (3.2)$$

Now,

$$\frac{\partial A(t)}{\partial t} = \int \int dz \, dy_1 \, W(z - y_1) \delta(x(t) - z) \int_0^t \delta(x(u) - y_1) \, du \quad (3.3)$$

Hence, we have

$$\langle \zeta | \hat{\rho}(T) - \hat{\rho}_0(T) | \zeta' \rangle = \int_0^T dt \int \int dz \, dy_1 \langle \zeta | \hat{\rho}_0(T - t) | z \rangle W(z - y_1)$$

$$\times \int_{\zeta'}^z D_t x \int_0^t \delta(x(u) - y_1) \, du \, e^{A(t)} \quad (3.4)$$

Next, add a term

$$A_J(T) = \int dz \, J(z) \int_0^T \delta(x(u) - z) \, du \quad (3.5)$$

to the action, and denote the resulting integral as

$$\langle \zeta | \tilde{I}(T) | \zeta' \rangle = \int_{\zeta'}^{\zeta} D_T x \exp[A(T) + A_J(T)] \quad (3.6)$$

$\hat{I}(T)$ reduces to $\hat{\rho}(T)$ when $J = 0$.

One can generate the path integral in Eq. (3.4), representing a correla-

tion function, by taking the functional derivative

$$\frac{\delta}{\delta J(y_1)} \langle z|\hat{I}(t)|\zeta'\rangle$$

The price that must be paid is the additional term

$$\frac{\partial A_J(t)}{\partial t} e^{A+A_J(t)} = \int dz\, J(z)\delta(x(t)-z)e^{A+A_J(t)} \tag{3.7}$$

This leads simply to a contribution $J(z)\langle z|\hat{I}(t)|\zeta'\rangle$.

Putting these elements together, we have the functional equation

$$\langle \zeta|\hat{I}(T) - \hat{\rho}_0(T)|\zeta'\rangle$$

$$= \int_0^T \langle \zeta|\hat{\rho}_0(T-t)|z\rangle \left[\int dy_1\, W(z-y_1)\frac{\delta}{\delta J(y_1)} + J(z) \right] \langle z|\hat{I}(t)|\zeta'\rangle \tag{3.8}$$

As was mentioned in the Introduction, for the Gaussian case we have used the standard generating function, and the results are well known.[17-19]

We may take Laplace transforms. Then

$$\langle \zeta|I(s) - \rho_0(s)|\zeta'\rangle$$

$$= \int dz\, \langle \zeta|\rho_0(s)|\zeta\rangle \left[\int dy_1\, W(z-y_1)\frac{\delta}{\delta J(y_1)} + J(z) \right]\langle z|I(s)|\zeta'\rangle \tag{3.9}$$

A more transparent form is

$$\langle \zeta|\rho_0^{-1}(s)I(s) - 1|\zeta'\rangle = \left[\int dy_1\, W(\zeta-y_1)\frac{\delta}{\delta J(y_1)} + J(\zeta) \right]\langle \zeta|I(s)|\zeta'\rangle \tag{3.10}$$

Here

$$\langle \zeta|1|\zeta'\rangle = \delta(\zeta - \zeta') \tag{3.11}$$

Let us recall that the mass operator is introduced by the definition

$$\langle \zeta|\hat{I}(T) - \hat{\rho}_0(T)|\zeta'\rangle$$

$$= \int\int dx_1\, dx_2 \int_0^T dt\, \langle \zeta|\hat{\rho}_0(T-t)|x_1\rangle$$

$$\times \int_0^t dt_1\, \langle x_1|\hat{\Sigma}_J(t-t_1)|x_2\rangle\langle x_2|\hat{I}(t_1)|\zeta'\rangle \tag{3.12}$$

Here $\hat{\rho}_0(T)$ is the free particle density matrix

$$\langle \zeta|\hat{\rho}_0(T)|\zeta'\rangle = (2\pi T)^{-d/2}\exp\left[-(\zeta-\zeta')^2/2T \right] \tag{3.13}$$

The convolution form in time implies simple products for the Laplace transforms. Using matrix notation,

$$\langle \zeta | \rho_0^{-1}(s)I(s) - 1 | s' \rangle = \langle \zeta | \Sigma_J(s)I(s) | \zeta' \rangle \tag{3.14}$$

$$\langle \zeta | I(s) - \rho_0(s) | \zeta' \rangle = \langle \zeta | \rho_0(s)\Sigma_J(s)I(s) | \zeta' \rangle \tag{3.15}$$

Thus the J-dependent mass operator is

$$\Sigma_J(s) = \rho_0^{-1}(s) - I^{-1}(s) \tag{3.16}$$

At $J = 0$, Σ_J is simply Σ. Then

$$\langle \zeta | \Sigma(s)\rho(s) | \zeta' \rangle = \int dy_1\, W(\zeta - y_1)\langle \zeta | \frac{\delta I}{\delta J(y_1)} \bigg|_{j=0} | \zeta' \rangle \tag{3.17}$$

3.2. Phonon Problems

We now derive the functional equations for the more complicated actions that occur when phonons have been eliminated, and where there is explicit time dependence. We start with the simplest ground-state polaron case, and then proceed to the thermal problems, emphasizing only the new points that arise.

Express the action of Eq. (2.9) at zero temperature for the phonons as

$$A(T) = \frac{1}{2} \int_0^T \int_0^T W[x(u) - x(u')] e^{-\omega|u - u'|}\, du\, du' \tag{3.18}$$

Reexpress this as

$$A(t) = \int \int dz\, dy_1\, W(z - y_1) \int_0^t du \int_0^u e^{-\omega(u - u')}\delta(x(u) - z)\delta(x(u') - z)\, du' \tag{3.19}$$

Now

$$\frac{\partial A(t)}{\partial t} = \int \int dz\, dy_1\, W(z - y_1)\delta(x(t) - z)\left[\int_0^t e^{-\omega(t - u')}\delta(x(u') - y_1)\, du' \right] \tag{3.20}$$

A useful generator can be introduced in at least two different ways. One is

$$A_J(T) = \int dz\, J(z)\left[\int_0^T e^{-\omega(T - u)}\delta(x(u) - z)\, du \right] \tag{3.21}$$

Then

$$\frac{\partial A(t)}{\partial t} e^{A + A_J(t)} = \int \int dz \, dy_1 \, W(z - y_1) \delta(x(t) - z) \frac{\delta}{\delta J(y_1)} e^{A + A_J} \quad (3.22)$$

The price that must be paid involves

$$\frac{\partial A_J(t)}{\partial t} = \int dz \, \delta(x(t) - z) - \omega \int dy_1 J(y_1) \left[\int_0^t e^{-\omega(t-u)} \delta(x(u) - y_1) \, du \right]$$

$$(3.23)$$

In the last term we insert a "stop" at time t, viz.,

$$1 = \int dz \, \delta(x(t) - z) \quad (3.24)$$

$$\frac{\partial A_J}{\partial t} e^{A + A_J} = \int dz \, \delta(x(t) - z) \left[J(z) - \omega \int dy_1 J(y_1) \frac{\delta}{\delta J(y_1)} \right] e^{A + A_J(t)}$$

$$(3.25)$$

We now have all the ingredients of the functional equation. The Laplace transform is

$$\langle \zeta | \rho_0^{-1}(s) I(s) - 1 | \zeta' \rangle$$

$$= \left\{ J(\zeta) + \int dy_1 \left[W(\zeta - y_1) \frac{\delta}{\delta J(y_1)} - \omega J(y_1) \frac{\delta}{\delta J(y_1)} \right] \right\} \langle \zeta | I(s) | \zeta' \rangle$$

$$(3.26)$$

The generalization to the thermally averaged polaron is immediate. The action is Eq. (2.9). Add the generating action

$$A_J(T) = \int \int dz \, d\alpha \, J(z \mid \alpha) \int_0^T e^{-\alpha \omega [T - u']} \delta(x(u') - z) \, du' \quad (3.27)$$

We find

$$\langle \zeta | \rho_0^{-1} I - 1 | \zeta' \rangle$$

$$= \int d\alpha_1 \left\{ J(\zeta \mid \alpha_1) + \int dy_1 \left[W(\zeta - y_1) \frac{\delta}{\delta J(y_1)} \right. \right.$$

$$\left. \left. - \alpha_1 \omega J(y_1 \mid \alpha_1) \frac{\delta}{\delta J(y_1)} \right] \right\} \langle \zeta | I | \zeta' \rangle$$

$$(3.28)$$

Finally the general thermal phonon action is given in Eq. (2.12). The generating action is

$$A_J(T) = \int dk \, dz \, d\alpha \left[\int_0^T e^{-\alpha\omega(k)(T-u)} \delta(x(u) - z) \, du \right] J(k|z|\alpha) \quad (3.29)$$

We then have the functional equation

$$\langle \zeta | \rho_0^{-1} I - 1 | \zeta' \rangle$$

$$= \int d(1) J(1) \delta(\zeta - y_1) \langle \zeta | I | \zeta' \rangle$$

$$+ \int d(1) \left[\tilde{W}(k_1 | \alpha_1) e^{ik_1(\zeta - y_1)} - \alpha_1 \omega_1 J(1) \right] \frac{\delta}{\delta J(1)} \langle \zeta | I | \zeta' \rangle \quad (3.30)$$

We use the notation

$$\omega_1 = \omega(k_1), \qquad J(1) = J(k_1 | y_1 | \alpha_1) \quad (3.31)$$

$$\frac{\delta}{\delta J(1)} = \frac{\delta}{\delta J(k_1 | y_1 | \alpha_1)} \quad (3.32)$$

In later sections the utility of these functional equations will be examined.

4. GAUSSIAN RANDOM POTENTIAL

Let us start the discussion with the time-independent Gaussian noise problem governed by the functional equation (3.10). Take functional derivatives and then set $J = 0$. Define the correlation functions

$$\langle \zeta | M(y_1, \ldots, y_n | s) | \zeta' \rangle = \langle \zeta | \frac{\delta^n I(s)}{\delta J(y_1) \ldots \delta J(y_n)} \bigg|_0 | \zeta' \rangle \quad (4.1)$$

One then finds a standard chain of equations for the M operators; note that $I(s)$ at $J = 0$ is $\rho(s)$:

$$\langle \zeta | \rho_0^{-1} I - 1 | \zeta' \rangle = \int dy_1 \, W(\zeta - y_1) \langle \zeta | M(y_1) | \zeta' \rangle \quad (4.2)$$

$$\langle \zeta | \rho_0^{-1} M(y_1) | \zeta' \rangle = \langle \zeta | \rho | \zeta' \rangle \delta(\zeta - \zeta') + \int dy_2 \, W(\zeta - y_2) \langle \zeta | M(y_1, y_2) | \zeta' \rangle \quad (4.3)$$

$$\langle \zeta | \rho_0^{-1} M(y_1, y_2) | \zeta' \rangle = \langle \zeta | M(y_2) | \zeta' \rangle \delta(y_1 - \zeta) + \langle \zeta | M(y_1) | \zeta' \rangle \delta(y_2 - \zeta')$$

$$+ \int dy_3 \, W(\zeta - y_3) \langle \zeta | M(y_1, y_2, y_3) | \zeta' \rangle \quad (4.4)$$

There is an obvious sequence of approximations, the most primitive being to neglect $M(y_1 y_2 | s)$ entirely. Then

$$\langle \zeta | M(y_1) | \zeta' \rangle = \langle \zeta | \rho_0 | y_1 \rangle \langle y_1 | \rho | \zeta' \rangle \quad (4.5)$$

$$W(\zeta - \zeta')$$

$$\langle \zeta | \Sigma(s) | \zeta' \rangle \quad \longrightarrow$$

$$\langle \zeta | \rho_0(s) | \zeta' \rangle$$

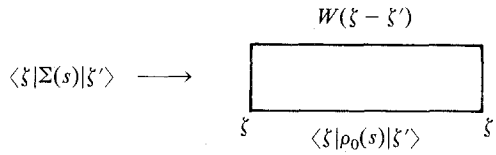ζ $\langle \zeta | \rho_0(s) | \zeta' \rangle$ ζ'

Fig. 1.

This is automatically of a form to yield a result for the mass operator. Inserting this result into Eq. (4.2)

$$\langle \zeta | \rho_0^{-1} \rho - 1 | \zeta' \rangle = \int dy_1 \, W(\zeta - y_1) \langle \zeta | \rho_0 | y_1 \rangle \langle y_1 | \rho | \zeta' \rangle \tag{4.6}$$

$$\langle \zeta | \Sigma | \zeta' \rangle = W(\zeta - \zeta') \langle \zeta | \rho_0(s) | \zeta' \rangle \tag{4.7}$$

This may be pictured as shown in Fig. 1.

In the next approximation we neglect $M(y_1, y_2, y_3)$. This leads to errors in the W^3 term of the mass operator expansion. Eliminating $M(y_1 y_2)$ gives a self-contained linear operator equation for $M(y_1)$.

$$\langle \zeta | \rho_0^{-1} M(y_1) | \zeta' \rangle = \langle \zeta | \rho | \zeta' \rangle \delta(y_1 - \zeta)$$

$$+ \int dy_2 \, W(\zeta - y_2) \langle \zeta | \rho_0 | y_2 \rangle \langle y_2 | M(y_1) | \zeta' \rangle$$

$$+ \int dy_2 \, W(\zeta - y_2) \langle \zeta | \rho_0 | y_1 \rangle \langle y_1 | M(y_2) | \zeta' \rangle \tag{4.8}$$

Replacing $M(y_1)$ by its lowest-order (W^0) value yields the W^2 accurate value of Σ:

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = W(\zeta - \zeta') \langle \zeta | \rho_0 | \zeta' \rangle + \int \int dy_1 \, dy_2 \ldots$$

$$\times \{ W(\zeta - \zeta') W(y_1 - y_2) + W(\zeta - y_2) W(y_1 - \zeta') \}$$

$$\times \langle \zeta | \rho_0 | y_1 \rangle \langle y_1 | \rho_0 | y_2 \rangle \langle y_2 | \rho_0 | \zeta' \rangle \tag{4.9}$$

The W^2 terms of Σ may be pictured as shown in Fig. 2. There is a second-order diagram that occurs in the direct expansion of the path integral expression for ρ in powers of the action (Fig. 3). This is suppressed (together with iterates), by going to the mass operator expansion.

$$W(\zeta - \zeta')$$

$$W(y_1 - y_2)$$

ζ y_1 y_2 ζ'

$+$

$$W(y_1 - \zeta')$$

ζ y_1 y_2 ζ'

Fig. 2.

$$W(\zeta - y_1) \qquad\qquad W(y_2 - \zeta')$$

[diagram]
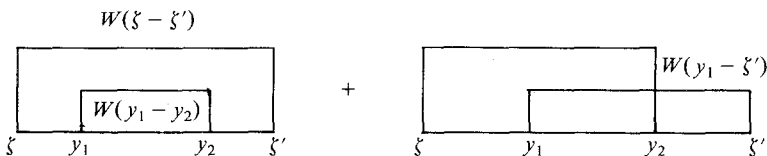
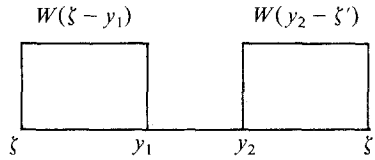$$\zeta \qquad\qquad y_1 \qquad\qquad y_2 \qquad\qquad \zeta'$$

Fig. 3.

The integral equation for $M(y_1|s)$ is complicated. The complete solution is equivalent to including classes of higher-order diagrams in the expression for Σ. However, one observation is in order. The two terms on the right-hand side of Eq. (4.8) have distinct structures. This makes it possible to do something beyond straightforward iteration. Take the Fourier transform

$$\langle k | \tilde{M}(y_1) | \zeta' \rangle = \int e^{ik\zeta} \langle \zeta | M(y_1) | \zeta' \rangle \, d\zeta \qquad (4.10)$$

$$\langle k | \tilde{M}(y_1) | \zeta' \rangle \tilde{\Delta}(k) = e^{iky_1} \langle y_1 | \rho | \zeta \rangle + \int e^{ik\zeta} \, d\zeta \int dy_2 \, W(\zeta - y_2) \langle \zeta | \rho_0 | y_1 \rangle$$
$$\times \langle y_1 | M(y_2) | \zeta' \rangle \qquad (4.11)$$

Here

$$\tilde{\Delta}(k) = \tilde{\rho}_0^{-1}(k|s) - \int dk_2 \, \tilde{W}(k - k_2) \tilde{\rho}_0(k_2|s) \qquad (4.12)$$

It is now possible to make a revised expansion. In lowest order

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = W(\zeta - \zeta) F(\zeta - \zeta') \qquad (4.13)$$

with

$$F(s) = \frac{1}{(2\pi)^d} \int \frac{e^{-ik\zeta} \, dk}{\tilde{\Delta}(k)} \qquad (4.14)$$

The "screening" of $M(y_1)$ by $\tilde{\Delta}(k)$ is associated with the first diagram of Fig. 2. However, this type of diagram does not occur when the mass operator is expressed in terms of exact propagators $\rho(s)$. This will be done in the next section. The expression in terms of exact propagators is both logically simpler and more accurate.

4.1. Bare Propagator Expansions for Phonon Problems

We now study the optical phonon problems using the functional equation (3.26). We use the notation

$$M(1, 2, \ldots | s) = M(y_1 \alpha_1 y_2 \alpha_2 | s)$$

for the functional derivatives at $J = 0$. The hierarchy is

$$\langle \zeta | \rho_0^{-1} \rho - 1 | \zeta' \rangle = \int d(1) \, W(\zeta - y_1 | \alpha_1) \langle \zeta | M(1) | \zeta' \rangle \qquad (4.15)$$

$$\langle \zeta | \left[\rho_0^{-1}(s) + \alpha_1 \omega \right] M(1 | s) | \zeta' \rangle \delta(\zeta - y_1)$$
$$+ \int d(2) \, W(\zeta - y_2 | \alpha_2) \langle \zeta | M(1,2 | s) | \zeta' \rangle \qquad (4.16)$$

$$\langle \zeta | \left[\rho^{-1}(s) + (\alpha_1 + \alpha_2) \omega \right] M(1,2 | s) | \zeta' \rangle$$
$$= \delta(\zeta - y_1) \langle \zeta | M(2 | s) | \zeta' \rangle + \delta(\zeta - y_2) \langle \zeta | M(1 | s) | \zeta' \rangle$$
$$+ \int d(3) \, W(\zeta - y_3 | \alpha_3) \langle \zeta | M(1,2,3 | s) | \zeta' \rangle \qquad (4.17)$$

The new point is the appearance of phonon-modified propagators

$$\rho_0^{-1}(s) + (\alpha_1 + \alpha_2) \omega = \rho_0^{-1}(s + (\alpha_1 + \alpha_2) \omega) \qquad (4.18)$$

Equation (4.16) may be rewritten as

$$\langle \zeta | M(1 | s) | \zeta' \rangle$$
$$= \langle \zeta | \rho_0(s + \alpha_1 \omega) | y_1 \rangle \langle y_1 | \rho(s) | \zeta' \rangle$$
$$+ \int d(2) \int \langle \zeta | \rho_0(s + \alpha_1 \omega) | z \rangle \, dz \, W(z - y_2) \langle z | M(1,2 | s) | \zeta' \rangle \quad (4.19)$$

Equation (4.17) is

$$\langle \zeta | M(1,2 | s) | \zeta' \rangle = \langle \zeta | \rho_0(s + (\alpha_1 + \alpha_2) \omega) | y_1 \rangle \langle y_1 | M(z) | \zeta' \rangle + 1 \rightleftarrows 2$$
$$+ \int d(3) \int dz \, \langle \zeta | \rho_0(s + (\alpha_1 + \alpha_2) \omega) | z \rangle$$
$$\times W(z - y_3) \langle z | M(1,2,3 | s) | \zeta' \rangle \qquad (4.20)$$

From this point we proceed just as in the Gaussian random case. To order W the mass operator is

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = \int d\alpha_1 \, W(\zeta - \zeta' | \alpha_1) \langle \zeta | \rho_0(s + \alpha_1 \omega) | \zeta' \rangle \qquad (4.21)$$

which may be pictured as shown in Fig. 4. The second-order correction may be read off from the diagrams in Fig. 5. The electron propagator between two points depends on the number of phonon lines above it.
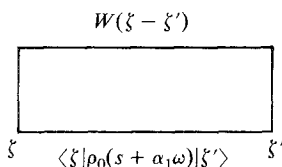
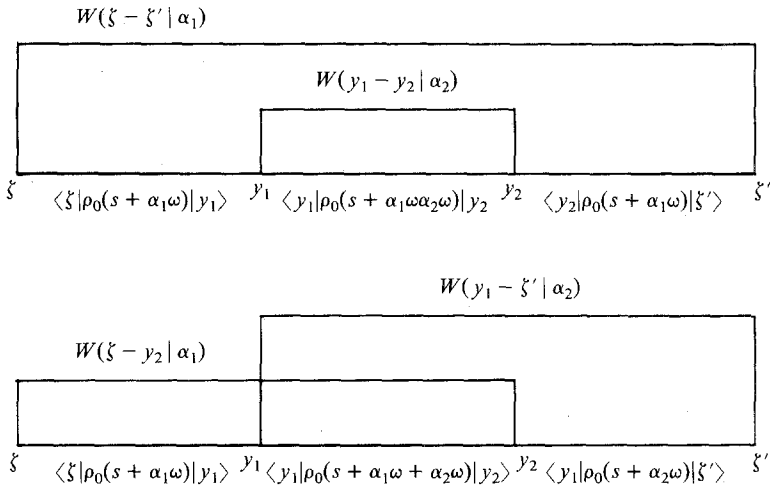$$W(\zeta - \zeta')$$

$$\zeta \qquad \langle \zeta | \rho_0(s + \alpha_1 \omega) | \zeta' \rangle \qquad \zeta'$$

Fig. 4.

$W(\zeta - \zeta' \mid \alpha_1)$

$W(y_1 - y_2 \mid \alpha_2)$

ζ $\langle \zeta | \rho_0(s + \alpha_1\omega) | y_1 \rangle$ y_1 $\langle y_1 | \rho_0(s + \alpha_1\omega\alpha_2\omega) | y_2 \rangle$ y_2 $\langle y_2 | \rho_0(s + \alpha_1\omega) | \zeta' \rangle$ ζ'

$W(y_1 - \zeta' \mid \alpha_2)$

$W(\zeta - y_2 \mid \alpha_1)$

ζ $\langle \zeta | \rho_0(s + \alpha_1\omega) | y_1 \rangle$ y_1 $\langle y_1 | \rho_0(s + \alpha_1\omega + \alpha_2\omega) | y_2 \rangle$ y_2 $\langle y_1 | \rho_0(s + \alpha_2\omega) | \zeta' \rangle$ ζ'

Fig. 5.

In the approximation that neglects $M(123)$, we eliminate $M(12)$ to find an equation for $M(1 \mid s)$. It is

$$\langle \zeta | \rho_0^{-1}(s + \alpha_1\omega)M(1) | \zeta' \rangle - \int d(2)\, W(\zeta - y_2 \mid \alpha_2)$$

$$\times \langle \zeta | \rho_0(s + \alpha_1\omega + \alpha_2\omega) | y_2 \rangle \langle y_2 | M(1) | \zeta' \rangle$$

$$= \langle \zeta | \rho(s) | \zeta' \rangle \delta(\zeta - y_1) + \int d(2)\, W(\zeta - y_2 \mid \alpha_2)$$

$$\times \langle \zeta | \rho_0(s + \alpha_1\omega + \alpha_2\omega) | y_1 \rangle \langle y_1 | M(2) | \zeta' \rangle \qquad (4.22)$$

In taking the Fourier transform we encounter

$$\tilde{\Delta}(k \mid \alpha_1) = s + \alpha_1\omega + \frac{k^2}{2} - \int \tilde{F}(k | 0 | s + \alpha_1\omega + \alpha_2\omega)\, d\alpha_2 \qquad (4.23)$$

Here

$$\tilde{F}(k | y_1 - y_2 | s + \alpha_1\omega + \alpha_2\omega)$$

$$= \int d\zeta\, e^{ik\zeta} W(\zeta + y_1 - y_2 \mid \alpha_2)\langle \zeta | \rho_0(s + \alpha_1\omega + \alpha_2\omega) | 0 \rangle \qquad (4.24)$$

The equation for $M(1)$ is

$$\langle k | \tilde{M}(1) | \zeta' \rangle \tilde{\Delta}(k \mid \alpha_1)$$

$$= e^{iky_1}\langle y_1 | \rho(s) | \zeta' \rangle$$

$$+ \int d\alpha_2\, dy_2\, \tilde{F}(k | y_1 - y_2 | s + \alpha_1\omega + \alpha_2\omega)e^{iky_1}\langle y_1 | M(2) | \zeta' \rangle \qquad (4.25)$$

Thus we can again make a W expansion with screened propagators.

Finally we study the general finite temperature action (3.30). The equations of the hierarchy at $J = 0$ are

$$\langle \zeta | \rho_0^{-1} \rho - 1 | \zeta' \rangle = \int d(1)\, \tilde{W}(k_1 | \alpha_1) e^{ik_1(\zeta - y_1)} \langle \zeta | M(1) | \zeta' \rangle \quad (4.26)$$

$$\langle \zeta | \left[\rho_0^{-1}(s) + \alpha_1 \omega_1 \right] M(1) | \zeta' \rangle = \langle \zeta | \rho(s) | \zeta' \rangle \delta(\zeta - y_1)$$
$$+ \int d(2)\, \tilde{W}(k_2 | \alpha_2) e^{ik_2(\zeta - y_2)} \langle \zeta | M(1,2) | \zeta' \rangle$$

$$(4.27)$$

$$\langle \zeta | \left[\rho_0^{-1}(s) + \alpha_1 \omega_1 + \alpha_2 \omega_2 \right] M(1,2) | \zeta' \rangle$$
$$= \delta(\zeta - y_1) \langle \zeta | M(2) | \zeta' \rangle + 1 \rightleftarrows 2$$
$$+ \int d(3)\, \tilde{W}(k_3 | \alpha_3) e^{ik_3(\zeta - y_3)} \langle \zeta | M(1,2,3) | \zeta' \rangle \quad (4.28)$$

Everything proceeds as in earlier cases. In lowest order

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = \int dk_1\, d\alpha_1\, \tilde{W}(k_1 | \alpha_1) e^{ik_1(\zeta - \zeta')} \langle \zeta | \frac{1}{\rho_0^{-1}(s) + \alpha_1 \omega(k_1)} | \zeta' \rangle$$

$$(4.29)$$

5. MASS OPERATORS AND EXACT PROPAGATORS

In the present section we analyze the mass operator $\Sigma(s)$ when it is expressed in terms of exact propagators $\rho(s)$. This then implies that a difficult nonlinear self-consistency problem is encountered. However, there is a gain both in logical simplicity and in accuracy. The lowest approximation is a simple coherent potential approximation applicable to the finite temperature case. Once one has a functional equation for $I(s)$ one can set in motion the machinery developed by Dyson, Feynman, and Schwinger. The first step is to find a functional equation for Σ_J.

5.1. Gaussian Random Potential

We multiply Eq. (3.10) by I^{-1} on the right-hand side and use $\Sigma_J = \rho_0^{-1} - I^{-1}$ to obtain

$$\langle \zeta | \Sigma_J | \zeta' \rangle = \int dy_1\, W(\zeta - y_1) \langle \zeta | \frac{\delta \Sigma_J}{\delta J(y_1)} I^{-1} | \zeta' \rangle + J(\zeta) \delta(\zeta - \zeta') \quad (5.1)$$

Now

$$\frac{\delta}{\delta J(y_1)} (II^{-1}) = 0 \quad (5.2)$$

implies

$$\frac{\delta I}{\delta J(y_1)} I^{-1} = I \frac{\delta \Sigma_J}{\delta J(y_1)} \tag{5.3}$$

So we have the functional equation for Σ_J

$$\langle \zeta | \Sigma_J | \zeta' \rangle = J(\zeta) \delta(\zeta - \zeta') + \int dy_1 \, W(\zeta - y_1) \langle \zeta | I \frac{\delta \Sigma_J}{\delta J(y_1)} | \zeta' \rangle \tag{5.4}$$

It involves the exact propagator I, rather than $\rho_0(s)$. Next, we want to take functional derivatives to form a hierarchy. Note that we repeatedly use

$$\frac{\delta I}{\delta J(y_1)} = I \frac{\delta \Sigma_J}{\delta J(y_1)} I$$

Define

$$\Phi(y_1) = I \frac{\delta \Sigma_J}{\delta J(y_1)} \tag{5.5}$$

We will frequently write $J(1)$ for $J(y_1)$, $\Phi(1)$ for $\Phi(y_1)$, etc. Taking functional derivatives and setting $J = 0$ yields the hierarchy

$$\langle \zeta | \Sigma_J | \zeta' \rangle = J(\zeta) \delta(\zeta - \zeta') + \int dy_1 \, W(\zeta - y_1) \langle \zeta | \Phi(1) | \zeta' \rangle \tag{5.6}$$

$$\langle \zeta | \Phi(1) | \zeta' \rangle$$

$$= \langle \zeta | I | \zeta' \rangle \delta(\zeta' - y_1) + \int dy_2 \int dz \, \langle \zeta | I | z \rangle W(z - y_2) \langle z | \frac{\delta \Phi(2)}{\delta J(1)} | \zeta' \rangle \tag{5.7}$$

$$\langle \zeta | \frac{\delta \Phi(2)}{\delta J(1)} | \zeta' \rangle = \langle \zeta | \Phi(1) I | \zeta' \rangle \delta(\zeta - y_2)$$

$$+ \int \int dz \, dy_1 \, \langle \zeta | \Phi(1) I | z \rangle W(z - y_1) \langle z | \frac{\delta \Phi(2)}{\delta J(1)} | \zeta' \rangle$$

$$+ \int dz \, \langle \zeta | I | z \rangle \int dy_3 \, W(z - y_3) \langle z | \frac{\delta \Phi(3)}{\delta J(2) \delta J(1)} | \zeta' \rangle \tag{5.8}$$

Note that we have interchanged 1 and 2 in the last equation, to prepare for insertion in the previous equation.

The crudest approximation is to neglect $\delta \Phi(2) | \delta J(1)$. Then since I at $J = 0$ is $\rho(s)$

$$\langle \zeta | \Sigma | \zeta' \rangle = W(\zeta - \zeta') \langle \zeta | \rho | \zeta' \rangle \tag{5.9}$$

which is pictured as shown in Fig. 6.

$$W(\zeta - \zeta')$$
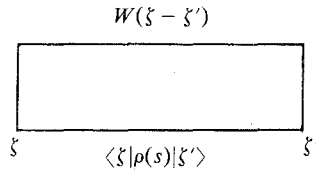

$$\langle \zeta | \rho(s) | \zeta' \rangle$$

Fig. 6.

In the next approximation we replace $\delta \Phi(2)/\delta J(1)$ by its value at $W = 0$. This leads to a linear equation for $\Phi(1)$

$$\langle \zeta | \Phi(1) | \zeta' \rangle = \langle \zeta | \rho | \zeta' \rangle \delta(\zeta' - y_1)$$
$$+ \int dz \, \langle \zeta | \rho | z \rangle W(z - \zeta') \langle z | \Phi(1) \rho | \zeta' \rangle \qquad (5.10)$$

If we replace $\Phi(1)$ by its zeroth-order value in the second term we get Σ to accuracy W^2. Relabeling the dummy variables, we find (at $J = 0$)

$$\langle \zeta | \Sigma | \zeta' \rangle = W(\zeta - \zeta') \langle \zeta | \rho | \zeta' \rangle$$
$$+ \int \int dy_1 \, dy_2 \, W(\zeta - y_2) W(y_1 - \zeta') \langle \zeta | \rho | y_1 \rangle \langle y_1 | \rho | y_2 \rangle \langle y_2 | \rho | \zeta' \rangle$$

$$(5.11)$$

The second term may be pictured as shown in Fig. 7. When we use exact propagators, only the completely linked second-order diagram occurs. This observation was made long ago by Edwards.[16]

The solution of the equation for $\Phi(1)$ corresponds to including an infinite number of additional graphs. The result of Σ is still in error in the W^3 term. The integral equation can be solved exactly for the case of one-dimensional white noise, when $W(x) = \lambda \delta(x)$. We find

$$\langle \zeta | \Phi(y_1) | \zeta' \rangle = \langle \zeta | \rho | \zeta' \rangle \left[\delta(\zeta' - y_1) + \frac{\lambda^2}{2\pi} \int e^{ik(y - \zeta')} \frac{\tilde{R}(k)}{1 - \lambda \tilde{R}(k)} dk \right] \qquad (5.12)$$
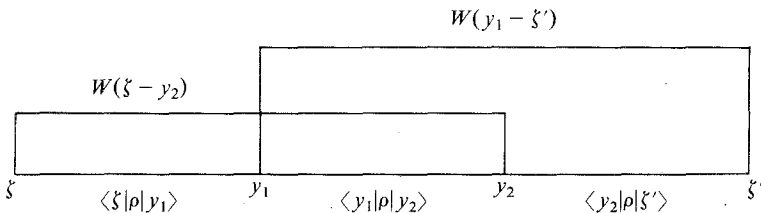
$$W(y_1 - \zeta')$$

$$W(\zeta - y_2)$$

$$\zeta \qquad \langle \zeta | \rho | y_1 \rangle \qquad y_1 \qquad \langle y_1 | \rho | y_2 \rangle \qquad y_2 \qquad \langle y_2 | \rho | \zeta' \rangle \qquad \zeta'$$

Fig. 7.

with

$$\tilde{R}(k) = \int dz \, e^{ikz} \langle z|\rho|0\rangle\langle 0|\rho|z\rangle \tag{5.13}$$

Then

$$\langle \zeta|\Sigma|\zeta'\rangle = \lambda\langle\zeta|\Phi(\zeta)|\zeta'\rangle$$

$$= \lambda\langle\zeta|\rho|\zeta'\rangle\left[\delta(\zeta - \zeta') + \frac{\lambda}{2\pi}\int e^{ik_1(\zeta-\zeta')}\frac{\tilde{R}(k_1)}{1-\lambda\tilde{R}(k_1)}dk_1\right] \tag{5.14}$$

and finally

$$\tilde{\Sigma}(k \mid s) = \lambda\langle 0|\rho|0\rangle + \frac{\lambda^2}{2\pi}\int\frac{\tilde{R}(k_1)}{1-\lambda\tilde{R}(k_1)}\tilde{\rho}(k+k_1 \mid s)\,dk_1 \tag{5.15}$$

5.2. Ground-State Polaron Mass Operator

We turn next to the ground-state polaron problem, where the functional equation for $I(s)$ is Eq. (3.26). This leads to the equation for Σ_J:

$$\langle\zeta|\Sigma_J(s)|\zeta'\rangle + \omega\int dy_1\langle\zeta|IJ(y_1)\frac{\delta\Sigma_J}{\delta J(y_1)}|\zeta'\rangle$$

$$= J(\zeta)\delta(\zeta-\zeta') + \int dy_1\,W(\zeta-y_1)\langle\zeta|\Phi(y_1)|\zeta'\rangle \tag{5.16}$$

Again $\Phi(y_1) = I\delta\Sigma_J \mid \delta J(y_1)$.

The equation for $\Phi(y_1)$ is now modified in an interesting way. We introduce

$$Q(s \mid \omega) = \left[\omega + I^{-1}(s)\right]^{-1} \tag{5.17}$$

At $J = 0$, $Q \to Q_0$,

$$Q_0(s \mid \omega) = \left[\rho_0^{-1}(s + \omega) - \Sigma(s)\right]^{-1} \tag{5.18}$$

Now rewrite the equation for $\Phi(1)$ as

$$\langle\zeta|\Phi(y_1)|\zeta'\rangle = \langle\zeta| Q(s \mid \omega)|\zeta'\rangle\delta(y_1 - \zeta')$$

$$+ \int dy_2\int dz\,\langle\zeta| Q(s \mid \omega)|z\rangle W(z-y_2)\langle z|\frac{\delta\Phi(2)}{\delta J(1)}|\zeta'\rangle$$

$$- \omega\int dy_2\langle\zeta| Q(s \mid \omega)J(2)\frac{\delta\Phi(1)}{\delta J(2)}|\zeta'\rangle \tag{5.19}$$

$$W(\zeta - \zeta')$$

$$\zeta \qquad \langle \zeta | Q_0(s \,|\, \omega) | \zeta' \rangle \qquad \zeta'$$
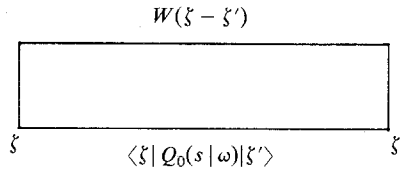
Fig. 8.

To lowest order in W, and going to the limit $J = 0$

$$\langle \zeta | \Sigma | \zeta' \rangle = W(\zeta - \zeta') \langle \zeta | \frac{1}{\rho_0^{-1}(s + \omega) - \Sigma(s)} | \zeta' \rangle \qquad (5.20)$$

This may be pictured as shown in Fig. 8. The electron propagator is modified by the phonon line above it.

The next equation is for $\delta\Phi(1)/\delta J(2)$. After some algebraic manipulation, one finds

$$\langle \zeta | [1 + \omega Q(s \,|\, \omega)] \frac{\delta\Phi(1)}{\delta J(2)} | \zeta' \rangle$$

$$= \langle \zeta | \frac{\delta Q(s \,|\, \omega)}{\delta J(1)} | \zeta' \rangle \delta(y_1 - \zeta')$$

$$+ \int dy_3 \int dz \, \langle \zeta | \frac{\delta Q(s \,|\, \omega)}{\delta J(2)} | z \rangle W(z - y_3) \langle z | \frac{\delta\Phi(3)}{\delta J(1)} | \zeta' \rangle$$

$$+ \int dy_3 \int dz \, \langle \zeta | Q(s \,|\, \omega) | z \rangle W(z - y_3) \langle z | \frac{\delta^2\Phi(3)}{\delta J(1)\delta J(2)} | \zeta' \rangle$$

$$- \omega \int dy_3 \langle \zeta | \left[\frac{\delta Q(s \,|\, \omega)}{\delta J(2)} J(3) + Q(s \,|\, \omega) J(3) \right] \frac{\delta^2\Phi(1)}{\delta J(3)\delta J(2)} | \zeta' \rangle$$

$$(5.21)$$

We will need this at $J = 0$. In addition we drop the term $\delta^2\Phi(s)/\delta J(1) \delta J(2)$. First we require an expression for $\delta Q(s \,|\, \omega)/\delta J(2)$. From

$$\frac{\delta}{\delta J(2)} [QQ^{-1}] = 0 \qquad (5.22)$$

$$\frac{\delta Q}{\delta J(2)} = Q \frac{\delta\Sigma(s)}{\delta J(2)} Q = \Phi(2) Q(s \,|\, \omega) \qquad (5.23)$$

Hence, at $J = 0$, the first three hierarchy equations are

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = \int dy_1 \, W(\zeta - y_1) \langle \zeta | \Phi(1) | \zeta' \rangle \tag{5.24}$$

$$\langle \zeta | \Phi(1) | \zeta' \rangle = \langle \zeta | Q_0(s | \omega) | \zeta' \rangle \delta(y_1 - \zeta')$$

$$+ \int dz \int dy_2 \langle \zeta | Q_0(s | \omega) | z \rangle W(z - y_2) \langle z | \frac{\delta \Phi(2)}{\delta J(1)} | \zeta' \rangle \tag{5.25}$$

$$\langle \zeta | \frac{\delta \Phi(1)}{\delta J(2)} | \zeta' \rangle = \langle \zeta | \frac{1}{1 + \omega Q_0} \Phi(2) Q_0 | \zeta' \rangle \delta(y_1 - \zeta')$$

$$\times \int dy_3 \int dz \langle \zeta | \frac{1}{1 + \omega Q_0} \Phi(2) Q_0 | z \rangle$$

$$\times W(z - y_3) \langle z | \frac{\delta \Phi(3)}{\delta J(1)} | \zeta' \rangle \tag{5.26}$$

If $\delta \Phi(1)/\delta J(2)$ is replaced by its value at $W = 0$, there is a self-contained equation for $\Phi(1)$:

$$\langle \zeta | \Phi(1) | \zeta' \rangle = \langle \zeta | Q | \zeta' \rangle \delta(y_1 - \zeta')$$

$$+ \int dz \langle \zeta | Q | z \rangle W(z - \zeta') \langle z | \frac{1}{1 + \omega Q} \Phi(1) Q | \zeta' \rangle \tag{5.27}$$

The W^2 correction to Σ is

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = W(\zeta - \zeta') \langle \zeta | Q_0(s | \omega) | \zeta' \rangle$$

$$+ \int \int dy_1 dy_2 \, W(\zeta - y_2) W(y_1 - \zeta') \langle \zeta | Q_0(s | \omega) | y_1 \rangle$$

$$\times \langle y_1 | Q_0(s | 2\omega) | y_2 \rangle \langle y_2 | Q_0(s | \omega) | \zeta' \rangle \tag{5.28}$$

with $Q_0^{-1}(s | n\omega) = \rho_0^{-1}(s + n\omega) - \Sigma(s)$. The expression for $\Sigma(s)$ may be pictured as in Fig. 9. We have the rule that the propagator between two points is $Q_0(s | n\omega)$ if there are n lines above the propagator.

There is an exact solution to the equation for $\Phi(1)$ for the case of a one-dimensional polaron with $W(x) = \lambda \delta(x)$. We set down the final result
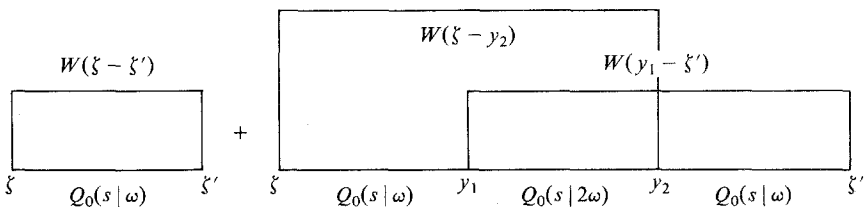

Fig. 9.

for $\tilde{\Sigma}(k\,|\,s)$. It is

$$
\tilde{\Sigma}(k_1\,|\,s) = \lambda\langle 0|\,\frac{1}{\rho_0^{-1}(s+\omega) - \Sigma(s)}\,|0\rangle
$$

$$
+ \frac{\lambda^2}{2\pi}\int\frac{dk_1}{\left[s + \omega + (k + k_1)^2/2 - \tilde{\Sigma}(k + k_1\,|\,s)\right]}\,\frac{\tilde{R}(k_1\,|\,s)}{1 - \lambda\tilde{R}(k_1\,|\,s)}
$$

$$(5.29)$$

Here

$$
\tilde{R}(k_1\,|\,s) = \int\frac{dk_2}{\left[s + 2\omega + k_2^2/2 - \tilde{\Sigma}(k_2\,|\,s)\right]}
$$

$$
\times\frac{1}{\left[s + \omega + (k_1 + k_2)^2/2 - \tilde{\Sigma}(k_1 + k_2\,|\,s)\right]}\qquad(5.30)
$$

This is of course accurate to order λ^2. But there is now a formidable self-consistency problem, particularly since the mass operator is dependent on the wave vector k.

We now consider the finite temperature polaron problem. The preceding results can be taken over directly if we interpret $J(1) = J(y_1\,|\,\alpha_1)$, $\int d(1) = \int\int dy_1\,d\alpha_1$. The equation for Σ_J is

$$
\langle\zeta|\Sigma_J|\zeta'\rangle + \omega\int d(1)\,\alpha_1\langle\zeta|IJ(1)\frac{\delta\Sigma_J}{\delta J(1)}\,|\zeta'\rangle
$$

$$
= \delta(\zeta - \zeta')\int d(1) J(1)\delta(y_1 - \zeta)
$$

$$
+ \int d(1)\,W(\zeta - y_1\,|\,\alpha_1)\langle\zeta|\Phi(1)|\zeta'\rangle\qquad(5.31)
$$

At $J = 0$

$$
\langle\zeta|\,Q_0^{-1}(s\,|\,\alpha_1\omega)\Phi(1)|\zeta'\rangle = \delta(\zeta - \zeta')\delta(y_1 - \zeta')
$$

$$
\times\int d(2)\,(\zeta - y_2\,|\,\alpha_2)\langle\zeta|\frac{\delta\Phi(2)}{\delta J(1)}\,|\zeta'\rangle\quad(5.32)
$$

The simplest coherent potential approximation is

$$
\langle\zeta|\Sigma|\zeta'\rangle = \int d\alpha_1\,W(\zeta - \zeta'\,|\,\alpha_1)\langle\zeta|\,Q_0(s\,|\,\alpha_1\omega)|\zeta'\rangle\qquad(5.33)
$$

The second-order correction to the mass operator involves the propagators $Q_0(s\,|\,\alpha_1\omega)$, $Q_0(s\,|\,\alpha_1\omega + \alpha_2\omega)$, $Q_0(s\,|\,\alpha_2\omega)$, with integrations over α_1 and α_2.

Again only a slight change of notation to treat the general finite temperature phonon problem. Let $J(1) = J(k_1|y_1|\alpha_1)$, $\omega_1 = \omega(k_1)$, $d(1) = dk_1\,dy_1\,d\alpha_1$, etc. Then we only have to replace

$$
W[\zeta - y_1\,|\,\alpha_1] \to \tilde{W}(k_1\,|\,\alpha_1)e^{ik_1(\zeta - y_1)}
$$

Thus

$$\langle \zeta | \Sigma_J | \zeta' \rangle + \int d(1)\, \alpha_1 \omega_1 \langle \zeta | IJ(1)\, \frac{\delta}{\delta J(1)} \Sigma_J | \zeta' \rangle$$

$$= \int d(1)\, J(1)\delta(\zeta - y_1)\delta(\zeta - \zeta')$$

$$+ \int d(1)\, \tilde{W}(k_1 | \alpha_1)e^{ik_1(\zeta - y_1)}\langle \zeta | \Phi(1) | \zeta' \rangle \qquad (5.34)$$

The equation for $\Phi(1) = \delta \Sigma_J / \delta J(k_1 | y_1 | \alpha_1)$ is

$$\langle \zeta | Q^{-1}(s | \alpha_1 \omega_1)\Phi(1) | \zeta' \rangle = \delta(y_1 - \zeta')\delta(\zeta' - \zeta')$$

$$+ \int d(2)\, \tilde{W}(k_2 | \alpha_2)e^{ik_2(\zeta - y_2)}\langle \zeta | \frac{\delta \Phi(2)}{\delta J(1)} | \zeta' \rangle$$

$$- \int d(2)\, \alpha_2 \omega_2 \langle \zeta | J(2)\, \frac{\delta \Phi(1)}{\delta J(2)} | \zeta' \rangle \qquad (5.35)$$

$$Q^{-1}(s | \alpha_1 \omega_1) = I^{-1}(s) + \alpha_1 \omega(k_1) \qquad (5.36)$$

The lowest approximation at $J = 0$ is

$$\langle \zeta | \Sigma(s) | \zeta' \rangle = \int d(1)\, \tilde{W}(k_1 | \alpha_1)e^{ik_1(\zeta - \zeta')}\langle \zeta | Q_0(s | \alpha_1 \omega_1) | \zeta' \rangle \quad (5.37)$$

To proceed to higher approximations use

$$\frac{\delta Q^{-1}}{\delta J(2)}(s | \alpha_1 \omega_1) = -\frac{\delta \Sigma}{\delta J(2)} = -I^{-1}\Phi(2) \qquad (5.38)$$

$$Q^{-1}(s | \alpha_1 \omega_1 + \alpha_2 \omega_2) = I_0^{-1}(s + \alpha_1 \omega_1 + \alpha_2 \omega_2) - \Sigma_J(s) \qquad (5.39)$$

At $J = 0$ this leads to

$$\langle \zeta | Q_0^{-1}(s | \alpha_1 \omega_1 + \alpha_2 \omega_2)\, \frac{\delta \Phi(1)}{\delta J(2)} | \zeta' \rangle$$

$$= \langle \zeta | I^{-1}(1)\Phi(2)\Phi(1) | \zeta' \rangle$$

$$+ \int d(3)\, \tilde{W}(3)e^{ik_3(\zeta - y_3)}\langle \zeta | \frac{\delta^2 \Phi(3)}{\delta J(2)\delta J(1)} | \zeta' \rangle \qquad (5.40)$$

Neglecting $\delta^2 \Phi(3)/\delta J(2)\delta J(1)$ we have an equation for $\Phi(1)$

$$\langle \zeta | Q_0^{-1}(s | \alpha_1 \omega_1)\Phi(1) | \zeta' \rangle$$

$$= \delta(y_1 - \zeta')\delta(\zeta - \zeta')$$

$$+ \int d(2)\, \tilde{W}(k_2 | \alpha_2)e^{ik_2(\zeta - y_2)}\langle \zeta | Q_0(s | \alpha_1 \omega_1 + \alpha_2 \omega_2)I^{-1}\Phi(1)\Phi(2) | \zeta' \rangle$$

$$(5.41)$$

This concludes our discussion of generalized coherent potential approximation, i.e., approximations to the mass operator in terms of exact propagators, so that one has self-consistent type equations for the determination of $\tilde{\Sigma}(k\,|\,s)$.

6. A SECOND TYPE OF GENERATING ACTION

We return to the ground-state polaron action and show that a different functional equation can be derived. Introduce the generating functional

$$B_K(T) = \int dz\, K(z)\left[\int_0^T du\, \delta(x(u) - z)e^{\omega u}\, du\right] \tag{6.1}$$

This differs from the previous $A_J(T)$ by a factor $e^{-\omega T}$. We find

$$\langle\zeta|\hat{I}(T) - \hat{\rho}_0(T)|\zeta'\rangle$$

$$= \int dz \int_0^T dt\, \langle\zeta|\hat{\rho}_0(T - t)|z\rangle$$

$$\times\left[\int dy_1\, W(z - y_1)e^{-\omega t}\frac{\delta}{\delta J(y_1)} + K(z)e^{\omega t}\right]\langle z|\hat{I}(t)|\zeta'\rangle \tag{6.2}$$

Taking the Laplace transform

$$\langle\zeta|\rho_0^{-1}(s)I(s) - 1|\zeta'\rangle = \int dy_1\, W[\zeta - y_1]\frac{\delta}{\delta K(y_1)}\langle\zeta|I(s + \omega)|\zeta'\rangle$$

$$+ K(\zeta)\langle\zeta|I(s - \omega)|\zeta'\rangle \tag{6.3}$$

While the equation has a simpler dependence on the functional derivative, it is a difference equation in the s variable. The bare propagator theory is even simpler than with the A_J generator. Thus the second equation of the hierarchy is, at $K = 0$

$$\langle\zeta|\rho_0^{-1}(s + \omega)\frac{\delta I(s + \omega)}{\delta K(y_1)}|\zeta'\rangle = \delta(\zeta - y_1)\langle\zeta|I(s)|\zeta'\rangle$$

$$\times\int dy_2\, W(\zeta - y_2)\langle\zeta|\frac{\delta^2 I(s + \omega)}{\delta K(y_2)\delta K(y_1)}|\zeta'\rangle \tag{6.4}$$

and we easily obtain our earlier results.

The functional equation for Σ_K, which leads to dressed propagator expansions, however, appears to be less convenient. We use

$$\frac{\delta I(s + \omega)}{\delta K(y_1)} = I(s + \omega)\frac{\delta\Sigma_K(s + \omega)}{\delta K(y_1)}I(s + \omega) \tag{6.5}$$

to derive

$$\langle \zeta | \Sigma_K(s) \cdot I(s) | \zeta' \rangle = K(\zeta)\langle \zeta | I(s+\omega) | \zeta' \rangle$$

$$+ \int W(\zeta - y_1) I(s+\omega) \frac{\delta \Sigma_K(s+\omega)}{\delta K(y_1)} \cdot I(s+\omega) | \zeta' \rangle$$

$$(6.6)$$

We have found the Σ_J functional equation to be easier to work with.

7. CONCLUSIONS

Our starting point has been the path integral for the density matrix that results when the phonon degrees of freedom are exactly eliminated. The aim is to provide approximations for the mass operator in terms of exact propagators. We do this by adding special generating functionals to the action and then constructing functional derivative equations.

It is possible to extend the procedure to compute averages of products of density matrices and also time–temperature Green's functions. This makes contact with the important work of Kadanoff, Langreth, and Rev-zen[21] on the transport properties of polarons.

A word of caution is in order. The field theory description presented here does not treat deep traps properly. For the Gaussian random potential problem the Laplace transform of the density matrix does not exist. If the covariance function $W(x)$ is a constant W_0, the density matrix $\hat{\rho}(\beta)$ has a term $\exp(W_0 \beta^2 / 2)$. If $W(x)$ has a Taylor series expansion in x^2, there is a term proportional to $\beta^{3/2}$. It would be desirable to have a theory that includes these asymptotic features as well as being in terms of exact propagators. One way to do this is to base the formalism on a quadratic trial action rather than on a free particle action. This extension will be discussed elsewhere.

For electron–phonon problems, there is no difficulty with the Laplace transforms. However, the exact propagator approach does not treat the strong-coupling (Pekar) limit of the polaron in a satisfactory manner. Again, a possible way to handle this is to use a quadratic trial action as the starting point. In this way one can embed the Feynman polaron theory in a systematic field theory approach.

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