SECOND ORDER CORRECTIONS TO THE VARIATIONAL APPROXIMATION TO FROLICH'S POLARON MODEL

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Abstract

Using Feynman's path integral variational principle with a general quadratic trial action, we obtain equations for the absorption function of Frolich's polaron model. We evaluate numerically this absorption function in several cases. To test the accuracy of the variational absorption function, we develop formulas for the second order corrections to the absorption function and evaluate these numerically.

Rather than evaluating the correction directly in the double path integral formalism, we make analytic continuations in time which reduce the amount of labor involved in deriving the expressions for the corrections. The method of analytic continuation in time is generalized in such a way as to allow application of the variational principle to nonlinear transport problems and time dependent problems.

Finally, we present the variational equations and the second order corrections to them for a somewhat more realistic model of an electron in a crystal.

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1. INTRODUCTION

1.1. History

The problem of getting reliable numbers from field theories when perturbative methods are inapplicable is of immense interest. A successful example of such a calculation is Feynman's [1] application of his path integral variational principle to find the energy and effective mass of an electron in a polarizable crystal. The calculation was actually done on an idealized model of a polaron * developed by Frolich [2]. This model has become a standard on which to try various methods of computation. We discuss the details of this model below.

Others extended Feynman's calculation to find the polaron free energy at nonzero temperatures. Feynman,Hellworth,Iddings,and Platzman [4] (referred to as FHIP in the following) used path integral techniques to obtain an expression for the electron's response to weak external fields (that is, it's impedance function) at all frequencies,temperatures, and coupling strengths.

A check on the accuracy of Feynman's original calculation was made by Marshall and Mills [5] who computed the second order corrections to the polaron's energy. They found that the correction was never more than two percent at any value of the coupling.

The purpose of this thesis is to improve the FHIP impedance calculation by using a more general trial action in the variational method and to obtain an estimate of the reliability of the variational impedance function by calculating the second order corrections to it. The variational equations we obtain for the impedance function have recently been obtained by others by a nonvariational method [6].

* Polaron is the term used for the quasiparticle consisting of an electron with its associated cloud of virtual phonons.

1.2. Frolich's Model

Frolich's model takes the electron part of the Lagrangian to be just $\frac{1}{2}m\dot{\mathbf{r}}^2$ where m is an effective mass and $\dot{\mathbf{r}}$ is the electron's velocity vector. This approximation has some justification for slow electrons in a crystal with sufficient symmetry. As far as the path integral approach is concerned, the electron kinetic energy could be generalized to say $\frac{1}{2}\sum_{i,j} m_{ij}\dot{x}_i\dot{x}_j$ where $\dot{x}_i$ is a component of the electron velocity and m_{ij} is an effective mass tensor. The effect of the crystal lattice on the electron could be better accounted for by including a periodic potential $V(\mathbf{r})$ in the electron Lagrangian. However,this would make it more difficult to find a calculationally tractable trial action for the variational method.

The main idealization which Frolich's model makes about the lattice portion of the Lagrangian is that the harmonic approximation is adequate. This is important for the path integral approach since it permits the lattice variables to be integrated away exactly. However,applying the variational inequality twice,we can approximately integrate the lattice variables and get an upper bound on the free energy even in the anharmonic case. We will say more about this later. For now, we stay with the Frolich model.

The electron interacts with the lattice via its electric field which attracts the positive ions and repels the negative ions. The electron interacts most strongly with lattice modes in which nearby ions of opposite sign move in opposite directions (optical modes). The Frolich model assumes that the electron interacts only with the optical phonons. To simplify further, the model assumes that the crystal has two ions per unit cell and that the optical phonon frequency does not vary with the wavevector $\mathbf{k}$. This wavevector independence of the phonon frequency is equivalent to no coupling between different unit cells. Let $\delta\mathbf{u}$ be the deviation from equilibrium of the vector from the negative to the positive ion

in a unit cell. The kinetic energy of the optical modes per unit volume of the crystal is then $\frac{1}{2}nM\left(\frac{d\,\delta\mathbf{u}}{dt}\right)^2$. Here n is the number density of unit cells and M is the reduced mass of the ions in a unit cell. For convenience we introduce rescaled phonon variables by $\mathbf{w}=\sqrt{nM}\,\delta\mathbf{u}$. $\mathbf{w}$ can be separated into its longitudinal and transverse pieces: $\mathbf{w}=\mathbf{w}_l+\mathbf{w}_t$. Here $\nabla\cdot\mathbf{w}_t=0$ and $\nabla\times\mathbf{w}_l=0$. We shall shortly see that only the longitudinal optical phonons (LO phonons) interact with the electron. Since we assume dispersionless LO phonons,the LO phonon Lagrangian can now be written as

$$L_{LO}=\frac{1}{2}\int\left(\dot{\mathbf{w}}_l^2-\omega_l^2\mathbf{w}_l^2\right)d^3\mathbf{r} \tag{1.2.1}$$

Here ω_l is the frequency of the longitudinal optical phonons.

It now remains to write down the electron-phonon interaction. Frolich's model divides the polarization of the crystal into the sum of two pieces $\mathbf{P}_l$ and $\mathbf{P}_t$. $\mathbf{P}_l$ is due to distortions of the lattice and is proportional to $\mathbf{w}$. $\mathbf{P}_t$ is due to distortion of the ions themselves. It is assumed that frequencies of interest are much less than the excitation frequencies of the ions. In this case we can write $\mathbf{P}_t=\frac{\varepsilon_\infty-1}{4\pi}\mathbf{E}$ where ε_∞ is the dielectric constant of the crystal with the ions held fixed and $\mathbf{E}$ is the total electric field. From $\nabla\cdot(\mathbf{E}+4\pi\mathbf{P})=0$ and the expression for $\mathbf{P}_t$ we now obtain

$$\nabla^2\varphi=4\pi\nabla\cdot\mathbf{P}=\frac{4\pi}{\varepsilon_\infty}\nabla\cdot\mathbf{P}_l \tag{1.2.2}$$

Since $\mathbf{P}_l$ is proportional to $\mathbf{w}$,we have

$$\nabla^2\varphi=4\pi C\nabla\cdot\mathbf{w}_l \tag{1.2.3}$$

Here φ is the electrostatic potential generated by a given deformation field $\mathbf{w}$

and C is a constant to be determined. For a particle in the crystal at $\mathbf{r}$ with charge q the interaction term in the Lagrangian will be $-q\,\varphi(\mathbf{r})$. To determine C we consider two heavy charged particles in the crystal. Their interaction energy is given by

$$\frac{1}{\varepsilon_0}\frac{q_1 q_2}{|\mathbf{r}_1-\mathbf{r}_2|} \tag{1.2.4}$$

Here ε_0 is the static dielectric constant of the crystal. If the ions are immobilized, the interaction energy of the two particles is

$$\frac{1}{\varepsilon_\infty}\frac{q_1 q_2}{|\mathbf{r}_1-\mathbf{r}_2|} \tag{1.2.5}$$

If we allow the ions to move, the effect of the optical phonons must be to restore (1.2.5) to (1.2.4). Thus if we write down the path integral for this system and integrate away the phonon variables, we should recover (1.2.4) as the interaction term between the two particles.

The action for several charged particles in a crystal is in Frolich's model

$$S = \int_{-\infty}^{+\infty} (L_{part} + L_{LO} - \sum_i q_i \varphi(\mathbf{r}_i))dt \tag{1.2.6}$$

where

$$L_{part} = \sum_i \frac{1}{2} m_i \dot{\mathbf{r}}_i^2 - \frac{1}{2}\sum_{i\neq j}\frac{q_i q_j}{\varepsilon_\infty |\mathbf{r}_i-\mathbf{r}_j|} \tag{1.2.7}$$

In (1.2.6) φ is linear in $\mathbf{w}_l$, as can be seen from (1.2.3). To find the effective action for the particles alone,the LO phonon variables must be integrated away. (units are such that $\hbar = 1$)

$$e^{iS_{eff}} = \int D(\textit{phonon variables})e^{iS} \tag{1.2.8}$$

To carry this out, define first new phonon variables $u(\mathbf{k})$ by

$$\mathbf{w}_l(\mathbf{r}) = \int \frac{d\mathbf{k}^3}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\mathbf{k}}{|\mathbf{k}|} u(\mathbf{k}) \tag{1.2.9}$$

Note that $u^*(\mathbf{k}) = -u(-\mathbf{k})$. Also let

$$\varphi(\mathbf{r}) = \int \frac{d\mathbf{k}^3}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\varphi}(\mathbf{k}) \tag{1.2.10}$$

(1.2.3) gives $-\mathbf{k}^2\hat{\varphi}(\mathbf{k}) = 4\pi i C u(\mathbf{k})$. (1.2.6) now becomes

$$S = \int_{-\infty}^{+\infty} \left\{ L_{part} + \frac{1}{2} \int \frac{d\mathbf{k}^3}{(2\pi)^3} [u^*(\mathbf{k})u(\mathbf{k}) - \omega_l^2 u^*(\mathbf{k})u(\mathbf{k})] - 4\pi q C i \sum_i \int \frac{d\mathbf{k}^3}{(2\pi)^3} \frac{u(\mathbf{k})}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{r}_i} \right\}$$

(1.2.11)

Now use the path integral

$$\int Dx \exp\left[i \int_{-\infty}^{+\infty} \left(\frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2 + \gamma x \right) dt \right] \propto \exp\left[-\frac{1}{4\omega} \int\int \gamma(t) e^{-i|t-s|} \gamma(s) dt ds \right]$$

(1.2.12)

to find that

$$\int Du e^{iS} \propto \exp\left[i \int L_{part}\, dt - \frac{4\pi^2 C^2}{\omega_l} \sum_{i,j} \int\int dt ds \int \frac{d\mathbf{k}^3}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}_i(t) - \mathbf{r}_j(s))}}{\mathbf{k}^2} e^{-i\omega_l|t-s|} \right]$$

(1.2.13)

Using $\int \frac{d\mathbf{k}^3}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathbf{k}^2} = \frac{1}{4\pi|\mathbf{r}|}$ we have

$$S_{eff} = \int L_{part}\, dt - \frac{\pi C^2}{\omega_l} \sum_{i,j} \int\int dt ds \frac{e^{-i\omega_l|t-s|}}{|\mathbf{r}_i(t) - \mathbf{r}_j(s)|} \tag{1.2.14}$$

For a slow heavy particle $\mathbf{r}(t)$ is nearly a constant for times of the order of ω_l^{-1}.

If such particles labeled by 1 and 2 are not too close to each other,then by using $\int e^{-i\omega|s|}=\frac{2}{i\omega}$,we find from S_{eff} that their interaction energy is

$$q_1 q_2\left(\frac{1}{\varepsilon_\infty}-\frac{4\pi C^2}{\omega_l^2}\right)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} \tag{1.2.15}$$

Comparing to (1.2.4) we have

$$\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}=\frac{4\pi C^2}{\omega_l^2} \tag{1.2.16}$$

This determines C. For further work it will be convenient to choose the units of time and distance in such a way that $m=1$ and $\omega_l=1$. Following Frolich,we define the dimensionless interaction strength or coupling constant

$$\alpha=\frac{1}{2}q^2\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)\left(\frac{2m}{\omega_l}\right)^{\frac{1}{2}} \tag{1.2.17}$$

The effective action for one particle in the lattice can now be written as

$$S_{eff}=\frac{1}{2}\int \dot{\mathbf{r}}^2 dt+\frac{i\alpha}{\sqrt{8}}\int\int dt\,ds\,\frac{e^{-i|t-s|}}{|\mathbf{r}(t)-\mathbf{r}(s)|} \tag{1.2.18}$$

The path integrals used to obtain S_{eff} are real time path integrals. They are matrix elements of e^{-iHt} where H is the Hamiltonian of the system. One may also consider imaginary time path integrals for the matrix elements of $e^{-\tau H}$. These are related to the real time path integrals by analytic continuation. It is these imaginary time path integrals to which Feynman's variational principle applies.

The free energy F of a system at temperature β^{-1} is given by $e^{-\beta F}=Tr\,e^{-\beta H}$. If q denotes the set of all system coordinates,then

$$Tr\,e^{-\beta H}=\int dq\,\langle q|e^{-\beta H}|q\rangle \tag{1.2.19}$$

Thus $e^{-\beta F}$ may be evaluated by imaginary time path integrals over paths which close on themselves after time β. The "action" which appears in these integrals is the time integral of the classical Hamiltonian of the system. Thus if $H=\frac{\mathbf{p}^2}{2m}+V(\mathbf{r})$, then

$$Tr\, e^{-\beta H} = \int D\mathbf{r} \exp\left[-\frac{m}{2}\int_0^\beta \dot{\mathbf{r}}^2 dt - \int_0^\beta V(\mathbf{r})dt\right] = \int D\mathbf{r}\, e^{-S} \tag{1.2.20}$$

The imaginary time action is obtained from the real time action by the replacement of t by $-it$. Thus (1.2.7), the particle Lagrangian, becomes*

$$L_{part} = \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{1.2.21}$$

The LO phonon Lagrangian (1.2.1) becomes

$$L_{LO} = \frac{1}{2}\int\left[\dot{w}_l^2 + \omega_l^2 w_l^2\right] d\mathbf{r}^3 \tag{1.2.22}$$

The interaction term is

$$L_{int} = \sum_i q_i \varphi(\mathbf{r}_i) \tag{1.2.23}$$

Finally, the action (1.2.11) becomes

$$S = \int_0^\beta \left\{ L_{part} + \frac{1}{2}\int \frac{d\mathbf{k}^3}{(2\pi)^3}\left[|\dot{u}(\mathbf{k})|^2 + \omega_l^2 |u(\mathbf{k})|^2\right] + 4\pi C i \sum_i \frac{d\mathbf{k}^3}{(2\pi)^3}\frac{u(\mathbf{k})}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{r}_i}\right\} dt \tag{1.2.24}$$

Now using the path integral

*We shall use the italic L for real time Lagrangians and the roman L for the corresponding imaginary time Lagrangians. The same convention will also apply to actions.

$$\int Dx\ \exp\left[-\frac{1}{2}\int_0^\beta (\dot{x}^2+\omega^2 x^2)d\tau+i\int_0^\beta \gamma x d\tau\right] = \frac{1}{2\sinh\left(\frac{\beta\omega}{2}\right)}\exp\left[-\frac{1}{2}\int_0^\beta\int_0^\beta \gamma(\tau)G_\omega(|\tau-\sigma|)\gamma(\sigma)\right]$$

(1.2.25)

where

$$G_\omega(\tau) = \frac{1}{2\omega}\left[\frac{e^{-\omega\tau}}{1-e^{-\omega\beta}}+\frac{e^{\omega\tau}}{e^{\omega\beta}-1}\right] \tag{1.2.26}$$

the $u(\mathbf{k})$'s may be integrated away and we obtain (after rescaling $\mathbf{r}$ and τ as before) for one particle

$$S = \frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau - \frac{\alpha}{\sqrt{2}}\int_0^\beta\int_0^\beta d\tau d\sigma \frac{G_1(|\tau-\sigma|)}{|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|} \tag{1.2.28}$$

We have dropped the subscript from S_{eff}. The action (1.2.28) will be the starting point for our further discussion and calculations.

2. FORMULATION OF THE PROBLEM AS A PATH INTEGRAL

2.1. Response Function

We can calculate such things as the absorption spectrum,mobility and effective mass for an electron in a polar crystal if we know the electron's response to a weak external force. We take the external field to be constant in space but variable in time. In this chapter we will present the details of this idea. We will also review how FHIP calculate the response function. Finally, we will present a method which allows a less laborious calculation of the response (when compared to the FHIP method) in the case that the crystal is initially in thermal equilibrium.

Weakness of the applied field implies that we can expand the response in powers of the field and retain only the terms which are linear in the field. This linearity in turn implies that we need only consider the effect of a brief pulse.

Frolich's polaron model and in particular the action given in (1.2.28) are invariant under rotations. The substitution $\mathbf{r}(t) \rightarrow R\mathbf{r}(t)$ makes no change in the value of S in (1.2.28). This implies that correlations such as $<x_i(\tau)x_j(\sigma)>$ are zero for $i \neq j$ and that there is no response in the y direction to an applied force in the x direction. Thus,in this chapter, we look at the response in the x direction to an impulse in the x direction. In chapter five we will give the equations which apply to an anisotropic crystal. Letting the applied force be $\gamma(t) = \gamma_0\delta(t)$,a term $-\gamma(t)x$ is added to the Hamiltonian. The effect of the pulse is to multiply the wavefunction of the system at a time just before $t = 0$ by $e^{i\gamma_0 x}$ to produce the wavefunction at a time just after $t = 0$. Subsequently the wavefunction evolves in accordance with the unperturbed system Hamiltonian H. If the system is initially in the state $|\Psi_i>$ with probability p_i,then at a time $t > 0$ we have for the expected position of the electron

$$\langle x(t)\rangle = \sum_i p_i \langle \Psi_i | e^{-i\gamma_0 x} e^{iHt} x e^{-iHt} e^{i\gamma_0 x} | \Psi_i \rangle \qquad (2.1.1)$$

Let $x(t) = e^{iHt} x e^{-iHt}$ and expand (2.1.1) to first order in γ_0

$$\langle x(t)\rangle = \sum_i p_i \langle \Psi_i | x(t) | \Psi_i \rangle + i\gamma_0 \sum_i \langle \Psi_i | [x(t), x(0)] | \Psi_i \rangle + \cdots \qquad (2.1.2)$$

We assume that there are no net currents flowing in the unperturbed system. In this case $\sum p_i \langle \Psi_i | x(t) | \Psi_i \rangle = constant$, which can be taken as zero. Now we define a response function

$$R(t) = \vartheta(t) \sum_i p_i \langle \Psi_i | [x(t), x(0)] | \Psi_i \rangle \qquad (2.1.3)$$

$\vartheta(t)$ is 1 for $t>0$ and 0 for $t<0$. The linear response to a general time varying force $\gamma(t)$ is now given by

$$\langle x(t)\rangle = i \int_{-\infty}^{+\infty} R(t-s)\gamma(s) ds \qquad (2.1.4)$$

Now we investigate some properties of $R(t)$. From (2.1.3) we see that $R(t)$ is pure imaginary. Consider the Fourier transform $\hat{R}(\lambda)$ of $R(t)$. Using the causality condition, $R(t) = 0$ for $t<0$, we have

$$\hat{R}(\lambda) = \int_0^{\infty} e^{i\lambda t} R(t) dt \qquad (2.1.5)$$

If our system is stable in the presence of a weak external force $\gamma(t)$, then $R(t)$ will not rise exponentially as $t \to \infty$. In this case, $\hat{R}(\lambda)$ will be analytic for all $\mathrm{Im}\,\lambda > 0$ since the integral (2.1.5) then converges absolutely. Using this information and Cauchy's theorem one finds that $\hat{R}(\lambda)$ may be represented as

$$\hat{R}(\lambda) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{Re}\,\hat{R}(\omega)}{\omega - \lambda} d\omega \quad , \mathrm{Im}\,\lambda > 0 \qquad (2.1.6)$$

We also note that since $R^*(t) = -R(t)$ we have from (2.1.5) for real λ that $\hat{R}^*(\lambda) = -\hat{R}(-\lambda)$ and

$$\mathrm{Re}\hat{R}(\lambda) = -\mathrm{Re}\,\hat{R}(-\lambda) \quad ,\lambda \textit{ real} \tag{2.1.7}$$

This allows us to write

$$\hat{R}(\lambda) = \frac{1}{i\pi}\int_0^\infty \frac{2\omega \mathrm{Re}\hat{R}(\omega)}{\omega^2-(\lambda+i0)^2}d\omega \tag{2.1.8}$$

In the following we denote $2\omega\mathrm{Re}\hat{R}(\omega)$ by $s(\omega)$.

To get a better idea of the significance of $R(t)$ and $\hat{R}(\lambda)$ insert $\sum_i |\Psi_i><\Psi_i| = 1$ into (2.1.3). Letting E_i be the eigenvalue of $|\Psi_i>$ and defining $\omega_{ni} = E_n - E_i$, we have

$$R(t) = -2i\sum_{i,n} p_i\, |<\Psi_i|x|\Psi_n>|^2 \sin(\omega_{ni}t)\vartheta(t) \tag{2.1.9}$$

Taking the Fourier transform of (2.1.9) yields (we put in a convergence factor $e^{-\varepsilon t}$ and later let $\varepsilon \to 0$)

$$\hat{R}(\lambda) = i\sum_{i,n} p_i\, |<\Psi_i|x|\Psi_n>|^2 \left\{\frac{1}{\lambda-\omega_{ni}+i0} - \frac{1}{\lambda+\omega_{ni}+i0}\right\} \tag{2.1.10}$$

$$= i\sum_{i,n} p_i\, |<\Psi_i|x|\Psi_n>|^2 \frac{2\omega_{ni}}{(\lambda+i0)^2-\omega_{ni}^2}$$

We see from (2.1.10) using $\frac{1}{x+i0} = P\frac{1}{x} - i\pi\delta(x)$ that

$$\mathrm{Re}\hat{R}(\lambda) = \frac{s(\lambda)}{2\lambda} = \sum_{i,n} p_i\, |<\Psi_i|x|\Psi_n>|^2 \left\{\pi\delta(\lambda-\omega_{ni}) - \pi\delta(\lambda+\omega_{ni})\right\} \tag{2.1.11}$$

Now apply a weak external force $\gamma(t) = \gamma_0\cos(\omega t)$ to the x coordinate of the system and ask at what rate the system absorbs energy. The answer is given by

first order time dependent perturbation theory. The transition rate from a state $|\Psi_i>$ to a state $|\Psi_n>$ is given by

$$W_{n\leftarrow i}(\omega) = \frac{\gamma_0^2}{2}\left\{\pi\delta(\omega-\omega_{ni})+\pi\delta(\omega+\omega_{ni})\right\}|<\Psi_i|x|\Psi_n>|^2 \qquad (2.1.12)$$

For each transition, the energy of the system changes by ω_{ni}. Thus $\omega_{ni}\, W_{n\leftarrow i}(\omega)$ gives the energy absorbed per unit time at frequency ω by the system in transitions from $|\Psi_i>$ to $|\Psi_n>$. Averaging over initial states and summing over final states, the total energy absorption rate at ω is $\sum_{n,i} p_i\, \omega_{ni}\, W_{n\leftarrow i}$ or

$$\frac{\omega\gamma_0^2}{2}\sum_{i,n} p_i\,|<\Psi_i|x|\Psi_n>|^2\left\{\pi\,\delta(\omega-\omega_{ni})-\pi\,\delta(\omega+\omega_{ni})\right\} = \frac{\gamma_0^2}{4}s(\omega) \qquad (2.1.13)$$

Thus $s(\omega)$ is proportional to the energy absorption rate, and (2.1.8),(2.1.5) show that the entire response function can be expressed in terms of it. Therefore we can concentrate on finding $s(\omega)$.

Next we derive a sum rule which will be important later. First observe that

$$\int_0^\infty s(\omega)d\omega = 2\pi\sum_{i,n} p_i\,|<\Psi_i|x|\Psi_n>|^2\omega_{ni} \qquad (2.1.14)$$

Choose units so that the mass associated with coordinate x is 1. $H = \frac{p^2}{2} + \cdots$, where p is the momentum conjugate to x. We suppose that the rest of H commutes with x, as it does for our case. This implies that $[[x,H],x] = 1$. Forming $\sum_i p_i <\Psi_i|[[x,H],x]|\Psi_i>$ and inserting $\sum_n |\Psi_n><\Psi_n| = 1$ gives the result

$$2\sum_i p_i\,|<\Psi_i|x|\Psi_n>|^2\omega_{ni} = 1 \qquad (2.1.15)$$

Comparing (2.1.15) with (2.1.14) gives

$$\int_0^\infty s(\omega)\frac{d\omega}{\pi} = 1 \tag{2.1.16}$$

If we examine (2.1.8) in the light of (2.1.16) we see that as $\lambda \to \infty$

$$\hat{R}(\lambda) \to \frac{i}{\lambda^2} \tag{2.1.17}$$

This says that at sufficiently high frequencies the electron responds as though it were free. Time is needed for the electron to interact appreciably with the phonons. Also,if we knew that $\hat{R}(\lambda)$ had the behavior given in (2.1.17), then (2.1.16) would follow.

2.2. Response from Path Integral:General Density Matrix

$R(t)$,as given in (2.1.3),can be rewritten as

$$R(t) = \sum_i p_i \langle \Psi_i | e^{iHt}\, x\, e^{-iHt}\, x\, | \Psi_i \rangle - \textit{complex conjugate} \tag{2.2.1}$$

Take $T_a \ll 0, T_b \gg 0$. The first term of (2.2.1) can be written as

$$\sum_i p_i \langle \Psi_i | e^{iH(T_b - T_a)} e^{-iH(T_b - t)}\, x\, e^{-iHt}\, x\, e^{iHT_a} | \Psi_i \rangle \tag{2.2.2}$$

Let q represent the coordinates of the system including x. Now

$$\langle q_f | e^{-iH(t_f - t_i)} | q_i \rangle = \int Dq_{fi}\, e^{iS[t_f, t_i]} \tag{2.2.3}$$

where if L is the Lagrangian associated with H,then $S[t_f, t_i] = \int_{t_i}^{t_f} L dt$ and the path integral is over all paths $q(t)$ which begin at $q_i = q(t_i)$ and end at $q_f = q(t_f)$. The notation Dq_{fi} means that we integrate over all paths with ends fixed at q_f and at q_i. On the other hand, taking the complex conjugate of (2.2.3) gives

$$<q_i|e^{iH(t_f-t_i)}|q_f> = \int Dq_{fi}\, e^{-iS[t_f,t_i]} \tag{2.2.4}$$

Note that the paths still run from q_i at time t_i to q_f at time t_f. Finally

$$<q_f|e^{-iH(t_f-t)}x\, e^{-iH(t-t_i)}x\,|q_i> = \int Dq_{fi}\, e^{iS[t_f,t_i]}x(t)x(0) \tag{2.2.5}$$

Combining (2.2.3),(2.2.4),(2.2.5) and letting

$$\rho = \sum_i |\Psi_i> p_i <\Psi_i| \tag{2.2.6}$$

gives

$$\int dq_a\, dq_{a'}\, Dq'_{ba'} Dq_{ba}\, e^{-iS'[T_b,T_a]+iS[T_b,T_a]}x(t)x(0)<q_a|\rho|q_{a'}> \tag{2.2.7}$$

$Dq'_{ba'}$ is associated with the primed action. The paths associated with the primed action run from $q_{a'}$ at T_a to q_b at T_b while the paths of the unprimed action run from q_a at T_a to q_b at T_b. Noting that $ix(t) = \left\{\frac{\delta}{\delta\gamma(t)}e^{i\int\gamma x}\right\}_{\gamma=0}$, we see that (2.2.7) is obtainable from

$$\int dq_a\, dq_{a'}\, Dq_{ba'} Dq_{ba}\, e^{-iS'+iS+i\int\gamma x}<q_a|\rho|q_{a'}> \tag{2.2.8}$$

When the system is in thermal equilibrium at temperature β^{-1},

$$\rho = \frac{e^{-\beta H}}{Tr\, e^{-\beta H}} \tag{2.2.9}$$

Going back to (2.2.2), consider the factor $e^{iHT_a}\rho\, e^{-iHT_a}$. If the density matrix was ρ at time T_a then this factor is the density matrix at time $t = 0$. However, as we let $T_a \to -\infty$, we can just as well start with the density matrix of the noninteracting system ($\alpha = 0$). We expect that the electron comes into equilibrium with the effectively infinite lattice in a finite time so that by $t = 0$ the density matrix is exactly that of the interacting system ($\alpha \neq 0$) in thermal equilibrium at the

original lattice temperature. This replacement allows the path integrals over the phonon variables to be carried out in a simple fashion.

The approach described in this section is used by FHIP to calculate the response function. However,in the special case that the system is initially in thermal equilibrium,it is possible to do the calculation more simply. We do it by first calculating some other functions ($\hat{g}(\lambda)$ and $f(\tau)$ below) and working back from them to $s(\omega)$. This method is described in the next section.

2.3. Response from Path Integral:Thermal Density Matrix

When the system is initially in thermal equilibrium,so that the density matrix is given by (2.2.9),we need to compute

$$\sum_i p_i \langle \Psi_i | e^{iHt} x e^{-iHt} x | \Psi_i \rangle = \frac{Tr\left[e^{-\beta H} e^{iHt} x e^{-iHt} x \right]}{Tr\, e^{-\beta H}} \qquad (2.3.1)$$

Note that this is the analytic continuation to $\tau = it$ of

$$g(\tau) = \frac{Tr\left[e^{-(\beta-\tau)H} x e^{-\tau H} x \right]}{Tr\, e^{-\beta H}} \qquad (2.3.2)$$

Equation (2.3.2) may be reexpressed in terms of path integrals as

$$g(\tau) = \langle x(\tau)x(0) \rangle = \frac{\int Dq\, x(\tau)x(0)\, e^{-S}}{\int Dq\, e^{-S}} \qquad (2.3.3)$$

Here $S = \int_0^\beta L d\tau$ where L is the imaginary time Lagrangian of the system and the path integration is over closed paths. For real τ and s in the range 0 to β we have $\langle x(\tau)x(s) \rangle = g(|\tau - s|)$. From (2.3.2) we can easily verify that for all complex τ

$$g(\beta - \tau) = g(\tau) \qquad (2.3.4)$$

Also since $g(\tau)$ is real on the real axis $g(\tau^*) = g^*(\tau)$. From this and (2.3.4) with τ replaced by $-\tau$,

$$g(\beta+\tau) = g^*(-\tau^*) \tag{2.3.5}$$

On the interval 0 to β we can expand $g(\tau)$ in terms of functions $e^{-i\lambda_\alpha\tau}$ with $\lambda_\alpha = \frac{2\pi\alpha}{\beta}$ and $\alpha = \ldots,-2,-1,0,1,2,\ldots$. It is important to note that while $g(\tau) = \beta^{-1}\sum_\alpha \hat{g}(\lambda_\alpha)e^{-i\lambda_\alpha\tau}$ for $0\le\tau\le\beta$, for $-\beta\le\tau\le\beta$ the sum gives $g(|\tau|)$. The Fourier sum is periodic in τ with period β while $g(\tau)$ does not have this property.

From (2.3.2) we obtain by inserting $\sum_i |\Psi_i><\Psi_i| = 1$ where necessary

$$g(\tau) = e^{\beta F}\sum_{i,n} e^{-\beta E_n} e^{-\tau\omega_{ni}} |<\Psi_i|x|\Psi_n>|^2 \tag{2.3.6}$$

Multiplying by $e^{i\lambda_\alpha\tau}$ and integrating over τ from 0 to β, we have

$$\hat{g}(\lambda_\alpha) = e^{\beta F}\sum_{i,n} |<\Psi_i|x|\Psi_n>|^2 \frac{e^{-\beta E_n} - e^{-\beta E_i}}{i\lambda_\alpha - \omega_{ni}} \tag{2.3.7}$$

where $\hat{g}(\lambda_\alpha) = \int_0^\beta g(\tau)e^{i\lambda_\alpha}d\tau$ This may be reexpressed as

$$\hat{g}(\lambda_\alpha) = \int_0^\infty \frac{s(\omega)}{\lambda_\alpha^2+\omega^2}\frac{d\omega}{\pi} \tag{2.3.8}$$

where $s(\omega)$ is given by (2.1.11). The analytic continuation of (2.3.7) to general λ which behaves as λ^{-2} when $\lambda\to\infty$ is

$$\hat{g}(\lambda) = \int_0^\infty \frac{s(\omega)}{\lambda^2+\omega^2}\frac{d\omega}{\pi} \tag{2.3.9}$$

Comparing this to (2.1.8) we see that $\hat{g}(-i\lambda) = \hat{R}(\lambda)$ and that $s(\omega)$ may be obtained by (as $\varepsilon\to 0$)

$$s(\omega) = \mathrm{Im} 2\omega \hat{g}(\varepsilon - i\omega) \tag{2.3.10}$$

Define now a function $f(\tau), 0 \leq \tau \leq \beta$, by

$$\hat{g}(\lambda_a) = \frac{1}{\lambda_a^2 + \hat{f}(\lambda_a)}$$

$$f(\tau) = \beta^{-1} \sum_a \hat{f}(\lambda_a) e^{-i\lambda_a \tau} \tag{2.3.11}$$

In the following we shall obtain the solution to our problem as a series for $f(\tau)$. This will allow us to find $\hat{f}(\lambda_a)$. However, to find $s(\lambda)$ or the response function $R(t)$,we need to know $\hat{f}$ for general values of λ. $\hat{g}(\lambda)$ will then be given by $\hat{g}(\lambda) = (\lambda^2 + \hat{f}(\lambda))^{-1}$. The problem is that specifying a function at a discrete set of points does not uniquely determine the analytic continuation of the function. However,the condition that $\hat{g}(\lambda) \to \lambda^{-2}$ as $|\lambda| \to \infty$ for all complex λ is sufficient to fix the physically correct analytic continuation. We now use this condition to continue $\hat{f}(\lambda_a)$ to $\hat{f}(\lambda)$. We assume that we are given $f(\tau)$ in the complex τ plane (at least for $\mathrm{Re}\tau > 0$). If we start with

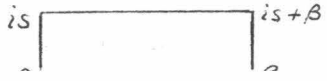
$$\hat{f}(\lambda_a) = \int_0^\beta e^{i\lambda_a \tau} f(\tau) d\tau \tag{2.3.12}$$

then an obvious attempt at $\hat{f}(\lambda)$ is

$$\hat{f}(\lambda) = \int_0^\beta e^{i\lambda \tau} f(\tau) d\tau \tag{2.3.13}$$

This has the problem that for some directions in the complex λ plane $\hat{f}(\lambda)$ rises exponentially as $|\lambda| \to \infty$. $\hat{g}(\lambda)$ then falls more rapidly than λ^{-2}.

It is possible to see how to correct the problem by changing the path of integration in (2.3.13). Suppose that $\mathrm{Re}\lambda > 0$ and consider the following contour in the τ plane:



As $s \to \infty$, the piece from is to $is+\beta$ goes to zero. We can now write

$$\hat{f}(\lambda) = i\int_0^{\infty} e^{-\lambda t} f(it)dt - i\, e^{i\lambda\beta}\int_0^{\beta} e^{-\lambda t} f(\beta+it)dt \qquad (2.3.14)$$

So far this $\hat{f}(\lambda)$ is the same as in (2.3.12). However, we have isolated the bad behavior. It is given by the $e^{i\lambda\beta}$ in the second term of (2.3.14). For $\lambda = \lambda_\alpha$ this factor is just 1. If we remove this factor, the new $\hat{f}(\lambda)$ will still have the correct values at $\lambda = \lambda_\alpha$ and it will have the correct behavior as λ goes to infinity. For $\mathrm{Re}\lambda<0$ we must construct a different expression, but we shall not need this.

On the real axis $f(\tau)$ is real and $f(\beta-\tau) = f(\tau)$. The first property implies $f(\tau^*) = f^*(\tau)$. The second property can be extended to the whole complex plane for $f(\tau)$ analytic. Thus $f(\tau)$ shares properties (2.3.4) and (2.3.5) with $g(\tau)$. In particular $f(\beta+it) = f^*(it)$ for real t. Thus

$$\hat{f}(\lambda) = -2\int_0^{\beta} e^{-\lambda t}\, \mathrm{Im} f(it)dt \qquad (2.3.15)$$

We can now summarize our calculational procedure. First we shall obtain $f(\tau)$ as a series

$$f(\tau) = f_0(\tau)+f_1(\tau)+f_2(\tau)+\cdots \qquad (2.3.16)$$

We shall obtain f_0 from a variational calculation. In this case f_1 will vanish and f_2 will be the result of calculating the second order perturbation about the trial action. It will be possible to continue the f's to complex τ (and therefore to find $\hat{f}(\lambda)$ from (2.3.15)). From (2.3.10) we are actually interested in $\lambda = \varepsilon - i\omega$ for ω real. Using (2.3.15)

$$\hat{f}(\varepsilon-i\omega) = -2\int_0^{\infty} e^{-\varepsilon t+i\omega t}\, \mathrm{Im} f(it) \qquad (2.3.17)$$

Finally, we compute $s(\omega)$ by

$$s(\omega) = \lim_{\varepsilon \to 0} \mathrm{Im} \frac{2\omega}{(\varepsilon - i\omega)^2 + \hat{f}(\varepsilon - i\omega)} \tag{2.3.18}$$

3. DEVELOPMENT OF THE APPROXIMATION

3.1. Variational Method and Perturbation Expansion

The path integral for $g(\tau)$ in (2.3.3) cannot be performed for the polaron action S given by (1.2.28). Thus we shall imitate S by a trial action S_0 and use Feynman's variational principle to pick out the best S_0

If A is a functional of the path $\mathbf{r}(t)$ of the system, then averages $\langle A\rangle_0$ are defined by

$$\langle A\rangle_0 = \frac{\int D\mathbf{r} A\, e^{-S_0}}{\int D\mathbf{r}\, e^{-S_0}} \tag{3.1.1}$$

Define $S_1 = S - S_0$ and note that $\int D\mathbf{r}\, e^{-S} = \langle e^{-S_1}\rangle_0 \int D\mathbf{r}\, e^{-S_0}$. The variational inequality states that*

$$\langle e^{-S_1}\rangle_0 \geq e^{-\langle S_1\rangle_0} \tag{3.1.2}$$

The best S_0 is now taken to be the one which maximizes the right hand side of (3.1.2). In terms of free energies F_0 and F defined by

$$e^{-\beta F} = \int D\mathbf{r}\, e^{-S} \tag{3.1.3}$$

$$e^{-\beta F_0} = \int D\mathbf{r}\, e^{-S_0}$$

*This follows from the fact that if x is a random variable with probability distribution $P(x)$ and $f(x)$ is any function which lies above any of its tangent lines (a convex function),then

$$\int P(x) f(x)\, dx = \langle f\rangle \geq f(\langle x\rangle)$$

To see this,note that $f(x) \geq f(x_0) + f'(x_0)(x - x_0)$ for any x_0. Averaging this over the distribution $P(x)$ gives $\langle f\rangle \geq f(x_0) + f'(x_0)(\langle x\rangle - x_0)$. Let $x_0 = \langle x\rangle$ to find $\langle f\rangle \geq f(\langle x\rangle)$ Since e^x always lies above its tangent lines, $\langle e^x\rangle \geq e^{\langle x\rangle}$. Finally note that

$$P(x) = \frac{\int D\mathbf{r}\, \delta(x - S_1)\, e^{-S_0}}{\int D\mathbf{r}\, e^{-S_0}}$$

is a probability distribution for the values of S_1.

we can rewrite (3.1.2) as

$$F \leq F_0 + \frac{1}{\beta} \langle S_1 \rangle_0 \tag{3.1.4}$$

In the limit of $\beta \to \infty$ this reduces to an upper bound for the ground state energy of the system.

The path integrals involving the action S given by (1.2.28) diverge as the volume of the system becomes infinite. This is because S is invariant under the transformation $\mathbf{r}(\tau) \to \mathbf{r}(t) + \Delta\mathbf{r}$. To avoid this problem we impose a weak harmonic oscillator potential $\frac{1}{2}\Omega^2\mathbf{r}^2$ on the electron. Although the free energies F and F_0 diverge as $\Omega \to 0$, we can obtain finite results by subtracting from each of them the free energy of an electron which is in a harmonic oscillator potential $\frac{1}{2}\Omega^2\mathbf{r}^2$ but which is not interacting with the lattice. In this way we obtain as $\Omega \to 0$ ΔF and ΔF_0 which are exact and approximate free energies of a polaron relative to an electron which does not interact with the optical phonons. The variational principle now applies to ΔF and ΔF_0

$$\Delta F \leq \Delta F_0 + \frac{1}{\beta} \langle S_1 \rangle_0 \tag{3.1.5}$$

The best S_0 is taken to be the one which minimizes the right hand side of (3.1.5). If S_0 is a trial action which minimizes the right hand side of (3.1.5) and we make a small variation in S_0 then first order change in the right hand side must be zero.

We now let the action be

$$S = \frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 \, d\tau + \frac{\Omega^2}{2}\int_0^\beta \mathbf{r}^2 \, d\tau - \frac{\alpha}{\sqrt{2}}\int_0^\beta\int_0^\beta \frac{G_1(\tau-\sigma)}{|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|} d\tau d\sigma \tag{3.1.6}$$

For the trial action we take

$$S_0 = \int_0^\beta \int_0^\beta d\tau d\sigma \, \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) g_0^{-1}(|\tau-\sigma|) \tag{3.1.7}$$

Here g_0^{-1} is inverse to a function g_0 in the sense that

$$\int_0^\beta g_0^{-1}(|\tau_1-\sigma|) g_0(|\sigma-\tau_2|) d\sigma = \delta(\tau_1-\tau_2) \tag{3.1.8}$$

for $0 \le \tau_1, \tau_2, s \le \beta$.

The path integral $\int D\mathbf{r} e^{-S_0 + \int \gamma \cdot \mathbf{r}}$ may be performed by analogy to the discrete Gaussian integral

$$\int d^N z \, e^{-\frac{1}{2}\sum_{i,j} A_{ij} z_i z_j + \sum_i z_i \gamma_i} = \frac{(2\pi)^{\frac{N}{2}}}{\sqrt{\det A}} e^{-\frac{1}{2}\sum_{i,j} \gamma_i A_{ij}^{-1} \gamma_j} \tag{3.1.9}$$

Here N is the dimension of the symmetric matrix A. g_0^{-1} corresponds to A_{ij} and g_0 to A_{ij}^{-1}. The result is

$$\int D\mathbf{r} e^{-S_0 + \int_0^\beta \gamma \cdot \mathbf{r} dt} = e^{-\beta F_0} e^{\frac{1}{2}\int_0^\beta \int_0^\beta dt ds \gamma(t) \cdot \gamma(s) g_0(|t-s|)} \tag{3.1.10}$$

$$<e^{\int_0^\beta \gamma \cdot \mathbf{r} dt}>_0 = e^{\frac{1}{2}\int_0^\beta \int_0^\beta dt ds \gamma(t) \cdot \gamma(s) g_0(|t-s|)}$$

Here $e^{-\beta F_0}$ is by (3.1.3) the value of the path integral in (3.1.10) with $\gamma = 0$. We shall evaluate $e^{-\beta F_0}$ later.

Noting that $\left[\frac{\delta^2}{\delta\gamma(\tau)\delta\gamma(\sigma)} <e^{\int \gamma \cdot \mathbf{r}}>_0\right]_{\gamma=0} = <\mathbf{r}(\tau)\mathbf{r}(\sigma)>_0$, we have from (3.1.10) that

$$<x_i(\tau)x_j(\sigma)>_0 = \delta_{ij} g_0(|\tau-\sigma|) \tag{3.1.11}$$

In this equation the x_i are the components of $\mathbf{r}$. (We use x and x_1 interchangeably.)

Since $<x(\tau)x(\sigma)>_0 = g_0(|\tau-\sigma|)$,$g_0(\tau)$ is for the action S_0 what $g(\tau)$ is for the action S. We define

$$\hat{g}_0(\lambda_a) = \int_0^\beta e^{i\lambda_a\tau} g_0(\tau) \tag{3.1.12}$$

As we did for $g(\tau)$,we can for $g_0(\tau)$ define related functions $\hat{f}(\lambda_a)$ and $f(\tau)$ by

$$\hat{f}_0(\lambda_a) = \frac{1}{\hat{g}_0(\lambda_a)} - \lambda_a^2 \tag{3.1.13}$$

$$f_0(\tau) = \beta^{-1}\sum_a \hat{f}_0(\lambda_a) e^{-i\lambda_a\tau}$$

In the time domain, the relations between $g(\tau)$ and $f(\tau)$ and between $g_0(\tau)$ and $f_0(\tau)$ following from (3.1.13) and (2.3.11) are

$$-\frac{d^2}{d\tau^2} g(|\tau-\sigma|) + \int_0^\beta f(|\tau-\tau'|) g(|\tau'-\sigma|) d\tau' = \delta(\tau-\sigma) \tag{3.1.14}$$

$$-\frac{d^2}{d\tau^2} g_0(|\tau-\sigma|) + \int_0^\beta f_0(|\tau-\tau'|) g_0(|\tau'-\sigma|) d\tau' = \delta(\tau-\sigma)$$

Comparing the second of the equations (3.1.14) and the equation (3.1.8) we see that $g_0^{-1}(|\tau-\sigma|) = -\frac{d^2}{d\tau^2}\delta(\tau-\sigma) + f_0(|\tau-\sigma|)$. The trial action can be written as

$$S_0 = \frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 + \frac{1}{2}\int_0^\beta\int_0^\beta \mathbf{r}(\tau)\cdot\mathbf{r}(\sigma) f_0(|\tau-\sigma|) d\tau d\sigma \tag{3.1.15}$$

Note that the kinetic terms in S_0 and S coincide. If one leaves the mass in the trial action as a free parameter, the variational method forces it to have the same value as in the true action. For this reason we have defined $f_0(\tau)$ in such a way that the kinetic terms in the two actions agree. When we say that the kinetic terms agree,what we really mean is that for very short times the kinetic term is

the dominant term in the action and these dominant terms in S and S_0 agree with each other. Equivalently,we may Fourier analyze the actions, rewriting them in terms of variables $\hat{\mathbf{r}}(\lambda_\alpha) = \int_0^\beta e^{i\lambda_\alpha \tau}\mathbf{r}(\tau)d\tau$ $(\lambda_\alpha = \frac{2\pi\alpha}{\beta}, \alpha integer)$. The kinetic term in S is now $\frac{1}{2\beta}\sum_\alpha \hat{\mathbf{r}}(\lambda_\alpha)\cdot\hat{\mathbf{r}}^*(\lambda_\alpha)\lambda_\alpha^2$. If we used a mass $m \neq 1$ in the trial action, the kinetic term there would be the S kinetic term just given multiplied by m. The large λ_α pieces of these kinetic terms make such a large contribution to $<S-S_0>_0$ that we are forced to $m = 1$ in the trial action. That $m = 1$ in the trial action implies that as $\lambda_\alpha \to \infty, \hat{g}_0(\lambda_\alpha) \to \lambda_\alpha^{-2}$.(For $m \neq 1$ it goes to $m\lambda_\alpha^{-2}$.)

An action like S_0 in (3.1.15) can be gotten from the action of a system which consists of a particle coupled by linear interaction terms to a set of harmonic oscillators. S_0 is obtained by integrating away the oscillator variables in the path integral for the particle-oscillator system. Since the particle-oscillator system is described by a Hamiltonian, we can repeat the discussion of the last chapter and derive dispersion relations,sum rules,etc. for the response function $R_0(t)$ and its Fourier transform $\hat{R}_0(\lambda)$ associated with the trial action S_0.

From the comments in the preceding paragraph we see that $\hat{R}_0(\lambda) \to \frac{i}{\lambda^2}$ as $\lambda \to \infty$ so that the absorption function $s_0(\lambda)$ for the system with action S_0 satisfies the same sum rule $\int_0^\infty \frac{d\omega}{\pi} s_0(\omega) = 1$ as does $s(\omega)$ for the system with action S.

Next we note that the righthand side of equation (3.1.4) is the beginning of a series for the free energy F. This series is obtained by writing

$$e^{-\beta F} = \int Dq e^{-S_0 - S_1} = \int Dq e^{-S_0} \sum_{n=0}^{\infty} \frac{(-S_1)^n}{n!} = e^{-\beta f_0} \sum_{n=0}^{\infty} (-1)^n \frac{<S_1^n>_0}{n!} \quad (3.1.16)$$

and then taking logarithms to second order on S_1 we have

$$\beta F = \beta F_0 + <S_1>_0 - \frac{1}{2}[<S_1^2> - <S_1>^2] + \cdots \quad (3.1.17)$$

From this expansion it is also possible to get an expansion for $g(\tau)$. First define $h(\tau-\sigma) = \Omega^2\delta(\tau-\sigma)-f_0(\tau-\sigma)$. Then S in (3.1.6) can be rewritten as

(3.1.18)

$$S=\frac{1}{2}\int \mathbf{r}(\tau)\mathbf{r}(\sigma)f_0(\tau-\sigma)+\left[\frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{1}{2}\int\int \mathbf{r}_\tau \mathbf{r}_\sigma h(\tau-\sigma) - \frac{\alpha}{\sqrt{2}}\int\int \frac{G_1(\tau-\sigma)}{|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|}\right]$$

Now generalize this by letting $h(\tau-\sigma)$ be independent of f_0. Denote the piece in bracket in (3.1.18) by A. Now vary f_0 leaving $h(\tau-\sigma)$ constant. Then

$$\delta(e^{-\beta F}) = \delta\int D\mathbf{r}\, e^{-A-\frac{1}{2}\int\int \mathbf{r}(\tau)\mathbf{r}(\sigma)f_0(\tau-\sigma)} \tag{3.1.19}$$

$$= \int D\mathbf{r}\left[-\frac{1}{2}\int\int \mathbf{r}(\tau)\mathbf{r}(\sigma)f_0(\tau-\sigma)\right] e^{-A-\frac{1}{2}\int\int \mathbf{r}(\tau)\mathbf{r}(\sigma)f_0(\tau-\sigma)}$$

On the other hand $\delta(e^{-\beta F}) = \delta(-\beta F)e^{-\beta F}$. Combining this and (3.1.19) using $\langle x_i(\tau)x_j(\sigma)\rangle = \delta_{ij}\, g(|\tau-\sigma|)$ we find that

$$\delta(\beta F) = \frac{3}{2}\int g(|\tau-\sigma|)\delta f_0(|\tau-\sigma|)d\tau d\sigma \tag{3.1.20}$$

If we vary βF_0 with respect to f_0 we find

$$\delta(\beta F_0) = \frac{3}{2}\int g_0(|\tau-\sigma|)\delta f_0(|\tau-\sigma|)d\tau d\sigma \tag{3.1.21}$$

If we vary both sides of the expansion (3.1.17) (with S given by (3.1.18) and h independent of f_0) we obtain a series for $g(|\tau-\sigma|)$. Once we have obtained the series we set $h(\tau-\sigma) = \Omega^2\delta(\tau-\sigma)-f_0(\tau-\sigma)$. This procedure gives us a perturbation expansion for g about any S_0. We shall call the expansion for g the g series.

$$g(\tau) = g_0(\tau)+g_1(\tau)+g_2(\tau)+\cdots \tag{3.1.22}$$

Experience with simple examples shows that it is better to transform the series

(3.1.22) for $g(\tau)$ into a series for $f(\tau)$. Thus if S is a harmonic oscillator action and S_0 is a different harmonic oscillator action, then the g series is an infinite series. The f series in this case terminates at f_1 and the result is exact. Other examples such as a single anharmonic oscillator show that the f series gives a qualitatively better picture of the spectrum.

Suppose that $f = f_0+f_1+f_2+f_3+\cdots$. Denote an equation such as (3.1.8) schematically by $g_0^{-1}g_0 = 1$. From (3.1.14) we have

$$g_0^{-1}(|\tau-\sigma|) = -\frac{d^2}{d\tau^2}\delta(\tau-\sigma) + f_0(|\tau-\sigma|)$$

and

$$g^{-1}(|\tau-\sigma|) = -\frac{d^2}{d\tau^2}\delta(\tau-\sigma) + f_1(|\tau-\sigma|)$$

Thus we can write

$$g^{-1} = g_0^{-1} + f_1 + f_2 + \cdots \qquad (3.1.23)$$

$$= g_0^{-1} + \Delta f$$

Inverting

$$g = (g_0^{-1}+\Delta f)^{-1} = g_0(1+\Delta f g_0)^{-1}$$

$$g = g_0-g_0\Delta f g_0+g_0\Delta f g_0\Delta f g_0-\cdots \qquad (3.1.24)$$

Comparing this with the g series (3.1.22) and equating items of equal order gives

$$g_1 = -g_0 f_1 g_0 \qquad (3.1.25)$$

$$g_2 = -g_0 f_2 g_0+g_0 f_1 g_0 f_1 g_0$$

Solving for f_1 and f_2 gives

$$f_1 = -g_0^{-1} g_1 g_0^{-1} \tag{3.1.26}$$

$$f_2 = -g_0^{-1}(g_2 - g_0 f_1 g_0 f_1 g_0) g_0^{-1}$$

The next section will discuss the variational calculation of f_0. The section after that will give the explicit construction of the g series and its reduction to the f series.

3.2. The variational equations

We begin by computing $\langle S-S_0\rangle_0 \equiv \langle S_1\rangle_0$. Using (3.1.18) for S and (3.1.15) for S_0, then S_1 is

$$S_1 = \frac{1}{2}\int_0^\beta\int_0^\beta \left[\mathbf{r}_\tau\cdot\mathbf{r}_\sigma h(|\tau-\sigma|) - \alpha\pi\sqrt{8}\int \frac{d^3\mathbf{k}}{2\pi^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}(\tau)-\mathbf{r}(\sigma))}}{\mathbf{k}^2} G_1(|\tau-\sigma|)\right] \tag{3.2.1}$$

where $\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathbf{k}^2} = \frac{1}{4\pi}\frac{1}{|\mathbf{r}|}$ has been used to rewrite the α term. From (3.1.11) $\langle \mathbf{r}(\tau)\cdot\mathbf{r}(\sigma)\rangle = 3g_0(|\tau-\sigma|)$. To evaluate $\langle e^{i\mathbf{k}\cdot(\mathbf{r}(\tau)-\mathbf{r}(\sigma))}\rangle_0$ use (3.1.10) with $\gamma(\mu) = i\mathbf{k}\delta(\mu-\tau) - i\mathbf{k}\delta(\mu-\sigma)$. The result is

$$\langle e^{i\mathbf{k}\cdot(\mathbf{r}(\tau)-\mathbf{r}(\sigma))}\rangle_0 = e^{-\mathbf{k}^2 D_0(|\tau-\sigma|)} \tag{3.2.2}$$

where $D_0(\tau)$ is defined by $D_0(\tau) = g_0(0) - g_0(\tau)$. This combination occurs repeatedly and also has the nice property that as the $\Omega^2\mathbf{r}^2$ potential used to confine the electron to a finite portion of the crystal vanishes $D_0(\tau)$ stays finite. So far we have

$$\langle S_1\rangle_0 = \int_0^\beta\int_0^\beta \left[\frac{3}{2}h(|\tau-\sigma|)g_0(|\tau-\sigma|) - \alpha\pi\sqrt{8}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{-\mathbf{k}^2 D_0(|\tau-\sigma|)}}{\mathbf{k}^2} G_1(|\tau-\sigma|)\right] \tag{3.2.3}$$

Making the replacement $\mathbf{k}^{-2} = \int_0^\infty e^{-u\mathbf{k}^2}du$, the $\mathbf{k}^2$ integral can be done. This

leaves a u-integral. The necessary integral is

$$\int_0^\infty \frac{du}{(u+A)^{\frac{3}{2}}} = 2A^{-\frac{1}{2}} \tag{3.2.4}$$

Finally, we may use the time translation invariance of the integrals to reduce the double time integrals to single integrals.

$$\langle S_1\rangle_0 = \beta\int_0^\beta \left[\frac{3}{2}h(|\tau|)g_0(|\tau|) - \frac{\alpha}{\sqrt{2\pi}}\frac{G_1(\tau)}{D_0^{\frac{1}{2}}(\tau)}\right]d\tau \tag{3.2.5}$$

Now we are almost ready to vary $f_0(\tau)$ to find the conditions for a minimum of $\beta F_0+\langle S_1\rangle_0$. First replace $h(\tau)$ by $\Omega^2\delta(\tau)-f_0(\tau)$. From (3.1.14) we find that when f_0 is varied the change in g_0 is given by $\delta g_0 = -g_0^{-1}\delta f_0 g_0^{-1}$ or in more detail by

$$\delta g_0(|\tau-\sigma|) = -\int_0^\beta\int_0^\beta g_0^{-1}(|\tau-\tau'|)\delta f_0(|\tau'-\sigma'|)g_0^{-1}(|\sigma'-\sigma|)d\tau' d\sigma' \tag{3.2.6}$$

Combining this with (3.1.21) which gives $\delta(\beta F_0)$ we obtain finally

$$f_0(\tau) = \Omega^2\delta(\tau) - \frac{\alpha}{3\sqrt{2\pi}}\left[\frac{G_1(\tau)}{D_0^{\frac{3}{2}}(\tau)} - \delta(\tau)\int_0^\beta \frac{G_1(\sigma)}{D_0^{\frac{3}{2}}(\sigma)}d\sigma\right] \tag{3.2.7}$$

This equation makes sense with $\Omega^2 = 0$, so we shall drop the Ω^2 term in the following. It is convenient to define a function $\kappa_0(\tau)$ by

$$\kappa_0(\tau) = \frac{\alpha}{3\sqrt{2\pi}}\frac{G_1(\tau)}{D_0^{\frac{3}{2}}(\tau)} \tag{3.2.8}$$

so that $f_0(\tau)$ will be given by

$$f_0(\tau) = -\kappa_0(\tau) + \delta(\tau)\int_0^\beta \kappa_0(\tau) \tag{3.2.9}$$

From this we have

$$\hat{f}_0(\lambda_\alpha) = \int_0^\beta (1-e^{i\lambda_\alpha\tau})\kappa_0(\tau)d\tau\ ,\ \lambda_\alpha = \frac{2\pi\alpha}{\beta},\quad \alpha integer \tag{3.2.10}$$

Following the methods of chapter 2 this may be continued away from the discrete valves λ_α. We now write down the cycle of equations which self consistently determine the quantities $D_0(it)$, $s_0(\omega)$, $\hat{f}_0(-i\lambda)$ ($s_0(\omega)$ is for the action S_0 what $s(\omega)$ was for S - the energy absorption function). Suppose we start with some $s_0(\omega)$ (this should obey the sum rule $\int_0^\infty \frac{d\omega}{\pi} s_0(\omega) = 1$) using the equivalent of (2.2.8) for $s_0(\omega)$ and $\hat{g}_0(\lambda_\alpha)$ and the relation $\frac{1}{\beta}\sum_\alpha \frac{e^{-i\lambda_\alpha\tau}}{\lambda_\alpha^2+\omega^2} = G_\omega(\tau)$ where $G_\omega(\tau)$ is given by (1.2.26) and noting $D_0(it) = g_0(0)-g_0(it)$, we can write

$$D_0(it) = \int_0^\infty \frac{d\omega}{\pi} s(\omega)\frac{1}{2\omega}\left[\frac{1-e^{-i\omega t}}{1-e^{-\beta\omega}} + \frac{1-e^{i\omega t}}{e^{\beta\omega}-1}\right] \tag{3.2.11}$$

From this $D_0(it)$ we may construct $\kappa_0(it)$ which we then use in the equivalent of (2.2.8) to find

$$\hat{f}_0(-i\lambda) = \frac{2\alpha}{3\sqrt{2\pi}}\int_0^\infty (e^{i\lambda s}-1)\mathrm{Im}\frac{G_1(is)}{D_0^2(is)}ds \tag{3.2.12}$$

Finally, referring to (2.2.18), we may complete the cycle by

$$s_0(\omega) = \mathrm{Im}\left[\frac{2\omega}{\hat{f}_0(-i\omega)-\omega^2}\right] \tag{3.2.13}$$

Of course, we can start this cycle of equations (3.2.11) - (3.2.13) with $D_0(it)$ or $\hat{f}_0(-i\lambda)$ just as well as with $s_0(\omega)$. These equations have been also derived in [6] by another method not connected with a variational principle.

Since one may also ask to know the free energy associated with a particular $s_0(\omega)$, we briefly stretch how βF_0 may be calculated.

It is sufficient to consider the path integral over closed paths $x(0) = x(\beta)$

$$Z = \int Dx e^{-\frac{1}{2}\int_0^\beta \dot{x}^2 - \frac{1}{2}\int_0^\beta\int_0^\beta x(\tau)x(\sigma)f(|\tau-\sigma|)d\tau d\sigma} \tag{3.2.14}$$

To avoid worrying about the normalization of Dx divide (3.2.14) by the corresponding path integral for the free energy of a harmonic oscillator of frequency ω.

$$\frac{1}{2\sinh\frac{\beta\omega}{2}} = \int Dx e^{-\frac{1}{2}\int_0^\beta \dot{x}^2 - \frac{\omega^2}{2}\int_0^\beta x^2} \tag{3.2.15}$$

Introduce new variables $\hat{x}_\alpha$ by $x(\tau) = \frac{1}{\beta}\sum_\alpha e^{-i\lambda_\alpha\tau}\hat{x}_\alpha$ ($\lambda_\alpha = \frac{2\pi\alpha}{\beta}$, α *integer*). Since $x(\tau)$ is real $\hat{x}_\alpha^* = \hat{x}_{-\alpha}$, so that the independent variables are $\mathrm{Re}\hat{x}_0$ and for $\lambda_\alpha>0$ $\mathrm{Re}\hat{x}_\alpha$, $\mathrm{Im}\hat{x}_\alpha$. Also, $f(|\tau-\sigma|) = \frac{1}{\beta}\sum_\alpha e^{-i\lambda_\alpha\tau}\hat{f}(\lambda_\alpha)$ and the $\hat{f}(\lambda_\alpha)$ are real. Letting $\hat{x}$ denote integration over the independent variables, the ratio of path integrals is

$$(2\sinh\frac{\beta\omega}{2})Z = \frac{\int D\hat{x}\, e^{-\frac{\hat{f}_0(0)}{2\beta}(\mathrm{Re}\hat{x}_0)^2}\prod_{\alpha>0} e^{-\frac{1}{2\beta}(\lambda_\alpha^2+\hat{f}_0(\lambda_\alpha))\left[(\mathrm{Re}\hat{x}_\alpha)^2+(\mathrm{Im}\hat{x}_\alpha)^2\right]}}{\int D\hat{x}\, e^{-\frac{\omega^2}{2\beta}(\mathrm{Re}\hat{x}_0)^2}\prod_{\alpha>0} e^{-\frac{1}{2\beta}(\lambda_\alpha^2+\omega^2)\left[(\mathrm{Re}\hat{x}_\alpha)^2+(\mathrm{Im}\hat{x}_\alpha)^2\right]}} \tag{3.2.16}$$

Numerator and denominator are each just a product of Gaussian integrals. Carrying out the integrations and using the formula $\sinh(\pi z) = \pi z\prod_{j=1}^{\infty}(1+\frac{z^2}{j^2})$ with $z = \frac{\beta\omega}{2\pi}$ we finally obtain

$$Z = \frac{1}{\beta}\frac{1}{\sqrt{\hat{f}_0(0)}}\prod_{\alpha>0}\frac{1}{\left[1+\frac{\hat{f}_0(\lambda_\alpha)}{\lambda_\alpha^2}\right]} \tag{3.2.17}$$

$-\beta F_0$ is the logarithm of (3.2.17). Using this and our result (3.2.5) for $<S_1>_0$ we have an expression for $\beta F_0+<S_1>$. Let $h(\tau-\sigma) = \Omega^2\delta(\tau-\sigma)-f_0(\tau-\sigma)$. Now we may treat the $\hat{f}_0(\lambda_\alpha)$ as variational parameters. In particular, if we find the best value of $\hat{f}(0)$ by

$$\frac{\delta}{\delta\hat{f}(0)}\left[\beta F_0+<S_1>_0\right] = 0 \tag{3.2.18}$$

we find that $\hat{f}(0) = \Omega^2$. For now we leave the other $\hat{f}(\lambda_\alpha)$' ($\alpha\neq 0$) arbitrary. If from $\beta F_0+<S_1>_0$ we subtract β times (free energy for electron in potential $\frac{\Omega^2}{2}\mathbf{r}\cdot\mathbf{r}$ but not interacting with the phonons) and then take the limit as $\Omega\to 0$ we get a finite result which is just an upper bound on difference in free energy between a polaron and an electron not interacting with the optical phonons. If we denote the actual value of this energy difference by ΔF, then we have

$$\beta\Delta F\leq 3\sum_{\alpha>0}\ln\left[1+\frac{\hat{f}(\lambda_\alpha)}{\lambda_\alpha^2}\right] - 3\sum_{\alpha>0}\frac{\hat{f}_0(\lambda_\alpha)}{\lambda_\alpha^2+\hat{f}(\lambda_\alpha)} - \frac{\beta\alpha}{\sqrt{2\pi}}\int_0^\beta \frac{G_1(\tau)}{D_0^{\frac{1}{2}}(\tau)}d\tau \tag{3.2.19}$$

The factors of 3 in the first two terms of the right hand side of (3.2.19) are due to the three degrees of freedom of the electron.

3.3. Second Order Calculation

First we work out the second order contribution to the free energy given by $-\frac{1}{2}\left[<S_1^2>_0 - <S_1>_0^2\right]$. Letting

$$A = \frac{1}{2}\int_0^\beta\int_0^\beta h(|\tau-\sigma|)\mathbf{r}(\tau)\cdot\mathbf{r}(\sigma)d\tau d\sigma \tag{3.3.1}$$

$$B = -\sqrt{8}\pi\alpha\int_0^\beta\int_0^\beta d\tau d\sigma\int\frac{d^3k}{(2\pi)^3}G_1(|\tau-\sigma|)\frac{e^{i\mathbf{k}\cdot(\mathbf{r}(\tau)-\mathbf{r}(\sigma)}}{k^2}$$

so that $S_1 = A + B$, we have to evaluate $\langle A^2\rangle_0 - \langle A\rangle_0^2$, $\langle B^2\rangle_0 - \langle B\rangle_0^2$, and $\langle AB\rangle_0 - \langle A\rangle_0\langle B\rangle_0$. A useful theorem in these evaluations is gotten by integration by parts (see [7])

$$\int Dq \frac{\delta Q}{\delta q(\tau)} e^{-S} = \int Dq\, Q \frac{\delta S}{\delta q(\tau)} e^{-S} \tag{3.3.2}$$

or

$$\left\langle \frac{\delta Q}{\delta q(\tau)} \right\rangle_S = \left\langle Q \frac{\delta S}{\delta q(\tau)} \right\rangle_S$$

Here S is any action with variables q and Q is a functional of the q. For the Gaussian action S_0 in (3.1.7) we find

$$\left\langle \frac{\delta Q}{\delta x_i(\tau)} \right\rangle_0 = \int_0^\beta g_0^{-1}(|\tau-\sigma|)\langle Q x_i(\sigma)\rangle_0 \tag{3.3.3}$$

or

$$\langle x_i(\tau) Q\rangle_0 = \int_0^\beta g_0(|\tau-\sigma|)\left\langle \frac{\delta Q}{\delta x_i(\sigma)} \right\rangle$$

Consider now the term $\langle B^2\rangle_0$. To evaluate this we first need to compute

$$\langle e^{i\mathbf{k}_1\cdot(\mathbf{r}(\tau_1)-\mathbf{r}(\sigma_1))} e^{i\mathbf{k}_2\cdot(\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2))}\rangle_0 \tag{3.3.4}$$

Letting $\gamma(\mu) = \sum_{j=1}^{2} i\mathbf{k}_j[\delta(\mu-\tau_i)-\delta(\mu-\sigma_i)]$

and using (3.1.10) and $D_0(\tau) = g_0(0) - g_0(\tau)$ we find that (3.3.4) is given by

$$\frac{1}{(2\pi^2)^2}\int\int \frac{d^3\mathbf{k}_1}{\mathbf{k}_1^2}\frac{d^3\mathbf{k}_2}{\mathbf{k}_2^2} e^{-\sum_{i,j=1}^{2}\mathbf{k}_i\mathbf{k}_j A_{ij}} \tag{3.3.5}$$

The A_{ij} are defined by

$$A_{ij} = \frac{1}{2}\Big[D_0(|\tau_i-\sigma_j|)+D_0(|\sigma_i-\tau_j|)-D_0(|\sigma_i-\sigma_j|)-D_0(|\tau_i-\tau_j|)\Big] \qquad (3.3.6)$$

To do the $\mathbf{k}$ integrals we use $\int_0^\infty du_i\, e^{-u_i \mathbf{k}_i\cdot\mathbf{k}_i} = \frac{1}{\mathbf{k}_i^2}$. The $\mathbf{k}$ integrals are then Gaussian integrals. Evaluating these and then performing the resulting integrals over u_1 and u_2, we finally obtain

$$<\frac{1}{|\mathbf{r}(\tau_1)-\mathbf{r}(\sigma_1)|}\,\frac{1}{|\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2)|}>_0 = \frac{1}{\pi(A_{12})}\sin^{-1}\left[\frac{A_{12}}{\sqrt{A_{11}A_{22}}}\right] \qquad (3.3.7)$$

In $<AB>_0$ we encounter

$$<\mathbf{r}(\tau_1)\cdot\mathbf{r}(\sigma_1)\,\frac{1}{|\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2)|}>_0 \qquad (3.3.8)$$

Applying (3.3.3) several times and using $\nabla^2\frac{1}{|\mathbf{r}-\mathbf{a}|} = -4\pi\delta^3(\mathbf{r}-\mathbf{a})$, we find that (3.3.8) is given by

$$<\mathbf{r}(\tau_1)\cdot\mathbf{r}(\sigma_1)>_0<\frac{1}{|\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2)|}>_0 \qquad (3.3.9)$$

$$-4\pi<\delta^3(\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2))>_0\Big[D_0(|\tau_1-\tau_2|)-D_0(|\tau_1-\sigma_2|)\Big]\Big[D_0(|\sigma_1-\tau_2|)-D_0(|\sigma_1-\sigma_2|)\Big]$$

The expectation of the delta function is found by using $\delta^3(\mathbf{r}) = \int\frac{d^3\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\mathbf{r}}$ and (3.1.10) to give

$$<\delta^3(\mathbf{r}(\tau)-\mathbf{r}(\sigma))>_0 = \frac{1}{8\pi^{\frac{3}{2}}}D_0^{-\frac{3}{2}}(|\tau-\sigma|) \qquad (3.3.10)$$

Also note that

$$<\mathbf{r}(\tau_1)\cdot\mathbf{r}(\sigma_1)\;\;\mathbf{r}(\tau_2)\cdot\mathbf{r}(\sigma_2)>_0 = <\mathbf{r}(\tau_1)\cdot\mathbf{r}(\sigma_1)>_0\;\;<\mathbf{r}(\tau_2)\cdot\mathbf{r}(\sigma_2)>_0 \qquad (3.3.11)$$

$$+3g_0(|\tau_1-\tau_2|)g_0(|\sigma_1-\sigma_2|)+3g_0(|\tau_1-\sigma_2|)g_0(|\tau_2-\sigma_1|)$$

Combining (3.3.1), (3.3.7), (3.3.9), (3.3.10), (3.3.11), and previous results for $\langle S\rangle_0$ we can finally write down $\beta\Delta F$ to second order.

Before doing this, however, we shall extend the schematic notation which we introduced earlier in equations (3.1.23) to (3.1.26). Thus symbols such as $a, b, \cdots$ will refer to $a(|\tau-\sigma|), b(|\tau-\sigma|), \cdots$ If we wish to be more explicit about some of the variables, we will write $(a)_{\tau\sigma}$ for $a(|\tau-\sigma|)$. A product notation ab will be used to denote integrals, so that $(ab)_{\tau\rho}$ will stand for $\int_0^\beta a(|\tau-\sigma|)b(|\sigma-\rho|)d\sigma$. If we wish to explicitly display integration over a variable, we will write $\int_\tau$ for $\int_0^\beta d\tau$. The notation $[a]$ will denote $\delta(\tau-\sigma)\int a(|\tau-\sigma'|)d\sigma'$.

With this notations the free energy to first order is

$$\beta\Delta F_0 + \frac{3}{2}\int_\tau (hg_0)_{\tau\tau} - \frac{\alpha}{\sqrt{2\pi}}\int_{\tau\sigma}\frac{(G_1)_{\tau\sigma}}{(D_0)_{\tau\sigma}^{\frac{1}{2}}} \tag{3.3.12}$$

The second order free energy is (κ_0 is defined in (3.2.8))

$$\frac{-3}{4}\int_\tau (g_0hg_0h)_{\tau\tau} + \frac{3}{2}\int_\tau (g_0hg_0\kappa_0)_{\tau\tau} \tag{3.3.13a}$$

$$-\frac{3}{2}\int_{\tau\sigma}(\kappa_0)_{\tau\sigma}(g_0hg_0)_{\tau\tau}$$

$$-\frac{\alpha^2}{4\pi}\int_{\tau_1\sigma_1\tau_2\sigma_2} G_1(|\tau_1-\sigma_1|)G_1(|\tau_2-\sigma_2|)q(\tau_1\sigma_1|\tau_2\sigma_2)$$

The function q is defined by

$$q(\tau_1\sigma_1|\tau_2\sigma_2) = \frac{1}{A_{12}}\left[\sin^{-1}\left[\frac{A_{12}}{\sqrt{A_{11}A_{22}}}\right] - \frac{A_{12}}{\sqrt{A_{11}A_{22}}}\right] \tag{3.3.13b}$$

with (from (3.3.6))

$$A_{11} = D_0(|\tau_1-\sigma_1|) \tag{3.3.13c}$$

$$A_{22} = D_0(|\tau_2-\sigma_2|)$$

$$A_{12} = \frac{1}{2}\left[D_0(|\tau_1-\sigma_2|)+D_0(|\sigma_1-\tau_2|)-D_0(|\sigma_1-\sigma_2|)-D_0(|\tau_1-\tau_2|)\right]$$

and

$$D_0(|\tau-\sigma|) = g_0(0)-g_0(|\tau-\sigma|)$$

The next step is to find the variation of the series (3.3.12) as we vary the function f_0 with h fixed. After setting $h(\tau) = \Omega^2\delta(\tau)-f_0(\tau)$ in the result (we shall take $\Omega = 0$), we obtain a series for $g(\tau)$. This series will then be transformed to an expansion for f. These expansions do not require that f_0 satisfy the variational equation (3.2.9), but we shall find that many terms drop out if (3.2.9) is satisfied.

From $gg_0^{-1} = 1$ (1 will represent the delta function $(1)_{\tau\sigma} = \delta(\tau-\sigma)$) and $-\frac{d^2}{dt^2}\delta(\tau-\sigma)+f_0(|\tau-\sigma|) = g_0^{-1}(|\tau-\sigma|)$ we have shown that $\delta g_0 = -g_0\delta f_0 g_0$. Since many of the terms involve D_0 's it is helpful to see what contributions such terms give when $D_0 \to D_0+\delta D_0$ as a result of $f_0 \to f_0+\delta f_0$. Let A represent such a term. Using $D_0(\tau) = g_0(0)-g_0(\tau)$ and $(g_0)_{\tau\tau} = (g_0)_{\sigma\sigma}$ we find that

$$\delta A = \int_{\tau\sigma}\frac{\delta A}{\delta(D_0)_{\tau\sigma}}(g_0\delta f_0 g_0)_{\tau\sigma} - \int_{\tau\sigma}\frac{\delta A}{\delta(D_0)_{\tau\sigma}}(g_0\delta f_0 g_0)_{\tau\tau} \tag{3.3.14}$$

Here the functional derivatives are to be taken as if $(D_0)_{\tau\sigma}$ is not symmetric in τ and σ. Since $\delta(\beta F) = \frac{3}{2}\int_\tau (g\,\delta f_0)_{\tau\tau}$, (3.3.14) leads to a contribution to the series for $(g)_{\tau\sigma}$ of

$$\frac{2}{3}\int_{\tau'\sigma'}(g_0)_{\tau\tau'}\left[\frac{\delta A}{\delta(D_0)_{\tau'\sigma'}}-\delta(\tau'-\sigma')\int_{\rho}\frac{\delta A}{\delta(D_0)_{\tau'\rho}}\right](g_0)_{\sigma'\sigma} \tag{3.3.15}$$

We note that the delta function term in (3.3.15) is completely determined by the other term. Applying (3.3.15) and $\delta g_0 = -g_0\delta f_0 g_0$ to (3.3.12) we find the g series to first order. Setting $h = -f_0$ and using the first of equations (3.1.26), we find that f_1, the first order correction to f_0 is given by

$$f_1 = -f_0-\kappa_0+[\kappa_0] \tag{3.3.16}$$

or more fully

$$f_1(|\tau-\sigma|) = -f_0(|\tau-\sigma|)-\kappa_0(|\tau-\sigma|)+\delta(\tau-\sigma)\int_0^{\beta}d\sigma'\kappa(|\tau-\sigma'|) \tag{3.3.17}$$

Here κ_0 is the function defined in (3.2.8). We note from (3.2.9) that for the best trial action S_0, f_0 satisfies $f_0+\kappa_0-[\kappa_0] = 0$, so that f_1 vanishes for the best S_0.

Before giving the second order terms in the f series we discuss the variation of the q - terms in (3.3.13a) in order to establish our notation. The variation of q is entirely due to the variations in A_{11}, A_{22}, A_{12}, so we may write

$$\delta q = q_{11}\delta A_{11}+q_{22}\delta A_{22}+q_{12}\delta A_{12} \tag{3.3.18}$$

The q_{ij} are given by

$$q_{11} = \frac{x}{2A_{11}A_{12}}\left[1-\frac{1}{\sqrt{1-x^2}}\right] \tag{3.3.19}$$

$$q_{22} = \frac{x}{2A_{22}A_{12}}\left[1-\frac{1}{\sqrt{1-x^2}}\right]$$

$$q_{12} = \frac{x}{A_{12}^2}\left[\frac{x}{\sqrt{1-x^2}}-\sin^{-1}x\right]$$

$$x = \frac{A_{12}}{\sqrt{A_{11}A_{22}}}$$

From (3.3.13a) and (3.3.19) we note some symmetries of the A_{ij} and q_{ij}. If τ_1 and σ_1 (in 3.3.13c) or τ_2 and σ_2 are interchanged then $A_{11}\rightarrow A_{11}$, $A_{22}\rightarrow A_{22}$, and $A_{12}\rightarrow -A_{12}$. The behavior of the q_{ij} under the same transformations is given by $q_{11}\rightarrow q_{11}$, $q_{22}\rightarrow q_{22}$, and $q_{12}\rightarrow -q_{12}$. If we interchange the pair $\tau_1\sigma_1$ with the pair $\tau_2\sigma_2$ we find that A_{22}, A_{11} and also q_{22}, q_{11} are interchanged while q_{12} and A_{12} are not changed. Using (3.3.18), (3.3.19), (3.3.15) and the symmetries just mentioned we can readily construct the contribution of the q - term in the free energy expansion to the g - series. From (3.1.26) the contribution to $(f)_{\tau\sigma}$ is

$$\frac{\alpha^2}{3\pi}\int_{\tau'\sigma'} G_1(|\tau-\sigma|)G_1(|\tau'-\sigma'|)q_{11}(\tau\sigma|\tau'\sigma') \qquad (3.3.20)$$

$$-\frac{\alpha^2}{3\pi}\int_{\tau'\sigma'} G_1(|\tau-\tau'|)G_1(|\sigma-\sigma'|)q_{12}(\tau\tau'|\sigma\sigma')$$

$$+\textit{delta function terms}$$

The rest of the second order contribution to $(f)_{\tau\sigma}$ is

$$((\kappa_0-[\kappa_0])g_0(\kappa_0-[\kappa_0]))_{\tau\sigma} \qquad (3.3.21)$$

$$-(L)_{\tau\sigma}((g_0f_0g_0)_{\tau\sigma}-(g_0f_0g_0)_{\tau\tau})$$

$$+\textit{delta function terms}$$

where

$$(L)_{\tau\sigma} = L(|\tau-\sigma|) = \frac{\alpha}{2\sqrt{2\pi}}\frac{G_1(|\tau-\sigma|)}{D_0^{\frac{5}{2}}(|\tau-\sigma|)} \qquad (3.3.22)$$

We note the delta term associated with the second term in (3.3.20) vanishes due to the antisymmetry of the integral in σ and σ'. The delta function terms associated with the first term in (3.3.21) also vanishes.

It seems strange that the first term in (3.3.21) survives. When we do perturbation theory with polynomial Lagrangians such terms always cancel out. This suggests that further simplifications may be possible. Suppose that we expand q_{12} in powers of x. The lowest order term is

$$\frac{1}{3}\frac{1}{A_{12}^2} = \frac{1}{3}\frac{A_{12}}{(A_{11}A_{22})^{\frac{3}{2}}} \tag{3.3.23}$$

By using the expressions (3.3.13c) for the A_{ij} and doing some rearranging we find that the contribution to the f series involving (3.3.23) cancels the first term in (3.3.21). Similarly, the lowest order term in q_{11} is

$$-\frac{1}{4}\frac{x^3}{A_{11}a_{12}} = -\frac{1}{4}\frac{A_{12}^2}{A_{11}^{\frac{5}{2}}A_{22}^{\frac{3}{2}}} \tag{3.3.24}$$

The contribution to the f series involving this piece of q_{11} combined with the second term in (3.3.21) is

$$-(L)_{\tau\sigma}\int_{\tau'\sigma'}(f_0+\kappa_0-[\kappa_0])_{\tau'\sigma'}(g_0)_{\tau\sigma'}((g_0)_{\sigma\tau'}-(g_0)_{\tau\tau'}) \tag{3.3.25}$$

Note the factor $+f_1 = -f_0-\kappa_0+[\kappa_0]$. We see that when we use the best S_0 so that $f_1 = 0$, the contribution from (3.3.25) vanishes. The corresponding delta function term also vanishes. We can in this case write the second order piece of f, that is f_2, as

$$f_2(|\tau-\sigma|) = -\kappa_2(|\tau-\sigma|)+\delta(\tau-\sigma)\int_{\sigma'}\kappa_2(|\tau-\sigma'|) \tag{3.3.26a}$$

where the function $\kappa_2(|\tau-\sigma|)$ is defined by

$$\kappa_2(|\tau-\sigma|) = \frac{\alpha^2}{3\pi}\int_{\tau'\sigma'}G_1(|\tau-\tau'|)G_1(|\sigma-\sigma'|)\bar{q}_{12}(\tau\tau'|\sigma\sigma') \tag{3.3.26b}$$

$$-\frac{\alpha^2}{3\pi}\int_{\tau'\sigma'} G_1(|\tau-\sigma|)g_1(|\tau'-\sigma'|)\bar{q}_{11}(\tau\sigma|\tau'\sigma')$$

where $\bar{q}_{12}$ and $\bar{q}_{11}$ are given by

$$\bar{q}_{11}(\tau_1\sigma_1|\tau_2\sigma_2) = \frac{x}{2A_{11}A_{12}}\left[1+\frac{x^2}{2}-\frac{1}{\sqrt{1-x^2}}\right] \tag{3.3.26c}$$

$$\bar{q}_{12}(\tau_1\sigma_1|\tau_2\sigma_2) = \frac{1}{A_{12}^2}\left[\frac{x}{\sqrt{1-x^2}}-\sin^{-1}x-\frac{x^3}{3}\right]$$

where

$$x = \frac{A_{12}}{\sqrt{A_{11}A_{22}}}$$

and as before

$$A_{11} = D_0(|\tau_1-\sigma_1|) \tag{3.3.26d}$$

$$A_{22} = D_0(|\tau_2-\sigma_2|)$$

$$A_{12} = \frac{1}{2}[D_0(|\tau_1-\sigma_2|)+D_0(|\tau_2-\sigma_1|)-D_0(|\tau_1-\tau_2|)-D_0(|\sigma_1-\sigma_2|)]$$

$D_0(\tau)$ is given by

$$D_0(\tau) = \int_0^\infty \frac{s_0(\omega)}{\pi}\frac{d\omega}{2\omega}\left[\frac{1-e^{-\omega\tau}}{1-e^{-\beta\omega}}+\frac{1-e^{\omega\tau}}{e^{\beta\omega}-1}\right] \tag{3.3.26e}$$

Here $s_0(\omega)$ is the absorption function for the trial action S_0. Note that this expression allows us to analytically continue $D_0(\tau)$ into the complex τ plane as long as $0\leq \mathrm{Re}\tau\leq\beta$.

The absorption function $s(\lambda)$, correct to second order is given by

$$s(\lambda) = \mathrm{Im}\left[\frac{2\lambda}{(0^+-i\lambda)^2+\hat{f}_0(-i\lambda)+\hat{f}_2(-i\lambda)}\right] \tag{3.3.27}$$

$\hat{f}_0(-i\lambda)$ is given by (3.2.12) and $\hat{f}_1(-i\lambda)$ is presumed to be zero. $\hat{f}_2(-i\lambda)$ is given by

$$\hat{f}_2(-i\lambda) = 2\int_0^\infty (e^{i\lambda s} - 1)\mathrm{Im}\kappa_2(is) \qquad (3.3.28)$$

$\kappa_2(is)$ is the continuation of $\kappa_2(\tau)$ given by (3.3.26b) for real τ to imaginary $\tau = is$.

4. NUMERICAL RESULTS

4.1. Solution of the Variational Equations

The first method of solution for the variational absorption function $s_0(\omega)$ which we used is based on the cycle of equations (3.2.11) to (3.2.13). In the actual program it is possible to start at several different points in this cycle. We shall briefly describe the program.

An array containing the values of $D_0(is)$ at equally spaced values of s is formed. From this a table of values of

$$\mathrm{Im}\,\frac{G_1(is)}{D_0^{\frac{3}{2}}(is)} \tag{4.1.1}$$

in the integrand of (3.2.12) is formed. This function falls off slowly as $s\to\infty$ and has a singularity at $s = 0$. To improve its behavior, we modify it by subtracting a function $\Phi(s)$ to get a table of values of

$$\left[\mathrm{Im}\,\frac{G_1(is)}{D_0^{\frac{3}{2}}(is)}\right]-\Phi(s) \tag{4.1.2}$$

The function $\Phi(s)$ is chosen so that it has the same singular behavior at $s = 0$ as the quantity in (4.1.1) and also falls off at ∞ in the same way as (4.1.1). $\Phi(s)$ is also chosen so that the integral

$$\frac{2\alpha}{3\sqrt{2\pi}}\int_0^\infty (e^{i\lambda s}-1)\Phi(s)ds \tag{4.1.3}$$

may be carried out analytically. The numerical integration of (4.1.2) multiplied by $\frac{2\alpha}{3\sqrt{2\pi}}(e^{i\lambda s}-1)$ is carried out by using a Fast Fourier Transform and the results are added to the results of (4.1.3) to form an array of $f_0(-i\lambda)$ values at

equally spaced values of λ. Equation (3.2.13) is now used to form a table of $s_0(\lambda)$. If an older version of this table exists, the entries are compared to see if they agree well enough that the iteration may be stopped. If the iterations are stopped, a table of $f_0(-i\lambda)$ is output. Otherwise a table of

$$s_0(\lambda) - u(\lambda) \tag{4.1.4}$$

is constructed, where $u(\lambda)$ has the same behavior as $s_0(\lambda)$ as $\lambda \to \infty$. The integral

$$\int_0^\infty \frac{d\omega}{\pi} u(\omega) \frac{1}{2\omega}\left[\frac{1-e^{-i\omega t}}{1-e^{-\beta\omega}} + \frac{1-e^{i\omega t}}{e^{\beta\omega}-1}\right] \tag{4.1.5}$$

is performed analytically while

$$\int_0^\infty \frac{d\omega}{\pi}[s_0(\omega)-u(\omega)] \frac{1}{2\omega}\left[\frac{1-e^{-i\omega t}}{1-e^{-\beta\omega}} + \frac{1-e^{i\omega t}}{e^{\beta\omega}-1}\right] \tag{4.1.6}$$

is done numerically. The results are added to form a table of values of $D_0(it)$. (see (3.2.11)). This is where we started. The program goes on this way until convergence is achieved.

Our second approach to the computation of $s_0(\omega)$ begins from the expression (3.2.19) for the free energy ΔF. We only worked out the $\beta = \infty$ case in this approach. In this case (3.2.19) becomes

$$\Delta F \leq 3\int_0^\infty \frac{d\lambda}{2\pi}\left[\ln\left(1+\frac{\hat{f}_0(\lambda)}{\lambda^2}\right) - \frac{\hat{f}_0(\lambda)}{\lambda^2+\hat{f}_0(\lambda)}\right] - \frac{\alpha}{\sqrt{2\pi}}\int_0^\infty \frac{e^{-\tau}}{D_0^{\frac{1}{2}}(\tau)} d\tau \tag{4.1.7}$$

$s_0(\omega)$ was assumed to have the form (for $\omega \geq 1$)

$$s_0(\omega) = C(\omega-1)^{\frac{1}{2}} R(\omega) \tag{4.1.8}$$

Here C is a constant and $R(\omega)$ is a rational function in ω. For $0<\omega\leq 1$, $s_0(\omega)$ is

taken to be zero. The factor $(\omega-1)^{\frac{1}{2}}$ was included because the threshold at $\omega = 1$ is known to have this form. Also, it is known that as $\omega\to\infty$, $s_0(\omega)\to\frac{4\alpha}{3}\omega^{-2.5}$. Thus the form (4.1.8) can have the correct behavior at $\omega\to1$ and as $\omega\to\infty$.

C and the roots of the numerator and denominator of $R(\omega)$ are taken as variational parameters. $D_0(\tau)$ is obtained (numerically) from

$$D_0(\tau) = \frac{a_0\tau}{2}+\int_1^\infty \frac{s_0(\omega)}{\pi}\frac{1}{2\omega}\left[1-e^{-\omega\tau}\right]d\omega \qquad (4.1.9)$$

with s_0 given by (4.1.8). a_0 is just $1-\int_1^\infty \frac{s_0(\omega)}{\pi}d\omega$. $\hat{f}(\lambda)$ is obtained analytically by evaluating (see (2.3.11) and (2.3.9))

$$\frac{1}{\lambda^2+\hat{f}(\lambda)} = \int_0^\infty \frac{s_0(\omega)}{\pi}d\omega\,\frac{1}{\lambda^2+\omega^2} \qquad (4.1.10)$$

The integrals in (4.1.7) are then evaluated numerically to find the right hand side of (4.1.7). A minimization program was then used to find the values of the parameters in $s_0(\omega)$ which give the smallest value for the right hand side of (4.1.7).

Some results for $\alpha = 5$ ($\beta = \infty$) are shown in figure 4.1.1. The value of $s_0(\omega)$ is plotted against ω. Curve 1 is the result of the iteration method (the first method described in this chapter). Curves 2 and 3 are both results of the minimization method. Curve 3 is apparently spurious for when the $s_0(\omega)$ of curve 3 is used as an input to the iteration method, the results rapidly converge to curve 1. Also, when a fit of the form (4.1.8) is made to curve 1 and the resulting parameters used as a first guess in the minimization method, curve 2 is the result. These results illustrates some of the pitfalls of minimization methods in general. The free energy is a functional of some function but is not very sensitive

to the form of the function in the vicinity of the minimum.

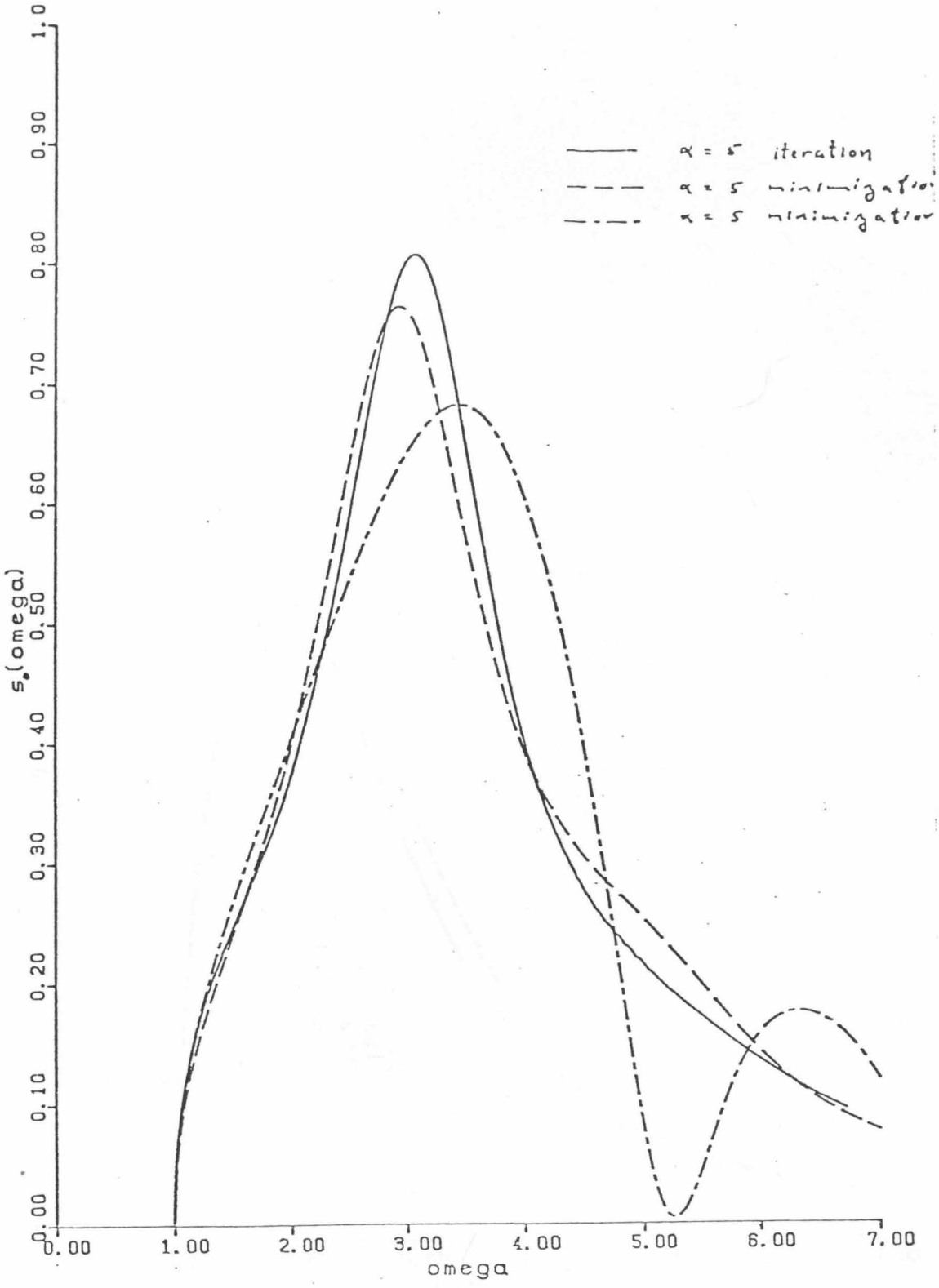

α = 5 iteration
α = 5 minimization
α = 5 minimization
s(omega)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.0
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.1.1

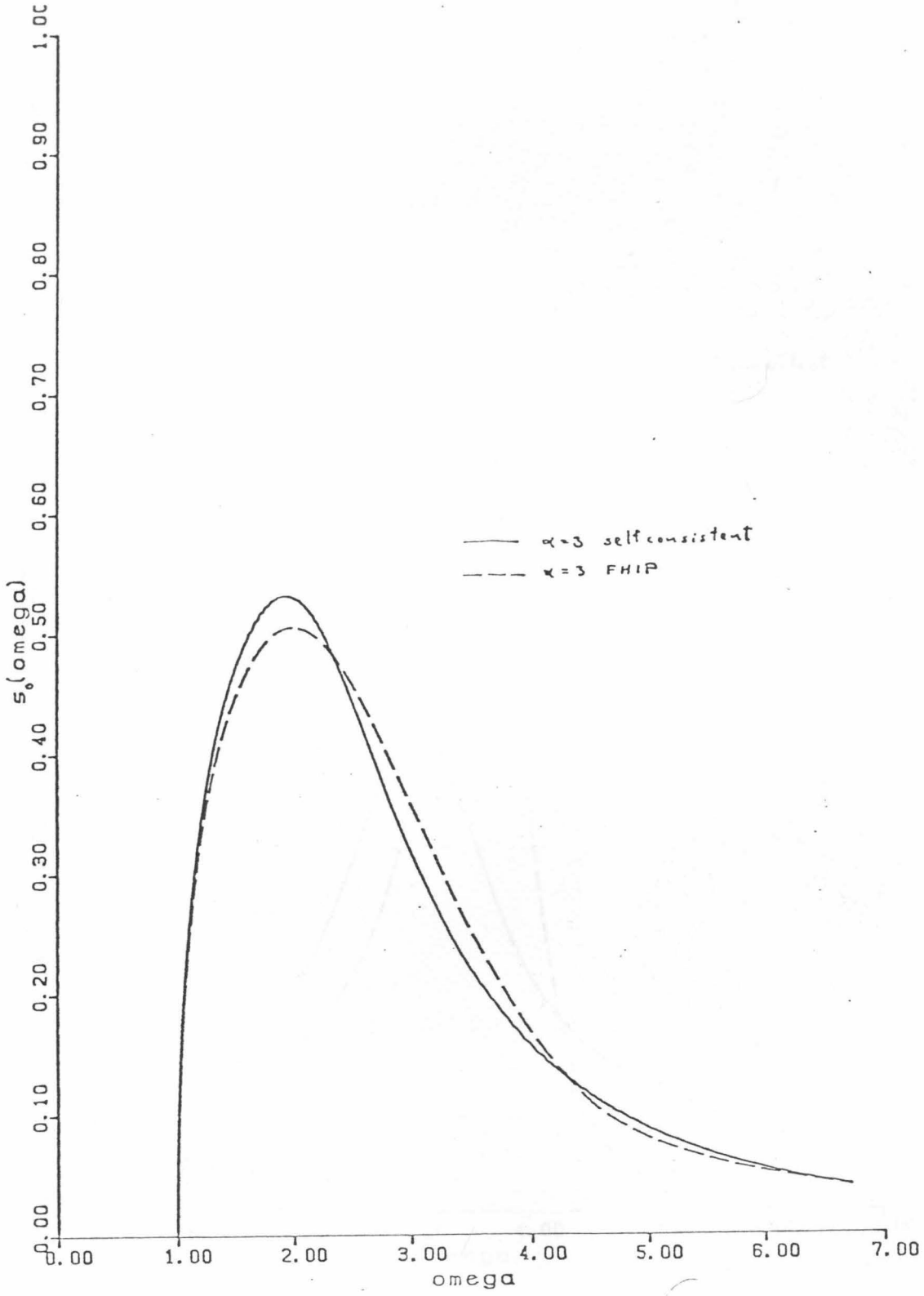

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
S_0(omega)
α=3 self consistent
α=3 FHIP
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.1.2

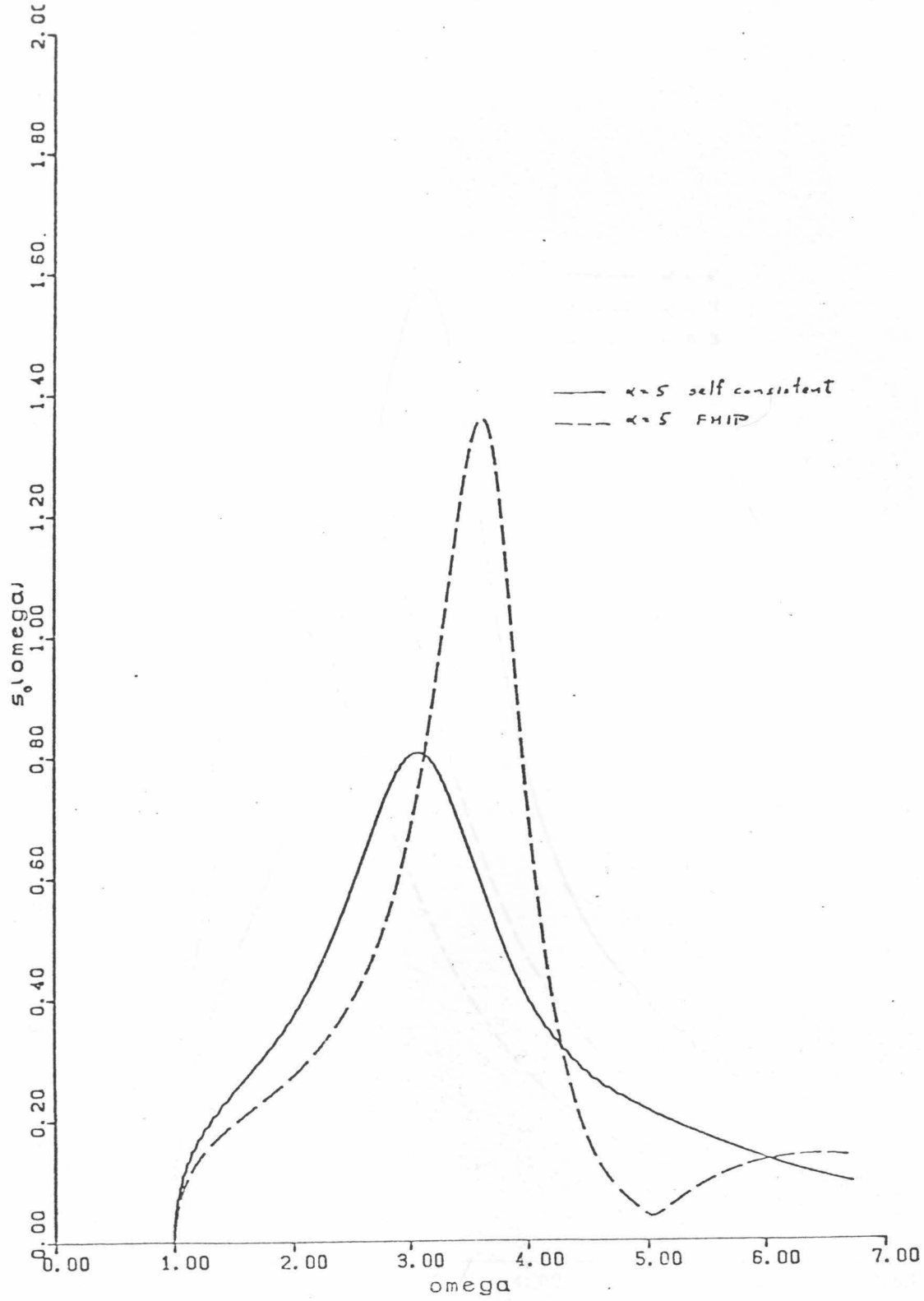

κ=5 self consistent
κ=5 FHIP
S(omega)
omega
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60
1.80
2.00
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00

Figure 4.1.3

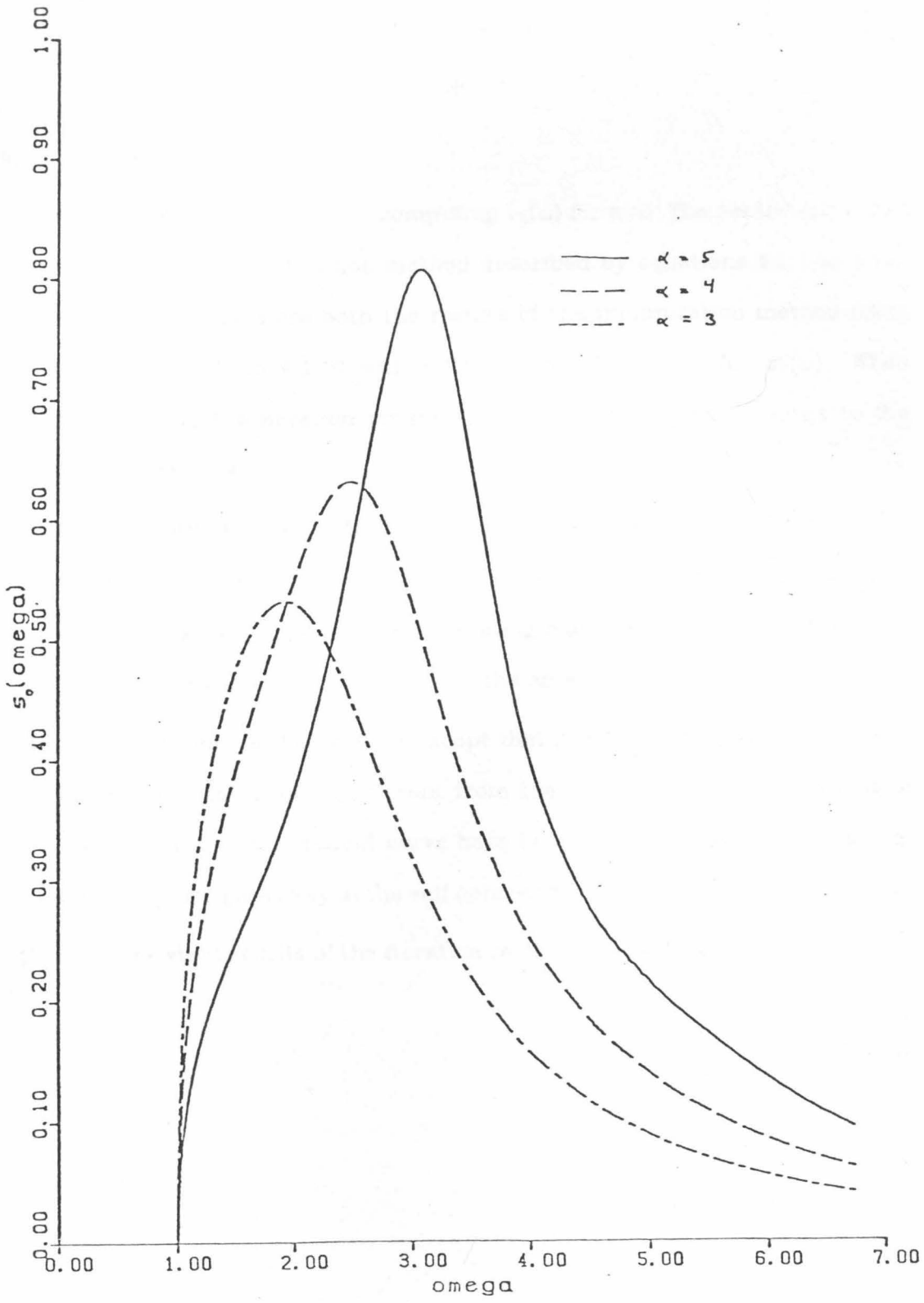

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
S_o(omega)
α = 5
α = 4
α = 3
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.1.4

Figure Captions

[1] Results from two methods of computing $s_0(\omega)$ for α=5. The continuous curve is the result of the iteration method described by equations 4.1.1 to 4.1.6. The dashed curves are both the results of the minimization method using equations 4.1.7 to 4.1.10 with different initial guesses for $s_0(\omega)$. When inserted into the iteration program both of these curves converge to the continuous curve.

[2] The continuous curve is the result of the iteration method for α=3. The dashed curve results from starting with an initial $s_0(\omega) = (1-a_1)\delta(\omega)+a_1\delta(\omega-\omega_1)$ and iterating once. a_1 and ω_1 are determined by minimizing the free energy. This is the ansatz used by FHIP.

[3] This is the same as figure 4.1.2 except that it is for α=5. Note that the self consistent $s_0(\omega)$ is quite different from the FHIP $s_0(\omega)$. Interpretations of the structure in the dashed curve have been given in [10],but we see that this structure goes away in the self consistent solution.

[4] Self consistent results of the iteration method for α= 3,4,5.

4.2. Second order correction

$s(\lambda)$, the absorption.function, is given correct to second order by (3.3.27). This requires the computation of $\hat{f}_2(-i\lambda)$ as in equation (3.3.28), which is

$$\hat{f}_2(-i\lambda) = 2\int_0^\infty (e^{i\lambda s}-1)\mathrm{Im}\kappa_2(is)ds \tag{4.2.1}$$

For real τ and σ, $\kappa_2(|\tau-\sigma|)$ is given by (3.3.26b) and the following equations. We need to continue these to imaginary $\tau = is$. A simple example illustrates how this may be done. If we wish to continue $a(\tau)$ given by

$$a(\tau) = \int_0^\infty e^{-\omega|\tau-\sigma|}d\sigma \tag{4.2.2}$$

into the complex τ plane, we can rewrite it as

$$a(\tau) = e^{-\omega\tau}\int_0^\tau e^{\omega\sigma}d\sigma + e^{\omega\tau}\int_\tau^\infty e^{-\omega\sigma}d\sigma \tag{4.2.3}$$

Now since the integrands are analytic and convergent, we are free to move the contours around. Thus $a(it)$ may be computed by

$$a(it) = e^{-i\omega t}\int_0^{it} e^{\omega\sigma}d\sigma + e^{i\omega t}\int_{it}^\infty e^{-\omega\sigma}d\sigma \tag{4.2.4}$$

Consider the contour C running from 0 to some complex τ and then to ∞. for σ_1, σ_2 on this contour write $\sigma_1 > \sigma_2$ if we encounter σ_2 first as we traverse the contour starting at 0. For complex τ and σ on C define $|\tau-\sigma|_C$ to be $\tau-\sigma$ if $\tau>\sigma$ and $\sigma-\tau$ if $\tau\leq\sigma$. Then for complex τ

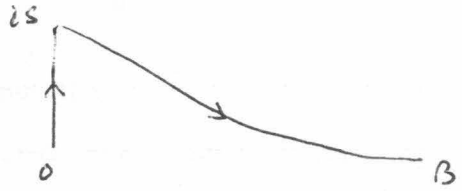
$$a(\tau) = \int_C e^{-\omega|\tau-\sigma|_C}d\tau \tag{4.2.5}$$

where τ must be on the contour C. With this notation $\kappa_2(is)$ is given by

$$\kappa(is) = \frac{\alpha^2}{3\pi}\int_{\tau'\sigma'} G_1(|is-\tau'|_C)G_1(\sigma')\bar{q}_{12}(is,\tau'|0,\sigma') \qquad (4.2.6)$$

$$-\frac{\alpha^2}{3\pi}\int_{\tau'\sigma'} G_1(is)G_1(|\tau'-\sigma'|_C)\bar{q}_{11}(is,0|\tau'\sigma')$$

Here τ', σ' are on a contour C such as:



We also have

$$\bar{q}_{12}(is,\tau'|0,\sigma') = \frac{1}{A_{12}^2}\left[\frac{x}{\sqrt{1-x^2}} - \sin^{-1}x - \frac{x^3}{3}\right] \qquad (4.2.7a)$$

with $x = \dfrac{A_{12}}{\sqrt{A_{11}A_{22}}}$ and

$$A_{11} = D_0(|is-\tau'|_C) \qquad (4.2.7b)$$

$$A_{22} = D_0(\sigma')$$

$$A_{12} = \frac{1}{2}\left[D_0(|is-\sigma'|_C) + D_0(\tau') - D_0(is) - D_0(|\tau'-\sigma'|_C)\right]$$

while for $\bar{q}_{11}$ we have

$$\bar{q}_{11}(is,0|\tau',\sigma') = \frac{x}{2A_{11}A_{12}}\left[1 + \frac{x^2}{2} - \frac{1}{\sqrt{1-x^2}}\right] \qquad (4.2.8a)$$

again with $x = \dfrac{A_{12}}{\sqrt{A_{11}A_{22}}}$ but with

$$A_{11} = D_0(is) \tag{4.2.8b}$$

$$A_{22} = D_0(|\tau'-\sigma'|_C)$$

$$A_{12} = \frac{1}{2}\left[D_0(|\tau'-\sigma'|_C) + D_0(\tau') - D_0(|is-\tau'|_C) - D_0(\sigma')\right]$$

$$D_0(\tau) = \int_0^\infty \frac{s_0(\omega)}{\pi} d\omega \, \frac{1}{2\omega}\left[\frac{1-e^{-\omega\tau}}{1-e^{-\beta\omega}} + \frac{1-e^{\omega\tau}}{e^{\beta\omega}-1}\right] \tag{4.2.9}$$

It is convenient to put these equations into a form in which the limit $\beta\to\infty$ is easily taken. Consider $G_1(\tau)$ as β becomes very large.

$$G_1(\tau) = \frac{1}{2}\left[\frac{e^{-\tau}}{1-e^{-\beta}} + \frac{e^{\tau}}{e^{\beta}-1}\right] \tag{4.2.10}$$

For fixed finite σ, $G_1(\sigma)$ and $G_1(\beta-\sigma)$ have finite limits as $\beta\to\infty$. Both limits are given by

$$G_1(\sigma) = G_1(\beta-\sigma) = \frac{e^{-\sigma}}{2} \qquad \beta\to\infty \tag{4.2.11}$$

We must also consider the behavior of $D_0(\tau)$ as $\beta\to\infty$. From (4.2.9) we see that for finite σ

$$D_0(\sigma) = D_0(\beta-\sigma) = \int_0^\infty \frac{s_0(\omega)}{\pi} d\omega \, \frac{1}{2\omega}\left[1-e^{-\omega\sigma}\right] \qquad \beta\to\infty \tag{4.2.12}$$

At $\beta=\infty$ (zero temperature) there are no optical phonon present initially in the crystal. The electron can absorb energy from the field at zero frequency (electron accelerated by a time constant field) or it can absorb energy from a time varying field and emit a phonon. However, this cannot happen until the frequency of the applied field is equal to or greater than the optical phonon frequency. From these consideration $s(\omega)$ has a delta function at $\omega = 0$ and is zero for $0<\omega<1$. Letting

$$a_1 = \int_1^\infty \frac{s_0(\omega)}{\pi} d\omega \tag{4.2.13}$$

and defining $a_0 = 1-a_1$ we find that at $\beta = \infty$, $D_0(\tau)$ has the form

$$D_0(\tau) = \frac{a_0\tau}{2} + \int_1^\infty \frac{s_0(\omega)}{\pi} d\omega \, \frac{1}{2\omega}\left[1-e^{-\omega\tau}\right] \tag{4.2.14}$$

Note that this becomes ∞ as $\tau\to\infty$.

Consider now the integrals in (4.2.6) and (4.2.7). Using (4.2.14), (4.2.12), and (4.2.11) we find that the integrand is now zero as $\beta\to\infty$ only if τ' or $\beta-\tau'$ and σ' or $\beta-\sigma'$ remain finite as $\beta\to\infty$. Denote the integrand in the sum of (4.2.6) and (4.2.7) by $I(is,\tau',\sigma')$ so that

$$\kappa_2(is) = \int_C d\tau' \int_C d\sigma' I(is,\tau',\sigma') \tag{4.2.15}$$

When $\beta\to\infty$ only the pieces of C near to 0 or β give any contribution. Let C_1 run from 0 to $\frac{\beta}{2}$. If τ is on C_1 take C_2 to be the set of all points $(\beta-\tau)$. C_1 and C_2 together form C. Rewrite each integral over C as

$$\int_C a(\tau)d\tau = \int_{C_1} a(\tau)d\tau + \int_{C_2} a(\tau)d\tau \tag{4.2.16}$$

$$= \int_{C_1} a(\tau)d\tau + \int_{C_1} a(\beta-\tau)d\tau$$

so that (4.2.15) becomes

(4.2.17)

$$\kappa_2(is) = \int_{C_1} d\tau' \int_{C_1} d\sigma' \left[I(is,\tau',\sigma') + I(is,\beta-\tau',\sigma') + I(is,\tau',\beta-\sigma') + I(is,\beta-\tau',\beta-\sigma')\right]$$

Finally use $D_0(\beta-\tau) = D_0(\tau)$, $G_1(\beta-\tau) = G_1(\tau)$ to rewrite the integrands. The $\beta\to\infty$

limit may now be taken. Of course, we may also use the form (4.2.17) for $\beta \neq \infty$. (4.2.17) is the form we actually used in the numerical computations.

To compute the second order corrections we did not use directly the table of values for $D_0(it)$ computed by the iteration method. Rather a fit was made to the $s_0(\omega)$ computed by the iteration method of the form

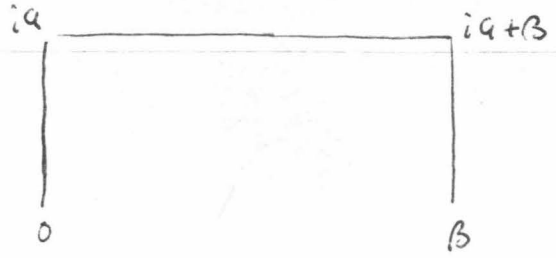
$$s_0(\omega) = 2\pi \sum_{i=0}^{n} A_i \omega(\omega-1)^{i+\frac{1}{2}} e^{-b(\omega-1)} \tag{4.2.18}$$

Here the A_i and b are parameters which we are free to vary. Figures 4.2.1 and 4.2.2 show the fits for $\alpha = 3$ and $\alpha = 5$ respectively. The $D_0(it)$ arising from (4.2.18) is given by

$$D_0(\tau) = \frac{a_0 \tau}{2} + \sum_{i=0}^{n} A_i (i+\frac{1}{2})! \left[b^{-i-\frac{3}{2}} - e^{-\tau}(b+\tau)^{-i-\frac{3}{2}} \right] \tag{4.2.19}$$

where $a_0 = 1 - a_1$ and $a_1 = \int_1^\infty \frac{s_0(\omega)}{\pi} d\omega$. An important feature of this $D_0(\tau)$ is that for $\tau = it$ and large t, the oscillating term in $D_0(\tau) = D_0(it) \to 0$ as $t \to \infty$.

To evaluate $\kappa_2(is)$ along the interval from $s=0$ to $s=\alpha$ we use a contour in the $\tau = is$ plane such as:



We split this contour into straight line segments. An integral along any segment may be done numerically by Gaussian integration. For each segment of contour we have a set of points and a weight for each point. Combining the points and

weights for all of the segments gives an array of points and an associated array of weights describing the contour. The integrals in (4.2.17) are carried out using these points and weights. Using a set of such contours a table of $\kappa_2(is)$ is built up. Similarly, a table of $\kappa_2(s)$ may be constructed using a contour lying along the real axis in the τ plane. Finally $\hat{f}_2(-i\lambda)$ is evaluated using (3.3.28) and $s(\lambda)$ is constructed from $\hat{f}_0(-i\lambda)+\hat{f}_2(-i\lambda)$.

In the path integral variational method, the trial action S_0 (or $s_0(\omega)$ from which we may construct the trial action) plays a role analogous to the wave function in the usual Hamiltonian variational method. At α=3 the second order correction to the polaron energy is one percent while at α=5 the correction is 1.5 percent. The second order corrections to the absorption function shown in figures 4.2.3 and 4.2.4 are quite reasonable in relation to the size of the energy corrections. For example,the difference in area under the variational curves and the corrected curves between $\omega = 1$ and $\omega = \infty$ is in each case less than 10 percent. For α=3 the correction is quite small except between ω=1.5 and ω=2.5 and in this range its maximum is 25 percent. For $\alpha = 5$ the location of the peak is shifted by about 10 percent and its width at half maximum is changed by about 20 percent.

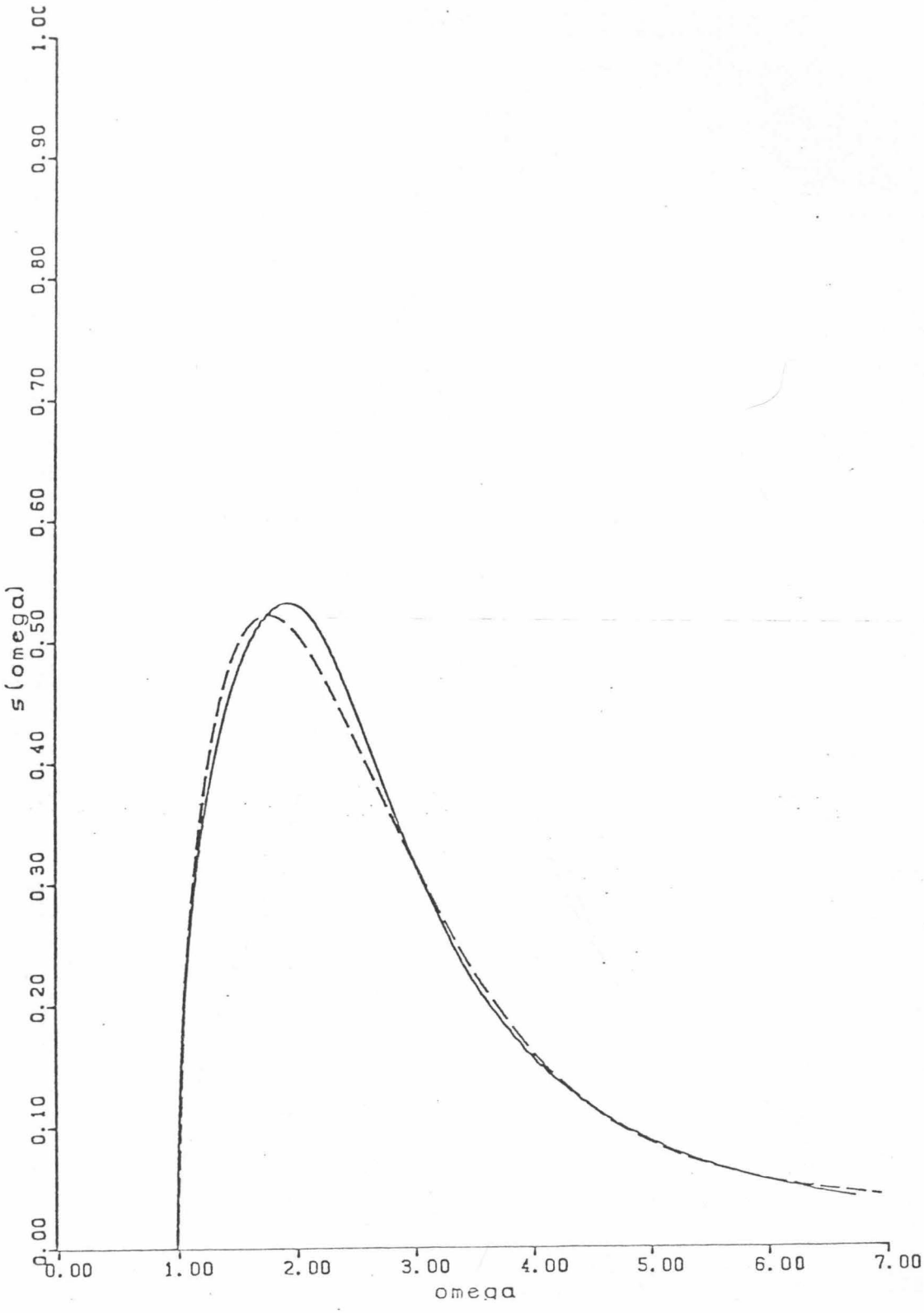

s(omega)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.2.1

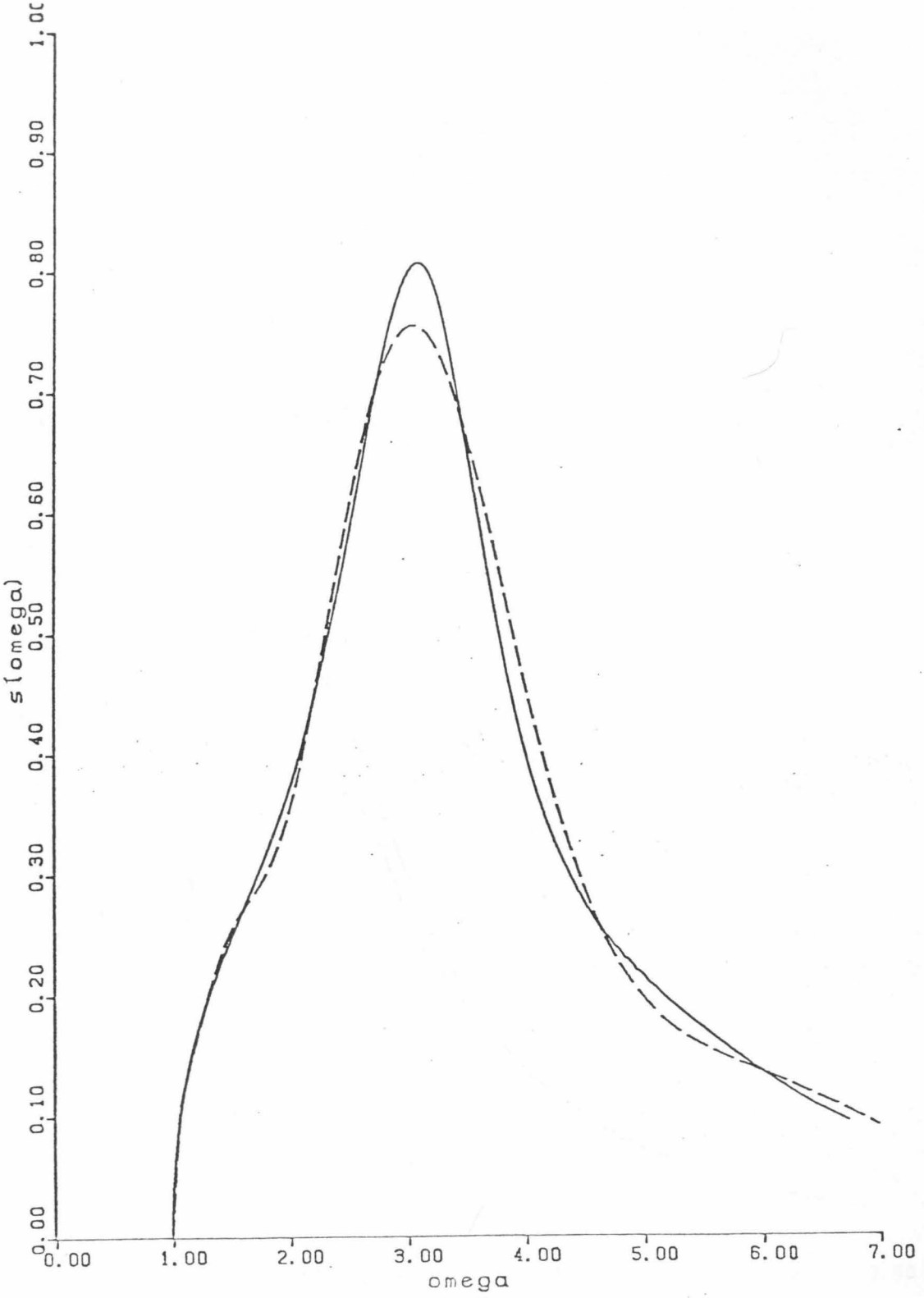

s(omega)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.2.2

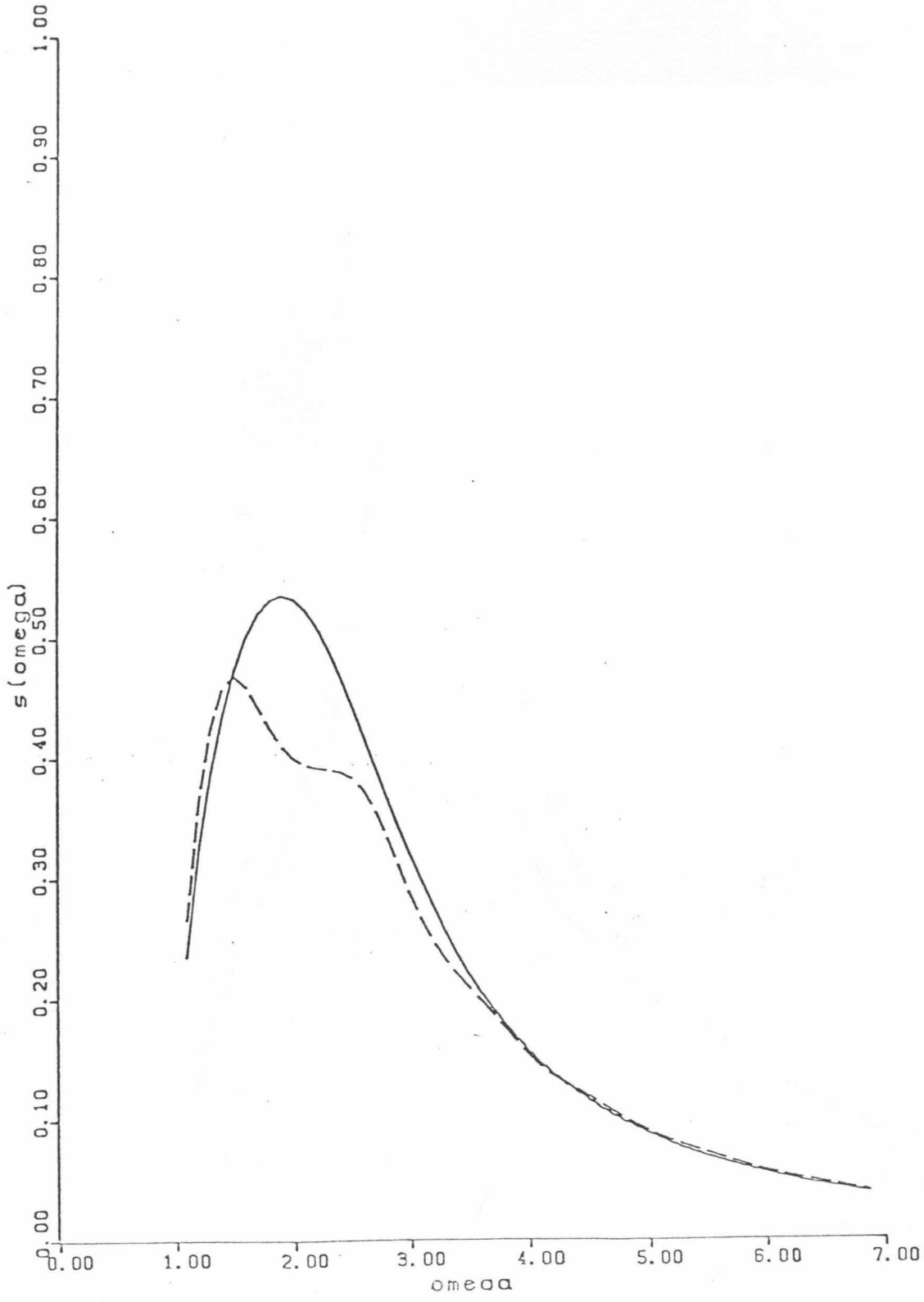

s(omega)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.2.3

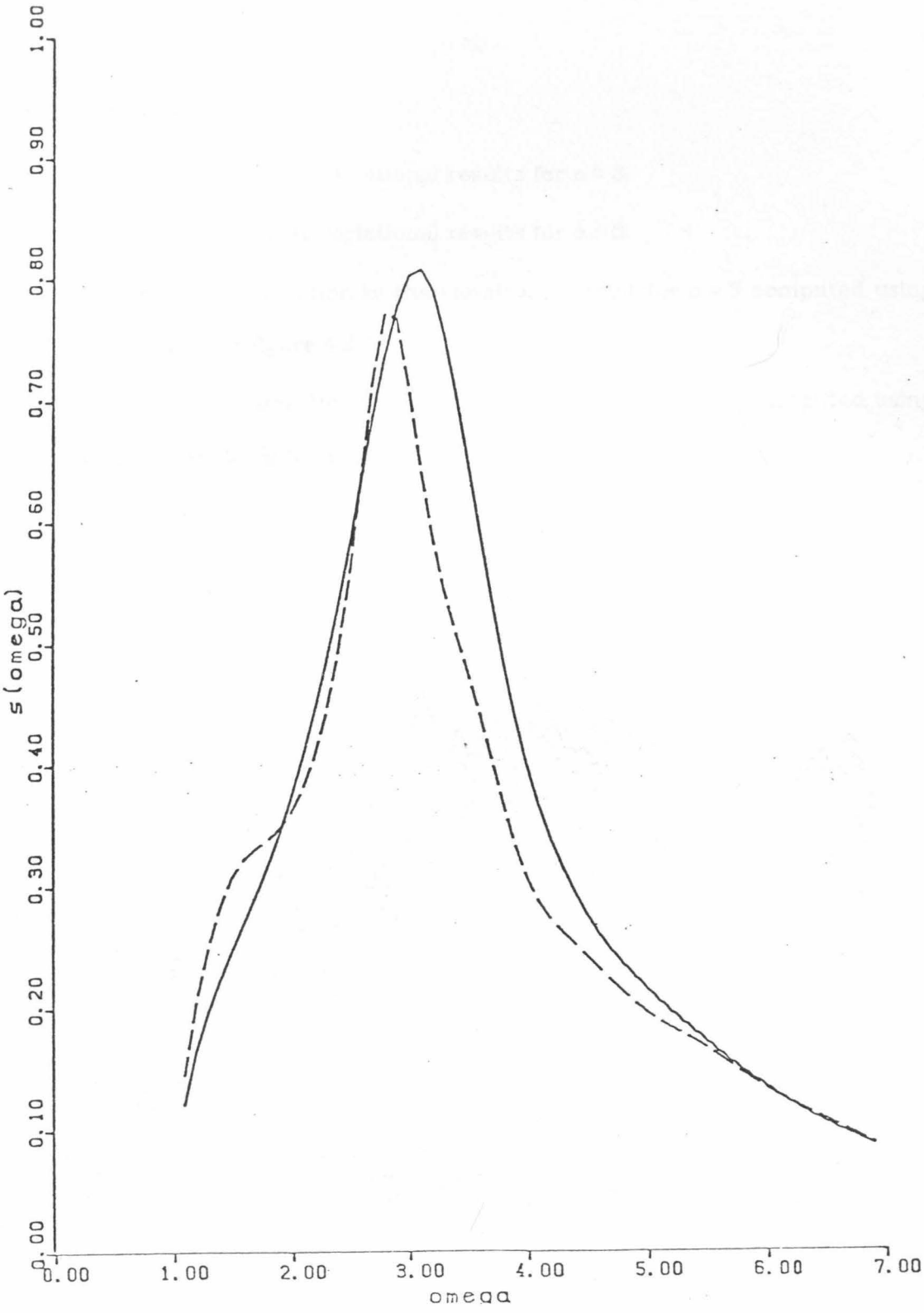

s(omega)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
omega

Figure 4.2.4

Figure Captions

[1] Fit of form (4.2.18) to variational results for $\alpha = 3$.

[2] Fit of form (4.2.18) to variational results for $\alpha = 5$.

[3] Second order correction to the variational result for $\alpha = 3$ computed using the fit shown in figure 4.2.1.

[4] Second order correction to the variational result for $\alpha = 5$ computed using the fit shown in figure 4.2.2.

5. FURTHER DEVELOPMENTS

5.1. Possibility of Improving the Method

To what extent can we remove the idealizations made in the Frolich model and still retain the ability to perform an accurate variational calculation for the free energy and the response functions?

The treatment of the crystal as a continuum is nonessential, as is the restriction to one type of phonon. The phonon dispersion relations can also be generalized. Of course, dropping these simplifications makes the numerical work more laborious, but this is a quantitative and not a qualitative difference. At least the solution of the variational equations could be carried out in a reasonable amount of time if one were sufficiently clever in formulating the numerical algorithms.

The most crucial idealizations which the Frolich model makes are that the lattice oscillations are harmonic and that the electron-phonon interaction is linear in the phonon variables. Of these, the latter is perhaps the more important approximation. The great virtue of Feynman's method of treating the polaron problem is that the phonon variables are intergrated away exactly. A variational calculation in which one tries to imitate the whole Frolich action by a Gaussian trial action cannot be expected to work as well as the Feynman method does. No coupling linear in both the electron and lattice variables can simulate correctly the distortion of the lattice by the electron.

If the electron-lattice coupling remains linear in the lattice variables but the lattice anharmonicity is taken into account in the lattice Lagrangian itself, we may still approximately integrate away the phonons in such a way that the variational inequality is preserved. Let S_l be the lattice action. Let the q denote the lattice variables and let the γ be functionals of the electron path

such that $\int \gamma \cdot q$ is the electron lattice coupling term. We need to do the path integral

$$\int Dq e^{-S_l + \int \gamma \cdot q} \tag{5.1.1}$$

When S_l is Gaussian this can be done. If S_l is not Gaussian then take a trial action of the form

$$S_0 - \int \gamma \cdot q \tag{5.1.2}$$

where S_0 is a Gaussian in the q's. The difference between $S_l - \int \gamma \cdot q$ and $S_0 - \int \gamma \cdot q$ is independent of the γ's. Finally, choose S_0 by minimizing $\beta F_{S_0} + <S_l - S_0>_{S_0}$. Here F_{S_0} is the free energy of S_0 alone (with the γ in (5.1.2) set to zero). This seems like a reasonable procedure and gives the exact result if S_l is Gaussian. Of course, it would be nicer to replace (5.1.2) by

$$\bar{S}_0 = S_0 - \int \bar{\gamma} \cdot q \tag{5.1.3}$$

where S_0 is again Gaussian but $\bar{\gamma}$ is different from γ. Now choose S_0 and $\bar{\gamma}$ so as to minimize

$$\beta F_{\bar{S}_0} + <S - \int \gamma \cdot q - \bar{S}_0>_{S_0} \tag{5.1.4}$$

The result is a set of nonlinear equations which, if solved, would give S_0 and $\bar{\gamma}$ as functionals of S_l and, more importantly, of γ. While we may solve these equations numerically to find S_0 and $\bar{\gamma}$ for a given γ, this is not of much use in writing down an effective action for the electron. Either the nonlinear equations resulting from the minimization of (5.1.4) must be solved explicitly for general γ or we must find an indirect method. To carry out a variational approximation to the electron effective action resulting from the approximate integration of the phonon variables, we need to calculate averages of quantities such as $\bar{S}_0$ and $\bar{\gamma}$ which

are given as implicit functionals of the electron path[*]

(since γ is a functional of the electron path). If this problem were solved, it would also be possible to treat the situation of an electron-phonon coupling non-linear in the phonon variables. In fact it might be possible to construct sequences of increasingly better variational approximations to a wide variety of problems. However, we have not discovered any way to solve the problem.

5.2. More General Method of Analytic Continuation

In this section we present a generalization of the method described in section 2.3. These generalizations allow us to treat nonthermal density matrices and to extend the path integral variational principle to a wider range of problems. To motivate the generalization we consider a particular problem.

A system consisting of an electron and a crystal has a Hamiltonian H. (H could be Frolich's Hamiltonian.) The system is initially in thermal equilibrium at temperature β^{-1}. At time $t=0$ a steady force $\mathbf{F}$ is applied to the electron. The Hamiltonian becomes $\overline{H} = H - \mathbf{F}\cdot\mathbf{r}$ ($\mathbf{r}$ is the electron position). No assumption is made that the force $\mathbf{F}$ is weak. We wish to compute $\langle \mathbf{r}(t) \rangle$. This function tells us how the electron responds to the force. In particular, it can tell us whether a steady state is reached in which the energy pumped into the electron by $\mathbf{F}$ is balanced by the energy lost by the electron due to interactions with phonons, etc.. We can also discover such things as the rate of energy dissipation at a given velocity, etc..

If the system is initially in state $|\Psi_i\rangle$ with probability p_i we have

$$\langle \mathbf{r}(t) \rangle = \sum_i p_i \langle \Psi_i | e^{i\overline{H}t} \mathbf{r} e^{-i\overline{H}t} | \Psi_i \rangle \qquad (5.2.1)$$

[*] The variational equations coming from the minimization of (5.1.4) provide the implicit relations between $S_0, \bar{\gamma}$, and the electron path.

This problem has been discussed by Thornber & Feynman [8].

For a thermal density matrix we have

$$\langle \mathbf{r}(t) \rangle = \frac{Tr\left[e^{-\beta H} e^{iHt}\, \mathbf{r}\, e^{-iHt}\right]}{Tr\, e^{-\beta H}} \tag{5.2.2}$$

(5.2.1) is the analytic continuation of

$$\sum_i p_i \langle \bar{\Psi}_i | e^{-\tau_2 \bar{H}}\, \mathbf{r}\, e^{-\tau_1 \bar{H}} | \bar{\Psi}_i \rangle \tag{5.2.3}$$

to $\tau_2 = -it$ and $\tau_1 = it$ while (5.2.2) is the analytic continuation of

$$\frac{Tr\left[e^{-\beta H} e^{-\tau_2 \bar{H}}\, \mathbf{r}\, e^{-\tau_1 \bar{H}}\right]}{Tr\, e^{-\beta H}} \tag{5.2.4}$$

again to $\tau_2 = -it$ and $\tau_1 = it$. In terms of path integrals (5.2.3) may be written as

$$\int Dq_{fi} \rho(q_f, q_i) e^{-\int_0^{\tau_1+\tau_2} L d\tau}\, \mathbf{r}(\tau_1) \tag{5.2.5}$$

Here the q are all the coordinates of the system including the electron coordinates. L is the classical energy associated with $\bar{H}$. $\rho(q_f, q_i) = \sum_i \langle q_f | \bar{\Psi}_i \rangle p_i \langle \bar{\Psi}_i | q_i \rangle$ and the path integral is over the path beginning at q_i and ending at q_f.

We can compute the path integral in (5.2.5) from path integrals of the form

$$\int Dq_{fi} \rho(q_f, q_i) e^{-\int_0^{\tau_1+\tau_2} L + \int_0^{\tau_1+\tau_2} \bar{\gamma}\cdot\mathbf{r}} \tag{5.2.6}$$

Here L is the imaginary time Lagrangian of the system with Hamiltonian H. To use (5.2.5) or (5.2.6) we need an expression for the density matrix $\rho(q_f, q_i)$. In

order to use a variational principle for the approximate calculation of (5.2.6) it is necessary that $\rho(q_f, q_i) \geq 0$.

The numerator of (5.2.4) requires the evaluation of the path integral

$$\int D_q e^{-\int_0^{\beta+\tau_1+\tau_2} L dt + \int_0^{\tau_1+\tau_2} \mathbf{F}\cdot\mathbf{r} + \int_0^{\beta+\tau_1+\tau_2} \gamma\cdot\mathbf{r}} \tag{5.2.7}$$

over all closed paths $q(0) = q(\beta+\tau_1+\tau_2)$. L has the same meaning in (5.2.7) as in (5.2.6). In the case that L is the imaginary time Lagrangian of the Frolich model, we integrate the phonon variables in (5.2.7) and find an effective action for the electron alone. The integral over the electron paths is now approximated using a trial action and the variational principle. The results must then be continued back to real times. The continuation process given in section 2.3 will not work in the present case because the action in (5.2.7) has explicit time dependence due to the term $\int_0^{\tau_1+\tau_2} \mathbf{F}\cdot\mathbf{r}$ even when $\gamma = 0$. The best trial action will also have explicit time dependence.

To see how to carry out the analytic continuation, we shall return to the problem of the weak response of an electron to a time varying field which we formulated in chapters 2 and 3. Although the effective action and the best trial action no longer have explicit time dependence in that case, the method of continuation in time will apply also to the path integral in (5.2.7).

The condition for the trial action given in (3.1.15) to be the best one with which to imitate the action (3.1.6) (with $D = 0$) was found to be from (3.2.7)

$$f_0(\tau) = -\frac{\alpha}{3\sqrt{2\pi}}\left[\frac{g_1(\tau)}{D_0^{\frac{3}{2}}(\tau)} + \delta(\tau)\int_0^{\beta}\frac{G_1(\tau)}{D_0^{\frac{3}{2}}(\tau)}d\tau\right] \tag{5.2.8}$$

with $D_0(\tau) = g_0(0) - g_0(\tau)$. In addition $g_0(\tau)$ and $f_0(\tau)$ are related by (3.1.14)

$$-\frac{d^2}{d\tau^2}g_0(|\tau-\sigma|)+\int_0^\beta f_0(|\tau-\tau'|)g_0(|\tau'-\sigma|)d\tau'=\delta(\tau-\sigma) \qquad (5.2.9)$$

To compute the real time response function $R_0(t)$ we need $g_0(it)$ since $R_0(t)=g_0(it)-g_0^*(it)$. (5.2.8) and (5.2.9) enable us to solve for $g_0(\tau)$ for τ real and in the interval $0\leq\tau\leq\beta$. In principle this is enough information to obtain the analytic continuation of $g_0(\tau)$ to all complex τ. However, it is difficult to see how to do this directly by means of (5.2.8) and (5.2.9). It is not clear how to treat the absolute values and especially the delta function $\delta(\tau-\sigma)$ as τ , σ, and τ' become complex.

To see what to do recall from equation (2.2.1) that we expressed the response function $R(t)$ in terms of

$$\sum_i p_i<\Psi_i|e^{iHt_1}xe^{-iHt_1}x|\Psi_i> \qquad (5.2.10)$$

or in terms of

$$Tr\left[e^{-\beta H}e^{iHt_1}xe^{-iHt_1}x\right] \qquad (5.2.11)$$

In chapter 2 we continued this to

$$Tr\left[e^{-\beta H}e^{\tau H}xe^{-\tau H}x\right] \qquad (5.2.12)$$

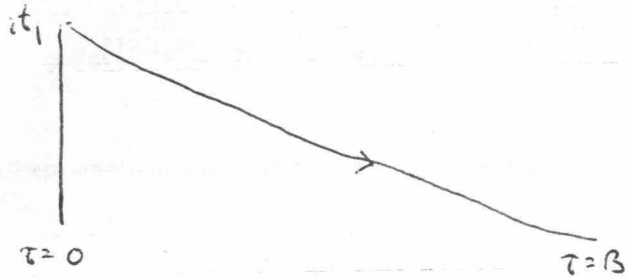
and expressed it as a single path integral. However (5.2.11) is also expressable as a single path integral if we merely allow the time variable to follow some contour in the complex t-plane (or τ plane). Thus (5.2.11) is

$$\int Dxe^{i\int_C Ldt}x(t_1)x(0) \qquad (5.2.13)$$

Here the contour C in the t-plane starts at $t = 0$, moves along the positive real axis to $t = t_1$, and then finally follows some contour to $t = -i\beta$.

L in (5.2.13) is the continuation of the real time Langrangian to times which lie along C. We must also impose on C the condition that Imt is decreasing as we traverse C from its beginning at $t = 0$ to its end at $t = -i\beta$ since otherwise the path integrals in (5.2.13) diverge.

It is convenient for us to work in the complex τ -plane where $\tau = it$. The contour C above is now $\bar{C}$



and the path integral (5.2.13) is now

$$\int Dx e^{-\int_C L d\tau} x(\tau_1)x(0) \qquad \tau_1 = it_1 \tag{5.2.14}$$

where L is the continuation of the imaginary time Lagrangian (which is the classical energy) of the system to τ along $\bar{C}$.

Order the contour $\bar{C}$ with 0 considered the least point and β the greatest point. If τ and σ are two points on this contour, write $\tau<\sigma$ if τ is encountered first as the contour is traversed from 0 to β, otherwise write $\tau\geq\sigma$. $|\tau-\sigma|_{\bar{C}}$ denotes $\tau-\sigma$ if $\tau\geq\sigma$ and $\sigma-\tau$ if $\tau<\sigma$.

Consider now the Gaussian action

$$S_0 = \int_C \dot{x}^2 d\tau + \frac{1}{2}\int_C\int_C f_0(|\tau-\sigma|_C)x(\tau)x(\sigma)d\tau d\sigma \tag{5.2.15}$$

$$= \int_C x(\tau)x(\sigma)g_0^{-1}(|\tau-\sigma|_{\bar{C}})$$

We wish to evaluate

$$<e^{\int_C \gamma(\tau)x(\tau)d\tau}>_0 = \frac{\int Dx e^{-S_0+\int_C \gamma(\tau)x(\tau)}}{\int Dx e^{-S_0}} \qquad (5.2.16)$$

By analogy to a discrete Gaussian integral such as (3.1.9) we need to find $g_0(|\tau-\sigma|_C)$ inverse to $g_0^{-1}(|\tau-\sigma|_C)$ in the sense that

$$\int_C g_0(|\tau-\sigma'|_C) g_0^{-1}(|\sigma'-\sigma|_C) d\sigma' = \delta_C(\tau-\sigma) \qquad (5.2.17)$$

Here $\delta_C(\tau-\sigma)$ is a representation of the identity. It satisfies

$$a(\tau) = \int_C \delta_C(\tau-\sigma) a(\sigma) d\sigma \qquad (5.2.18)$$

for τ and σ on C and $a(\tau)$ a test function on C. (5.2.17) may also be written as

$$-\frac{d^2}{d\tau^2} g_0(|\tau-\sigma|_C) + \int_C f_0(|\tau-\sigma'|_C) g_0(|\sigma'-\sigma|_C) = \delta_C(\tau-\sigma) \qquad (5.2.19)$$

And this is the generalization of (5.2.9) which we need. Let's check that we get its correct results. Define C to the contour shown below Let τ and σ be on the left piece of the contour and let $\tau = it$, $\sigma = is$. $\sigma' = is'$ on left piece of contour while $\sigma' = is'+\beta$ on right piece of contour. By using (5.2.19) and its complex conjugate and the relations $g_0(\beta-\tau) = g_0(\tau)$, $f_0(\beta-\tau) = f_0(\tau)$, $g_0^*(\tau) = g_0(\tau^*)$, $f_0^*(\tau) = f_0(\tau^*)$ which are true for complex τ, we arrive at an equation

$$\frac{d^2}{dt^2} R_0(|t-s|) - 2\int_s^t \mathrm{Im} f_0(it-is') R_0(|s'-s|) ds' = -2i\delta(t-s) \qquad (5.2.20)$$

Here R_0 is the response function given by $R_0(t) = g_0(it) - g_0^*(it)$ for $t>0$ and $R_0(t) = 0$ for $t<0$. (5.2.20) implies that

$$\frac{d^2}{dt^2} R_0(t) - 2\int_{-\infty}^t \mathrm{Im} f_0(it-is) R_0(s) ds = -i\delta(t) \qquad (5.2.21)$$

Substituting $R_0(t) = \int_{-\infty}^{+\infty} e^{-i\lambda t} \frac{d\lambda}{2\pi} \hat{R}_0(\lambda)$ into (5.2.21) we find that

$$\hat{R}_0(\lambda) = \frac{i}{\lambda^2 + 2\int_0^\infty [Im f_0(is)] e^{i\lambda s} ds} \tag{5.2.22}$$

so that from (2.1.11), the absorption function is

$$s_0(\lambda) = \mathrm{Re}\, 2\lambda \hat{R}_0(\lambda) = \mathrm{Im} \frac{2\lambda}{-\lambda^2 - 2\int_0^\infty [Im f_0(is)] e^{i\lambda s} ds} \tag{5.2.23}$$

comparing to (2.3.18) we see that

$$\hat{f}_0(-i\lambda) = -2\int_0^\infty e^{i\lambda s} \mathrm{Im} f_0(is) ds \tag{5.2.24}$$

which is just (2.3.17). Thus we have recovered the results of chapter 2 on analytical continuation by means of a different approach. The utility of this approach is that it allows the application of the variational method to problems such as the electron in a constant arbitrary strength electric field discussed earlier in this section. The method of analytic continuation in section 2.3 cannot be used for this problem. Also, the idea of working with the analytically continued path integrals such as given in (5.2.7) in order to evaluate expressions such as (5.2.2) seems to have the advantage that the computational labor involved working with the analytically continued path integrals is less than the labor involved on working with a direct path integral representation of the original problem.

5.3. More Realistic Model

In this section we present the variational and second order equations for a generalized version of Frolich's model.

We retain the assumption of a harmonic lattice. However we do not make the continuum approximation nor do we make any assumptions about the phonon dispersion relations or about the types of phonons coupled to the electron. We do assume that the electron-phonon coupling is linear in the phonon variables.

For the electron we initially assume that the energy is of the form

$$\frac{1}{2}\sum_{i,j} m_{i,j}\dot{x}_i\dot{x}_j + V(\mathbf{r}) \tag{5.3.1}$$

Here $\mathbf{r}$ is the positron vector of the electron and the x_i are the components of $\mathbf{r}$. $V(\mathbf{r})$ may be a periodic potential or it may include contributions due to impurities, etc. By a combination of an orthogonal transformation and a rescaling of coordinates one may always bring (5.3.1) into the form

$$L_{elec} = \frac{1}{2}\sum_{i}(\dot{x}'_i)^2 + V'(\mathbf{r}') \tag{5.3.2}$$

Here $\mathbf{r}'$, x'_i are the new coordinates. In the following we shall drop the primes on the new coordinates and take (5.3.2) as our starting point for the electron portion of the energy.

We work with a very large crystal with N unit cells and use periodic boundary conditions. $\mathbf{N}$ will denote the position of a unit cell and $\sqrt{M_\alpha}X_{\mathbf{N}\alpha}$ will be the displacement from equilibrium of the α^{th} atomic coordinate in the unit cell at $\mathbf{N}$. M_α is the mass associated with the α^{th} coordinate. In terms of the $X_{\mathbf{N}\alpha}$, the lattice energy is (retaining only quadratic terms in the potential)

$$L_{latt} = \frac{1}{2}\sum_{\mathbf{N}\alpha}\dot{X}^2_{\mathbf{N}\alpha} + \frac{1}{2}\sum_{\mathbf{N}_1\alpha_1\mathbf{N}_2\alpha_2} X_{\mathbf{N}_1\alpha_1}X_{\mathbf{N}_2\alpha_2}J_{\alpha_1\alpha_2}(\mathbf{N}_1-\mathbf{N}_2) \tag{5.3.3}$$

We define $\hat{J}_{\alpha_1\alpha_2}(\mathbf{k})$ by

$$J_{\alpha_1\alpha_2}(\mathbf{N}) = \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{N}}\hat{J}_{\alpha_1\alpha_2}(\mathbf{k}) \tag{5.3.4}$$

The $\mathbf{k}$ sums will always be over a unit cell in $\mathbf{k}$ space. Because $J_{\alpha\beta}(\mathbf{N})$ is real and $J_{\beta\alpha}(\mathbf{N}) = J_{\alpha\beta}(-\mathbf{N})$, $\hat{J}_{\alpha\beta}(\mathbf{k})$ has the properties

$$\hat{J}_{\alpha\beta}(\mathbf{k}) = \hat{J}^*_{\alpha\beta}(-\mathbf{k}) \tag{5.3.5}$$

$$\hat{J}_{\alpha\beta}(\mathbf{k}) = \hat{J}^*_{\beta\alpha}(\mathbf{k})$$

Note that $\hat{J}_{\alpha\beta}(\mathbf{k})$ is a Hermitian matrix. For each $\mathbf{k}$ we have $\varepsilon^{\lambda}_{\alpha}(\mathbf{k})$ and $\omega_{\lambda}(\mathbf{k})$ such that

$$\sum_{\beta}\hat{J}_{\alpha\beta}(\mathbf{k})\varepsilon^{\lambda}_{\beta}(\mathbf{k}) = \omega^2_{\lambda}(\mathbf{k})\varepsilon^{\lambda}_{\alpha}(\mathbf{k}) \tag{5.3.6}$$

We now define new variables $q_{\mathbf{k}\lambda}$ by

$$X_{\mathbf{N}\alpha} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}\lambda} q_{\mathbf{k}\lambda}\varepsilon^{\lambda}_{\alpha}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{N}} \tag{5.3.7}$$

Note that $q_{\mathbf{k}\lambda} = q_{-\mathbf{k}\lambda}$. $\omega_{\lambda}(\mathbf{k})$ is the frequency of a phonon of type λ as a function of its wave vector $\mathbf{k}$ and $\varepsilon^{\lambda}_{\alpha}(\mathbf{k})$ is a phonon "polarization". In terms of the q's the lattice energy is

$$L_{latt} = \frac{1}{2}\sum_{\mathbf{k}\lambda}\left(\dot{q}_{\mathbf{k}\lambda}\dot{q}_{-\mathbf{k}\lambda} + \omega^2_{\lambda}(\mathbf{k})q_{\mathbf{k}\lambda}q_{-\mathbf{k}\lambda}\right) \tag{5.3.8}$$

The most general electron-lattice interaction which does not involve time derivatives and is linear in the $X_{\mathbf{N}\alpha}$ and is invariant under simultaneous displacement of the electron and the displacements field $X_{\mathbf{N}\alpha}$ by a lattice vector $\mathbf{M}$ is

$$L_{int} = \sum_{N\alpha} U_\alpha(\mathbf{r}-\mathbf{N}) X_{N\alpha} \tag{5.3.9}$$

The reciprocal lattice vectors **G** satisfy

$$e^{i\mathbf{G}\cdot\mathbf{N}} = 1 \tag{5.3.10}$$

for all lattice vectors **N**. Once we chose a unit cell in **k** -space any vector **q** can be uniquely decomposed into the sum of a reciprocal lattice vector **G** and a vector **k** within the unit cell. Any periodic function ($f(\mathbf{r}) = f(\mathbf{r}+\mathbf{N})$ for all **N**) can be written as $f(\mathbf{r}) = \sum_{\mathbf{G}} \hat{f}_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$. Now define

$$\hat{B}_{k\lambda}(\mathbf{G}) = \sum_\alpha (\varepsilon_\alpha^\lambda(\mathbf{k}))^* \int d^3\mathbf{r} e^{-i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} U_\alpha(\mathbf{r}) \tag{5.3.11}$$

Note that $\hat{B}^*_{k\lambda}(\mathbf{G}) = \hat{B}_{-k\lambda}(-\mathbf{G})$. The interaction energy can now be rewritten as

$$L_{int} = \frac{1}{\sqrt{N}} \sum_{k\lambda} q_{-k\lambda} B_{k\lambda}(\mathbf{G}) e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} \tag{5.3.12}$$

Now we have established our notation and formulated a total energy $L = L_{elec} + L_{latt} + L_{int}$ for the system. The next step is to integrate away the lattice variables and arrive at an effective imaginary time action S for the electron. That is,

$$e^{-S} = \int Dq e^{-\int_0^\beta (L_{elec} + L_{int} + L_{latt}) d\tau} \tag{5.3.13}$$

where the integration is over all closed q paths $q_{k\lambda}(0) = q_{k\lambda}(\beta)$.

With the aid of the path integral given in (1.2.25) we may carry out the integration in (5.3.13) and find

$$S = \frac{1}{2}\int_0^\beta [\dot{\mathbf{r}}^2 + V(\mathbf{r})]d\tau \qquad (5.3.14)$$

$$-\frac{1}{2}\int_0^\beta\int_0^\beta d\tau_1 d\tau_2 \frac{1}{N}\sum_{\mathbf{k}\lambda}\sum_{\mathbf{G}_1\mathbf{G}_2} e^{i[(\mathbf{G}_1+\mathbf{k})\cdot\mathbf{r}(\tau_1)-(\mathbf{G}_2+\mathbf{k})\cdot\mathbf{r}(\tau_2)]} G_{\mathbf{k}\lambda}(|\tau_1-\tau_2|)\cdot B_{\mathbf{k}\lambda}(\mathbf{G}_1)B_{\mathbf{k}\lambda}(\mathbf{G}_2)$$

where

$$G_{\mathbf{k}\lambda}(\tau) = \frac{1}{2\omega_\lambda(\mathbf{k})}\left[\frac{e^{-\tau\omega_\lambda(\mathbf{k})}}{1-e^{-\beta\omega_\lambda(\mathbf{k})}} + \frac{e^{\tau\omega_\lambda(\mathbf{k})}}{e^{\beta\omega_\lambda(\mathbf{k})}-1}\right] \qquad (5.3.15)$$

The second term in (5.3.14) can also be written as

$$-\frac{1}{2}\int_0^\beta\int_0^\beta W(\mathbf{r}(\tau_1),\mathbf{r}(\tau))d\tau_1 d\tau_2 \qquad (5.3.16)$$

If a lattice vector **N** is added both arguments of $W(\mathbf{a},\mathbf{b})$ then its value remains unchanged

$$W(\mathbf{a},\mathbf{b}) = W(\mathbf{a}+\mathbf{N},\mathbf{b}+\mathbf{N}) \qquad (5.3.17)$$

This is not true if we add on an arbitrary vector **R** to **a**+**b**. This is due to the $\mathbf{G}_1\neq 0$ and $\mathbf{G}_2\neq 0$ terms in (5.3.14). The presence of these terms and the periodic potential $V(\mathbf{r})$ makes it difficult to formulate a good trial action for the problem. We have formulated some possible trial actions, but have not derived the variational equations or done any other calculations with these. For this reason we only consider those cases in which it is reasonable to take $V(\mathbf{r}) = 0$ and to drop the $\mathbf{G}_1,\mathbf{G}_2\neq 0$ terms in the second term of (5.3.14). Thus the action we consider is

$$S = \frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 - \frac{1}{2}\int_0^\beta\int_0^\beta d\tau d\sigma \frac{1}{N}\sum_{\mathbf{k}\lambda} e^{i\mathbf{k}\cdot(\mathbf{r}(\tau)-\mathbf{r}(\sigma))}|B_{\mathbf{k}\lambda}|^2 G_{\mathbf{k}\lambda}(|\tau-\sigma|) \qquad (5.3.18)$$

For a trial action we now take

$$S_0 = \frac{1}{2}\int_0^\beta \dot{r}^2 + \frac{1}{2}\int_0^\beta\int_0^\beta d\tau d\sigma \sum_{i,j} f_{0,ij}(|\tau-\sigma|)x_i(\tau)x_j(\sigma) \qquad (5.3.19)$$

As in equation (3.1.18), it is convenient to rewrite S as

$$S = \frac{1}{2}\int_0^\beta\int_0^\beta \sum_{i,j} f_{0,ij}(|\tau-\sigma|)x_i(\tau)x_j(\sigma) + \qquad (5.3.20)$$

$$\frac{1}{2}\int_0^\beta \dot{r}^2 d\tau + \frac{1}{2}\int_0^\beta\int_0^\beta \sum_{i,j} h_{ij}(|\tau-\sigma|)x_i(\tau)x_j(\sigma)$$

$$-\frac{1}{2}\int_0^\beta\int_0^\beta d\tau d\sigma \frac{1}{N}\sum_{k\lambda} |B_{k\lambda}|^2 G_{k\lambda}(|\tau-\sigma|)e^{ik\cdot(r(\tau)-r(\sigma))}$$

Here we eventually set $h_{ij} = -f_{0,ij}$. For the purpose of computing the series expansion of $g_{ij}(|\tau-\sigma|) = \langle x_i(\tau)x_j(\sigma)\rangle$, the h_{ij} are initially allowed to be arbitrary functions as h was in chapter 3.

For the trial action S_0, note that if we define $g_{0,ij}(\tau)$ by

$$-\frac{d^2}{d\tau^2} g_{0,ij}(|\tau-\sigma|) + \int_0^\beta \sum_k f_{0,ik}(|\tau-\sigma'|)g_{0,kj}(|\sigma'-\sigma|)d\sigma' = \delta_{ij}\delta(\tau-\sigma) \qquad (5.3.21)$$

then

$$g_{0,ij}(|\tau-\sigma|) = \langle x_i(\tau)x_j(\sigma)\rangle_0 \qquad (5.3.22)$$

where $\langle\rangle_0$ denotes an average taken with e^{-S_0} as a weight. (As in (3.1.1).)

$S_1 = S-S_0 \equiv A+B$ is now given by

$$A = \frac{1}{2}\int_0^\beta\int_0^\beta h_{ij}(|\tau-\sigma|)x_i(\tau)x_j(\sigma)d\tau d\sigma \qquad (5.3.23)$$

$$B = -\frac{1}{2}\int_0^\beta\int_0^\beta d\tau d\sigma \frac{1}{N}\sum e^{ik\cdot(r(\tau)-r(\sigma))}|B_{k\lambda}|^2 G_{k\lambda}(\tau-\sigma)$$

To evaluate $\langle S_1\rangle_0$ and $\langle S_1^2\rangle_0 - \langle S_1\rangle_0^2$ we need the results

$$\langle e^{i\mathbf{k}(\mathbf{r}(\tau)-\mathbf{r}(\sigma))}\rangle_0 = e^{-\sum_{i,j} k_i k_j D_{0,ij}(|\tau-\sigma|)} \tag{5.3.24}$$

where $D_{0,ij}(|\tau-\sigma|) = g_{0,ij}(|\tau-\sigma|)$ and

$$\langle e^{i\mathbf{k}_1\cdot(\mathbf{r}(\tau_1)-\mathbf{r}(\sigma_{\cdots 1}))} e^{i\mathbf{k}_2\cdot(\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2))}\rangle_0 = e^{-\sum_{i,j}^{2}\sum_{\alpha,\beta} k_{\alpha i} k_{\beta j}(A_{\alpha\beta})_{ij}(\tau_\alpha\sigma_\alpha|\tau_\beta\sigma_\beta)} \tag{5.3.25}$$

where now

$$(A_{\alpha\beta})_{ij}(\tau_\alpha\sigma_\alpha|\tau_\beta\sigma_\beta) = \tag{5.3.26}$$

$$\frac{1}{2}\Big[D_{0,ij}(|\tau_\alpha-\sigma_\beta|) + D_{0,ij}(|\tau_\beta-\sigma_\alpha|) - D_{0,ij}(|\sigma_\alpha-\sigma_\beta|) - D_{0,ij}(|\tau_\alpha-\tau_\beta|)\Big]$$

Note that, in particular

$$(A_{\alpha\alpha})_{ij}(\tau_\alpha\sigma_\alpha|\tau_\alpha\sigma_\alpha) = D_{0,ij}(|\tau_\alpha-\sigma_\alpha|) \tag{5.3.27}$$

If F_0 is the free energy associated with S_0 and F is the free energy associated with S, then to first order in S_1 we have

$$\beta F = \beta F_0 + \frac{1}{2}\int_0^\beta\int_0^\beta \sum_{i,j} h_{ij}(|\tau-\sigma|) g_{0,ij}(|\tau-\sigma|) d\tau d\sigma \tag{5.3.28}$$

$$-\frac{1}{2}\int_0^\beta\int_0^\beta d\tau d\sigma \frac{1}{N}\sum_{\mathbf{k}\lambda} |B_{\mathbf{k}\lambda}|^2 G_{\mathbf{k}\lambda}(|\tau-\sigma|) e^{-\sum_{i,j} k_i h_j D_{0,ij}(|\tau-\sigma|)}$$

If we set $h_{ij} = -f_{0,ij}$ and then set the first order variation in the right hand side of (5.3.28) to zero for an arbitrary variation in $f_{0,ij}$, we find the condition

$$f_{0,ij}(\tau) = -k_{0,ij}(\tau) + \delta(\tau)\int_0^\beta k_{0,ij}(\sigma) d\sigma \tag{5.3.29a}$$

where

$$k_{0,ij}(\tau) = \frac{1}{N}\sum_{\mathbf{k}\lambda} |B_{\mathbf{k}\lambda}|^2 k_i k_j G_{\mathbf{k}\lambda}(\tau) e^{-\frac{1}{2}\sum_{i,j} k_i k_j D_{0,ij}(\tau)} \qquad (5.3.29b)$$

for the free energy to be a minimum.

If the states of the whole system (before we integrate away the phonon variables) can be taken as real (which is true for the Hamiltonian associated with $L_{elect}+L_{int}+L_{latt}$), then we find that $R_{ij}(t)$, the response of the coordinate x_i to a kick in the j direction at zero time, satisfies

$$R_{ij}(t) = R_{ji}(t) \qquad (5.3.30)$$

$R_{ij}(t)$ is given by

$$R_{ij}(t) = \langle x_i(t)x_j(0)\rangle - \langle x_i(t)x_j(0)\rangle^* \qquad (5.3.31)$$

$$= g_{ij}(t) - g_{ij}^*(t)$$

The same comments apply to $R_{0,ij}(t)$, the response function associated with the trial function S_0.

$$R_{0,ij}(t) = g_{0,ij}(t) - g_{0,ij}^*(t) \qquad (5.3.32)$$

$$R_{0,ij}(t) = R_{0,ji}(t)$$

If we apply a weak external force $\gamma_0 \mathbf{n}\cos\omega t$ to the electron ($\mathbf{n}$ is a unit vector), so that there is is an extra term $-\gamma_0 \mathbf{n}\cdot\mathbf{r}\cos\omega t$ in the Hamiltonian, we find by an application of time dependent perturbation theory that the rate of energy absorption is proportional to (at frequency λ)

$$\sum_{i,j} n_i n_j s_{ij}(\lambda) \qquad (5.3.33)$$

where

$$s_{ij}(\lambda) = 2\lambda \mathrm{Re}\hat{R}_{ij}(\lambda) \tag{5.3.34}$$

If

$$\hat{f}_{0,ij}(\lambda_\alpha) = \frac{1}{\beta}\int_0^\beta e^{i\lambda_\alpha \tau} f_{0,ij}(\tau)d\tau \qquad \lambda_\alpha = \frac{2\pi\alpha}{\beta},\ \alpha\ an\ integer \tag{5.3.35}$$

then the analytic continuation of $\hat{f}_{0,ij}(\lambda_\alpha)$ to general values of λ may be obtained by methods discussed in section 2.3 or in the previous section 5.2. We now write down the cycle of equations for the solution of the variational problem. Starting with $s_{0,ij}(\omega)$ as in equation (3.2.11), we have

$$D_{0,ij}(it) = \int_0^\infty \frac{d\omega}{\pi} s_{0,ij}(\omega)\frac{1}{2\omega}\left[\frac{1-e^{-i\omega t}}{1-e^{-\beta\omega}} + \frac{1-e^{i\omega t}}{e^{\beta\omega}-1}\right] \tag{5.3.36}$$

From this we construct $k_{0,ij}(it)$ by means of (5.3.29b). Then

$$\hat{f}_{0,ij}(-i\lambda) = 2\int_0^\infty (e^{i\lambda s}-1)\mathrm{Im}k_{0,ij}(is) \tag{5.3.37}$$

Finally, we recover $s_{0,ij}(\omega)$ from

$$s_{0,ij}(\omega) = \mathrm{Im}\,2\omega\left[\hat{f}_0(-i\omega)-\omega^2\right]^{-1}_{ij} \tag{5.3.38}$$

the inverse referring to the matrix inverse of $\hat{f}_0(-i\omega)-\omega^2$.

Now we turn to the second order corrections to the variational results. As in chapter 3, the first order corrections vanish.

First we extend the notation discussed on page 34 of the third chapter. Let g_0, h, f_0, etc. stand for the matrices $g_{0,ij}$, h_{ij}, $f_{0,ij}$, etc.. Extend the meaning of the product notation ab so that

$$(ab)_{\tau\rho,ik} = \sum_j \int_\sigma a_{ij}(|\tau-\sigma|)b_{jk}(|\sigma-\rho|) \tag{5.3.39}$$

Using the expansion (3.1.17) with S_1 as given in (5.3.23) and applying (5.3.25) we find after some work that the free energy to second order is given by the first order free energy in (5.3.28) plus

$$-\frac{1}{4}\sum_i\int_\tau (g_0hg_0h)_{\tau\tau,ii}+\frac{1}{2}\sum_i(g_0hg_0k_0)_{\tau\tau,ii}-\int_{\tau_1\sigma_1\tau_2\sigma_2}P(\tau_1\sigma_1|\tau_2\sigma_2) \quad (5.3.40a)$$

where

$$(A_{11})_{ij}=D_{0,ij}(|\tau_1-\sigma_1|) \quad (5.3.40b)$$

$$(A_{22})_{ij}=D_{0,ij}(|\tau_2-\sigma_2|)$$

$$(A_{12})_{ij}=\frac{1}{2}\Big[D_{0,ij}(|\tau_1-\sigma_2|)+D_{0,ij}(|\tau_2-\sigma_1|)-D_{0,ij}(|\tau_1-\tau_2|)-D_{0,ij}(|\sigma_1-\sigma_2|)\Big]$$

and where P is given by

$$P(\tau_1\sigma_1|\tau_2\sigma_2)= \quad (5.3.40c)$$

$$\frac{1}{8}\frac{1}{N}\sum_{\mathbf{k}_1\lambda_1}\frac{1}{N}\sum_{\mathbf{k}_2\lambda_2}|B_{\mathbf{k}_1\lambda_1}|^2|B_{\mathbf{k}_2\lambda_2}|^2G_{\mathbf{k}_1\lambda_1}(|\tau_1-\sigma_1|)G_{\mathbf{k}_2\lambda_2}(|\tau_2-\sigma_2|)$$

$$\times e^{-\sum_\alpha k_{\alpha i}k_{\alpha j}(A_{\alpha\alpha})_{ij}}\Big[e^{-(A_{12})_{ij}(k_{1i}k_{2j}+k_{1j}k_{2i})}-1\Big]$$

Now f_0 is varied while keeping h constant. We use the relation

$$\delta g_0=-g_0\delta f_0 g_0 \quad (5.3.41)$$

and for a term T which depends on D_0's we use the analogue of (3.3.14)

$$\delta T=\int_{\tau\sigma}\sum_{ij}\frac{\delta T}{\delta(D_0)_{\tau\sigma,ij}}(g_0\delta f_0 g_0)_{\tau\sigma,ij}-\int_{\tau\sigma,ij}\frac{\delta T}{\delta(D_0)_{\tau\sigma,ij}}(g_0\delta f_0 g_0)_{\tau\tau,ij} \quad (5.3.42)$$

The contribution to the f series from such a term comes out to be (specifically the contribution to $(f)_{\tau\sigma,ij}$)

$$-2\left[\frac{\delta T}{\delta(D_0)_{\tau\sigma,ij}} - \delta(\tau-\sigma)\int_\rho \frac{\delta T}{\delta(D_0)_{\tau\rho,ij}}\right] \tag{5.3.43}$$

After the second order contribution to the f series is worked out, we specialize to the case that (see (3.3.16))

$$f_1 \equiv -f_0 - \kappa_0 + [\kappa_0] = 0 \tag{5.3.44}$$

where κ_0 is given now by (5.3.29b). This is just the statement that f_0 is the variational f_0.

Taking into account the vanishing of terms due to (5.3.44) and other cancellations discussed in chapter 3, we may now write down the second order contribution to the f series in the case that f_0 is given by the variational equations (5.3.29) and (5.3.36) to (5.3.38).

$$(f_2)_{\tau\sigma,ij} = -(\kappa_2)_{\tau\sigma,ij} + \delta(\tau-\sigma)\int_\rho (\kappa_2)_{\tau\rho,ij} \tag{5.3.45a}$$

and κ_2 is given by two terms. First we have

$$-\frac{1}{2}\int_{\tau\sigma'} \frac{1}{N}\sum_{\mathbf{k}_1\lambda_1} \frac{1}{N}\sum_{\mathbf{k}_2\lambda_2} |B_{\mathbf{k}_1\lambda_1}|^2 |B_{\mathbf{k}_2\lambda_2}|^2 G_{\mathbf{k}_1\lambda_1}(|\tau-\sigma|) G_{\mathbf{k}_2\lambda_2}(|\tau'-\sigma'|) \tag{5.3.45b}$$

$$\times\ e^{-\sum_{\alpha ij} k_{\alpha i} k_{\alpha j} (A_{\alpha\alpha})_{ij}} k_{1i} k_{1j} \left\{ e^{-\sum_{lk} (A_{12})_{lk} (k_{1l} k_{2k} + k_{1l} k_{2k})} - \frac{1}{2}\left[\sum_{lk} (A_{12})_{lk} (k_{1l} k_{2k} + k_{1k} k_{2l})\right]^2 - 1 \right\}$$

where

$$(A_{11})_{ij} = D_{0,ij}(|\tau-\sigma|) \tag{5.3.45c}$$

$$(A_{22})_{ij} = D_{0,ij}(|\tau'-\sigma'|)$$

$$(A_{12})_{ij} = \frac{1}{2}\left[D_{0,ij}(|\tau-\sigma'|) + D_{0,ij}(|\tau'-\sigma|) - D_{0,ij}(|\tau-\tau'|) - D_{0,ij}(|\sigma-\sigma'|)\right]$$

The second term is given by

$$-\frac{1}{2}\int_{\tau'\sigma'}\frac{1}{N}\sum_{\mathbf{k}_1\lambda_1}\frac{1}{N}\sum_{\mathbf{k}_2\lambda_2}|B_{\mathbf{k}_1\lambda_1}|^2|B_{\mathbf{k}_2\lambda_2}|^2 G_{\mathbf{k}_1\lambda_1}(|\tau-\sigma'|)G_{\mathbf{k}_2\lambda_2}(|\tau'-\sigma'|) \quad (5.3.45d)$$

$$\times\ e^{-\sum_{\alpha ij}k_{\alpha i}k_{\alpha j}(A_{\alpha\alpha})_{ij}}(k_{1i}k_{2j}+k_{1j}+k_{2i})\left[e^{-(A_{12})_{ij}(k_{1i}k_{2j}+k_{1j}k_{2i})+\sum_{lk}(A_{12})_{lk}(k_{1l}k_{2k}+k_{1k}k_{2l})}\right]$$

where now

$$(A_{11})_{ij} = D_{0,ij}(|\tau-\sigma'|) \quad (5.3.45e)$$

$$(A_{22})_{ij} = D_{0,ij}(|\tau'-\sigma|)$$

$$(A_{12})_{ij} = \frac{1}{2}\left[D_{0,ij}(|\tau-\sigma|)+D_{0,ij}(|\tau'-\sigma'|)-D_{0,ij}(|\tau-\tau'|)-D_{0,ij}(|\sigma-\sigma'|)\right]$$

To evaluate $\kappa_2(it)$ we proceed as in chapter 4. The integrals from 0 to β are replaced by integrals along a contour C which runs from 0 to β through it. The absolute values $|\tau-\sigma|$ are replaced by $|\tau-\sigma|_C$ as defined in section 5.2 or in chapter 4.

6. CONCLUSION

In this thesis we have treated Frolich's polaron model by Feynman's path integral variational method and have calculated corrections to the variational approximation. Following Feynman, we first integrate away the lattice variables in a path integral for the free energy of the system and obtain an effective imaginary time action for the electron alone. This effective action is then imitated by general quadratic trial action. The path integral variational inequality gives an upper bound on the true free energy of the system as a functional of the trial action. Minimizing this upper bound yields a set of variational equations for the functions which appear in the trial action.

Rather than working with real time double path integrals as FHIP [4] do, we work with the imaginary time path integrals for the free energy and obtain results for real time functions by carrying out an analytical continuation. In chapter 2 this analytical continuation is carried out by working with the absorption function $s(\lambda)$. $s(\lambda)$ is proportional to the rate of energy absorption by the electron in a weak spatially uniform time varying field of frequency λ. Other functions of interest such as the response function of the electron $R(t)$ may be expressed in terms of this absorption function. The method of working with imaginary time path integrals rather than real time double path integrals saves a great deal of computational labor.

We obtain equations which may be solved numerically for the variational approximation $s_0(\lambda)$ to the absorption function. Some numerical results for $s_0(\lambda)$ are presented. We also compute corrections to $s_0(\lambda)$ which are second order in the difference between the trial action and the true action.

The same equations but different numerical results for $s_0(\lambda)$ have been obtained by Klyukanov, Muntyan, and Pokatilov [6] using a nonvariational method. Our numerical results disagree with theirs in that they obtain an

absorption function with two peaks at, for example, $\alpha = 4$ and temperatures as high as $\beta = 4$ (β^{-1} = temperature) while we only have a single peak for $\alpha = 4$ even at zero temperature.

We next compute the second order corrections to $s_0(\lambda)$ as a test of the accuracy of $s_0(\lambda)$. We only obtain results for moderate α (up to $\alpha = 5$). For these values of α the corrections are reasonable in comparison to the second order corrections of the free energy. This is discussed more fully at the end of chapter four. It would be of interest to see how large the corrections are for large values of α. From other examples to which we have applied the variational method, we expect that for large α, the corrections are of the same relative size as for moderate α.

There are many problems in which much greater accuracy is needed than the variational method seems capable of attaining. It would be very useful to find ways of systematically increasing the accuracy of the variational method. At present it is a one shot approximation, and if the accuracy is insufficient, there is not very much which can be done to improve it. *

In section 5.2 we present a generalization of the method of analytic continuation used in chapter 2. This generalization would allow us to use the path integral variational principle to choose the best trial action in the problem of a polaron in a space-time constant electric field (this field may be strong) discussed by Thornber and Feynman [8]. In their paper Thornber and Feynman lacked a principle by which to choose a quadratic action to imitate the true action. We have not yet applied the method of section 5.2 to this problem of a polaron in a strong constant electric field, nor have we investigated in what other problems this method may be of use. Also, the reasoning of section 5.2 is

* This is not true for systems of a finite number of degrees of freedom at nonzero temperature. In that case there exists a series of better and better variational inequalities.

very nonrigorous and it is necessary to investigate under what conditions the methods discussed there might fail.

In section 5.3 we present the variational equations and the second order corrections to them for a more realistic version of an electron in a crystal lattice. We retain the assumption that the lattice is harmonic. Within the frame work of this assumption the biggest flaw in the treatment of section 5.3 is that we cannot deal effectively with the periodicity of the crystal lattice. It would be useful to find a trial action which could in some way imitate the effect of periodic crystal potential $V(\mathbf{r})$ in which the electron moves.

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