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The Low-Lying States of a System of Polarons in the Landau-Pekar Adiabatic Approximation.

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ABSTRACT

An effective interaction potential for a pair of polarons is derived in a Landau-Pekar adiabatic approximation. The possibility of formation of bound states of two polarons is discussed. The low-lying energy states of a system of Landau-Pekar polarons interacting with the derived effective potential are investigated by employing approximation models including a body-centered cubic lattice of polarons, a Hartree-Fock gas of polarons, and a Hartree-Fock gas of polarons weakly coupled to a polaron plasma. The low-lying energy states based on these models are examined numerically for a specific test case intended to describe polarons in an ionic crystal with a polaron coupling constant large enough that the Landau-Pekar approximation may be expected to be appropriate. It is found that, for a wide range of polaron densities, the plasma-coupled gas model yields the best results among the models treated.
INTRODUCTION

The quantum mechanical description of a system of electrons in a polarizable medium is of considerable physical interest. It is the object of this paper to describe the low-lying energy states of such a system for selected values of the electron density and other parameters.

If an electron moves slowly through a polarizable medium, then the electron together with the accompanying polarization field which it induces may be described as a single quasi-particle called a polaron. The polaron is characterized by a self-energy and an effective mass, both of which may be calculated in various approximations.

In the first chapter the Frölich Hamiltonian for a single polaron is examined and the Landau-Pekar polaron theory is reviewed. The Frölich Hamiltonian is generalized to describe a pair of polarons and the Landau-Pekar approximation is used to derive an adiabatic approximation for a two-polaron interaction potential. A Hamiltonian is thereby obtained to describe a system of electrons in a polarizable medium as a system of polarons interacting via the two-body potential and in a uniform background of positive charge.

In succeeding chapters, three approximation models are studied to describe the low-lying states of the many-polaron system. In Chapter Two the system is treated as a body-centered cubic lattice.
in Chapter Three as a Hartree-Fock gas, and in Chapter Four as a
Hartree-Fock gas weakly coupled to a polaron plasma. In Chapters
Two through Five, analytical descriptions of the three models are
obtained but not carried to fruition with the extensive numerical
work required. In the final chapter a set of values of the
parameters involved is selected to characterize a test case chosen
to describe a system of conduction electrons strongly coupled to
the lattice modes of an ionic crystal. For this particular set
of values and for a range of values of electron density, a numerical
investigation is made as to which of the three models may be the
most suitable for describing the low-lying energy states of the
system.
1. The Frohlich Single-Polaron Hamiltonian

Consider a single electron moving in an isotropic, homogeneous, polarizable medium. The electric field which acts upon the particle may be regarded as being composed of two partial fields. One of these is an electric field which varies over microscopic distances and which cancels in a process of averaging over a macroscopic region. If the electron moves slowly enough through the medium, the electronic wavelength will be much greater than the distance between the microscopic entities comprising the medium and electron diffraction and reflection will not occur. It will be assumed that this is the case and that the effect of the microscopically varying electric field on the motion of the electron may be taken into account by attributing to the electron a mass, \( m_p \), which may differ from the mass the electron would have in free space. In a crystalline solid, for instance, the microscopically varying field is the periodic field due to the lattice constituents, regarded as static, and the effective mass is the Bloch mass. The component of the electric field which survives the averaging process may be described as the sum of the electric displacement, \( \mathbf{D}(\mathbf{r}) \), due to the free charges, and \( (-4\pi \mathbf{P}(\mathbf{r})) \), where \( \mathbf{P}(\mathbf{r}) \) is the macroscopic polarization field.
Since the electric displacement due to the electron is longitudinal, the electron can induce only a longitudinal polarization in the medium. It will be assumed that there is no transverse polarization present. It will also be assumed that the longitudinal polarization with which the electron significantly interacts may be divided into two parts, a low-frequency part which arises from modes of the medium all of which will be assumed to have a common angular frequency $\omega$, and a high-frequency part arising from all other modes, which are assumed to have frequencies large compared to $\omega$. The response of the polarization field to an external electric field with frequency low compared to $\omega$ may be described by a static dielectric constant $\varepsilon_0$; the response to fields with frequencies large compared to $\omega$ but small compared to the smallest frequency of the high frequency modes may be described by a high frequency dielectric constant $\varepsilon_\infty$.

The forces exerted on the electron by the high-frequency modes are negligible compared to those exerted by the low-frequency modes provided the electron moves slowly enough. The reason for this is that the high-frequency part of the polarization field induced by a slowly moving electron is able to accommodate itself instantaneously to the position of the electron, thus providing a spherically symmetric polarization field centered on the electron. By symmetry, such a field can exert no force. Therefore only the low-frequency modes need be taken into account in describing the dynamics of a single electron.
The entity composed of a slowly moving electron in a polarizable medium and the accompanying induced longitudinal polarization field is called a polaron. The Hamiltonian which was proposed by Frohlich to describe a single polaron is, in units in which $2m^* = \hbar = \omega = 1$,

$$
H = -\left[ \frac{\hbar}{\partial x^2} \right] \dot{x} + \sum_v b_v^+ b_v + i \left( \frac{e}{\hbar c} \right)^2 \sum_v v \left[ b_v^+ e^{-i v \cdot x} - b_v e^{+i v \cdot x} \right],
$$

where

$$\alpha = \left( \frac{e}{\omega} \right)^{1/2} \frac{\hbar}{\epsilon_0} \frac{\hbar \omega}{m^*} \left( \epsilon_{\infty}^{-1} - \epsilon_o^{-1} \right) \tag{1.2}$$

and

$$\begin{bmatrix}
    b_v & b_v^+
\end{bmatrix} = \delta_{v, v'}. \tag{1.3}$$

In Eq.(1.1) the first term is the operator for the kinetic energy of the electron, whose position is $x$. The second term is the energy of the polarization field in the absence of interaction with the electron, and the last term is the energy of interaction of the electron with the polarization field. The operator $b_v^+$ creates a longitudinal polarization field quantum of wave vector $v$. The dimensionless parameter $\alpha$ is called the polaron coupling constant, and $S$ is the normalization volume which is to be taken infinitely
large, in which limit

$$S^{-1} \sum_{\nu} \rightarrow (8 \pi^3)^{-1} \int d^3 \nu$$

(1.4)
2. The Landau-Pekar Approximation

A strong coupling variational approximation to the ground state of the Hamiltonian of Eq. (1.1) has been developed by Landau and Pekar. (See also References 1 and 6.)

If the coupling is large, then according to Eq. (1.2) the natural frequency, \( \omega \), of the polarization field will be small (other quantities in Eq. (1.2) regarded as fixed). The polarization field will then react slowly to the electron's motion and the electron will find itself situated in a deep, almost static potential well. Accordingly, Landau and Pekar employ a variational ground state trial wave function of the form

\[
\psi = \Xi_0(\mathbf{x} - \mathbf{y}) \phi(\mathbf{y}),
\]

where \( \mathbf{y} \) is the arbitrarily chosen center of the well, where \( \Xi_0 \) is an electronic wave function independent of the polarization field coordinates, and where \( \phi \) is a polarization field amplitude independent of the electron coordinate \( \mathbf{x} \). Ideally, \( \Xi_0 \) and \( \phi \) should be chosen in such a way that

\[
E_0 \equiv \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle \tag{1.6}
\]

is a minimum. For any choice of \( \Xi_0 \), the \( \phi \) which minimizes \( E_0 \) is

\[
\phi = \exp \left[ -i \sum_{\mathbf{y}} \left( f_\mathbf{y} b_\mathbf{y}^\dagger + f_{\mathbf{y}}^* b_\mathbf{y} \right) \right] \phi_0, \tag{1.7}
\]
where

$$\mathcal{F}_y = \left(4\pi \alpha / \varepsilon \right)^{1/2} \varepsilon^{-1} \int d^3 \mathbf{y} \exp \left( -i \mathbf{y} \cdot \mathbf{V} \right) | \Omega_0 (\mathbf{x} - \mathbf{y}) |^2 / \langle \Omega_0 | \Omega_0 \rangle \tag{1.8}$$

and where $\phi_o$ is the vacuum state of the polarization field. The resulting value of $E_0$ is

$$E_o = \langle \Omega_0 | \Omega_0 \rangle \int d^3 \mathbf{x} \Omega_0^* (\mathbf{x} - \mathbf{y}) \left( -i \frac{\partial}{\partial \mathbf{x}} \right) \Omega_0 (\mathbf{x} - \mathbf{y}) - \sum \left\{ \frac{\partial}{\partial \mathbf{y}} \right\} \right|^2. \tag{1.9}$$

In practice, the function $\Omega_0 (\mathbf{x} - \mathbf{y})$ is chosen to represent a ground state wave function for an electron trapped in a potential well with center at $\mathbf{y}$. For example, if

$$\Omega_0 (\mathbf{r}) = \exp \left( -\beta \mathbf{r}^2 / 2 \right), \tag{1.10}$$

then the value of $E_o$ for the optimum choice of $\beta$ is

$$- \alpha^2 / 3\pi. \tag{1.11}$$

The Landau-Pekar approximation can be extended to obtain a polaron effective mass, $m_p = m_e m_B$, where

$$\mu = 1 + 2 \alpha^{-1} \pi^{-2} \int d^3 \mathbf{y} \left| \int d^3 \mathbf{z} \right| \left. \Omega_0 (\mathbf{z}) \right|^2 \left| \exp \left( i \mathbf{z} \cdot \mathbf{V} \right) \right|^2. \tag{1.12}$$

For the choice of $\Omega_0$ given in Eq. (1.10),

$$\mu = 0.0200 \alpha^4 + 1. \tag{1.13}$$
3. The Effective Two-Polaron Interaction Potential

In Appendix 1 the two-polaron Hamiltonian is derived by an argument which closely parallels the derivation of the single-polaron Hamiltonian given in Reference 1. The result is

\[ H = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} + \sum_{\gamma} b_\gamma^+ b_\gamma + Z \alpha \, p \left[ x_1 - x_2 \right]^{-1} + i \left( \frac{4\pi \alpha}{\hbar} \right)^{\frac{1}{2}} \sum_{\gamma} v_\gamma \left[ b_\gamma^+ \left( e^{-i 2\gamma \cdot x_1} + e^{-i 2\gamma \cdot x_2} \right) - b_\gamma \left( e^{i 2\gamma \cdot x_1} + e^{i 2\gamma \cdot x_2} \right) \right] \]

where

\[ p = \left[ 1 - \frac{\varepsilon_\infty}{\varepsilon_0} \right]^{-1} \]

and \( x_1 \) and \( x_2 \) are the coordinates of the two electrons. In Eq. (1.14), the first two terms represent the kinetic energy of the electrons, the third term represents the energy of the polarization field in the absence of interaction with the electrons, the fourth term represents the Coulomb interaction energy of two point charges in a medium of dielectric constant \( \varepsilon_\infty \), and the last term represents the interaction energy between the electrons and the polarization field.

The Landau-Pekar approximation is easily generalized to the two-polaron case. The variational ground state approximate trial wave function is chosen in the form

\[ \psi = \chi_0 \left( x_1, y_1, x_2, y_2 \right) \phi \left( y_1, y_2 \right) \]
analogous to Eq.(1.5), where $\Omega$ is independent of the polarization field variables and $\phi$ is independent of the electron coordinates $x_1$ and $x_2$. The coordinates $y_1$ and $y_2$ represent points to which the pair of electrons are self-trapped in the Landau-Pekar picture and therefore locate the centers of the polarons.

For arbitrary $\Omega_o$, the factor $\phi$ which minimizes

$$E_o = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

is the exact ground state wave function of

$$\bar{H} = \iint d^3 x_1 d^3 x_2 \Omega_o^* H \Omega_o.$$ 

(1.18)

Then $E_o = E_1 - E_4$, where

$$E_1 = \iint d^3 x_1 d^3 x_2 \Omega_o^* \left[ -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} + 2p \kappa |x_1 - x_2|^2 \right] \Omega_o \frac{\langle \Omega_o | \Omega_o \rangle}{\langle \Omega_o | \Omega_o \rangle}.$$ 

(1.19)

and

$$E_4 = \sum \nu \nu^2 \Omega_o^* (\nu) \Omega_o (\nu) \frac{1}{\langle \Omega_o | \Omega_o \rangle}.$$ 

(1.20)

with

$$d \Omega_o (\nu) = \left(\frac{4\pi}{2}\right) \iint d^3 x_1 d^3 x_2 \left( e^{i\nu \cdot \xi_1} + e^{i\nu \cdot \xi_2} \right) |\Omega_o (x_1, y_1, x_2, y_2)|^2.$$ 

(1.21)
The trial electronic wave function $\Omega_\circ$ is chosen to be

$$\Omega_\circ = \Omega_A \pm \Omega_B \quad (1.22)$$

where

$$\Omega_A = e^{-\frac{\beta}{2}(|x_1 - y_1|^2 + |x_2 - y_2|^2)} \quad (1.23)$$

$$\Omega_B = e^{-\frac{\beta}{2}(|x_1 - y_2|^2 + |x_2 - y_1|^2)} \quad (1.24)$$

and where the upper (lower) sign is to be used if the pair of electrons is in a spin singlet (triplet) state. With this choice of $\Omega_\circ$, one finds that $E_0 = E_0^+ (y/\beta) = E_1 - E_4$, where

$$E_1^+ = \left\{ \beta \pm 4 \alpha \mp \frac{\beta}{2} \left[ \left( \frac{1}{5} \right) \frac{1}{\sqrt{y}} \int f(2 \omega) \right] \pm \frac{1}{1 \pm \exp(-\omega^2)} \right\}$$

$$E_4^+ = 2 \frac{1}{\sqrt{\pi}} \left\{ \left( \frac{2}{\beta \pi} \right)^{\frac{1}{2}} \left( \frac{1}{\sqrt{y}} \int f(2 \omega) \right) + \left( \frac{2}{\beta \pi} \right)^{\frac{1}{2}} \exp(-2 \omega^2) \right\}$$

In Eqs. (1.25) and (1.26), $y = |x_1 - x_2|$ is the distance separating the two polaron centers, $w = y (\beta / 2)^{\frac{1}{2}}$, and the function $f$ is defined as

$$f(u) = \frac{1}{\sqrt{\pi}} \int_0^u e^{-x^2} dx = \frac{1}{\sqrt{\pi}} e^{-u^2 / 2} \quad (1.27)$$
The functions $E^+_0(y, \beta)$ must be numerically minimized with respect to the variational parameter, $\beta$, to yield the optimum ground-state energy $E^+_0(y)$. This minimization is done numerically with the aid of some analytical detail discussed in Appendix 2.

Analytic minimization of $E^+_0(y, \beta)$ with respect to $\beta$ for asymptotically large $y$ reveals that

$$E^+_0(y) \sim \frac{2\alpha(y-1)}{y^2} - \frac{2\alpha^2}{3\pi y}.$$  \hfill (1.28)

The second term of Eq. (1.28) is twice the self-energy of a single polaron, Eq. (1.11), calculated in the Landau-Pekar approximation. The first term of Eq. (1.28) is equivalent to

$$E^2 / \epsilon_o y.$$  \hfill (1.29)

Thus the effect of the low-frequency polarization is to replace $\epsilon_\infty$ by $\epsilon_o$ in the Coulombic potential energy at asymptotic separations and to modify the form of the interaction potential energy otherwise.

If $y$ is set to zero, the energy $E^+_0(y, \beta)$ may then be analytically minimized with respect to $\beta$ to yield

$$E^+_0(y = 0) = \frac{2\alpha^2}{3\pi} (4p - p^2 - 4).$$  \hfill (1.30)

and
Further analysis shows that these values are attained with vanishing derivative with respect to y.

The function

$$V(y) = \sqrt{E} + \frac{2\alpha^2}{3\pi},$$

(1.32)

where $P_{12}^s$ and $P_{12}^t$ are the singlet and triplet projection operators,

$$V_s(y) = E_{o}^+ (y) + \frac{2\alpha^2}{3\pi},$$

(1.33)

and

$$V_t(y) = E_{o}^- (y) + \frac{2\alpha^2}{3\pi},$$

(1.34)

is an adiabatic approximation for the interaction potential energy of a pair of polarons with coordinates $y_1$ and $y_2$ and each with an effective mass given by Eq.(1.13). In the language of second quantization, $V(y)$, given in Eq.(1.32), may be expressed as

$$V = \frac{1}{4} \sum_{\lambda, \beta, \sigma, \sigma'} \left\{ \left[ \widetilde{V}_s (\lambda) + \widetilde{V}_t (\lambda) \right] \mathcal{C}_{\lambda, \beta, \sigma, \sigma'} \mathcal{C}_{\lambda, \beta, \sigma, \sigma'}^{+} \mathcal{C}_{\lambda, \beta, \sigma, \sigma'} \mathcal{C}_{\lambda, \beta, \sigma, \sigma'}^{+} \right\}$$

(1.35)

$$+ \left[ \widetilde{V}_s (\lambda) - \widetilde{V}_t (\lambda) \right] \mathcal{C}_{\lambda, \beta, \sigma, \sigma'}^{+} \mathcal{C}_{\lambda, \beta, \sigma, \sigma'} \mathcal{C}_{\lambda, \beta, \sigma, \sigma'} \mathcal{C}_{\lambda, \beta, \sigma, \sigma'}^{+} \right\}$$
where $\mathcal{C}^{\dagger}_{\mathbf{q}, \sigma'}$ and $\mathcal{C}^\sigma_{\mathbf{q}, \sigma'}$ are creation and destruction operators for a polaron of wavevector $\mathbf{q}$ and an internal electron in spin state denoted by $\sigma'$, and where a tilde denotes a Fourier transform according to the definition

$$
\tilde{V}(\mathbf{q}) = \mathcal{S}^{-1} \int d^3x \ V(x) \mathcal{E}^{\dagger \mathbf{q} \cdot x}.
$$

The many-polaron system is assumed to exist against a background of a uniform static distribution of positive charge sufficient to electrically neutralize the system. The effect of the background is to add to the potential energy of the system a dynamically constant term representing the self-energy of the positive charge and the interaction energy of the positive charge with the polarons. By choice of reference of measurement of the energy of the system, it is convenient to choose this additive constant by calculating it as though the positive charge interacts with itself via the two-polaron potential and with polarons via the negative of the two-polaron potential. With this choice, one simply deletes from Eq. (1.35) the terms for which $p=0$ to obtain the potential energy of the system.

Graphs of $V_{s}(y)$ and $V_{v}(y)$ for selected sets of polaron parameters are shown in Figure 1.
\[ \alpha = 12 \]
\[ p = 1.2 \]

**FIGURE 1a**

- **Numerical Calculation**
- **Approximation**

Graph showing the relationship between \( \frac{V_s}{V_{os}} \) and \( \frac{V_f}{V_{of}} \) with \( y/\lambda \) as the x-axis.
Note change from linear to logarithmic scale at $y = 1.0$

$V_y$ (in polaron units)

$y$ (in polaron units)

FIGURE 1b
As illustrated in Figure lb, if $p$ (whose least meaningful value is unity) lies in the range $1 < p < p_c$, where $p_c$ is a critical value lying somewhere between 1.01 and 1.1, then $V_s(y)$ exhibits a negative minimum for $y > 0$, whereas $V_t(y)$ remains positive. Figure la is typical for $1.1 < p < 2$. If $p > 3$, $V_s(y)$ possesses a negative minimum at $y=0$ and if $p > 4.345$, both potential have negative minima at $y=0$. The possible negative minima of these potentials can be capable of supporting bound states. For example the potential well shown in Figure lb supports a tightly bound ground state of a pair of polarons the mass of each of which is determined by Eq. (1.13) to be 207 in the unit system ($\hbar = \omega = 2m_B = 1$) being used here. The binding energy of this state may be estimated easily to be about 1.4 by use of the simple harmonic approximation. Since this binding energy is only somewhat less than depth, 1.7, of the well, the simple harmonic approximation is adequate at least to predict confidently that the well supports at least one tightly bound bipolaron state.

The formation of multipolaron bound states will not be considered further here since for the values $\omega = 12$ and $p = 1.2$ to be used for numerical calculations in Chapter 5, the potentials are everywhere repulsive as shown in Figure la. The potentials shown in Figure la differ by at most about 10% so that the two-polaron interaction is almost spin independent. Moreover, for these values of $\omega$ and $p$, the potentials, $V_s(y)$ and $V_t(y)$, may be approximated as indicated in Figure la by the analytic form
\[ \mathbf{V}(\gamma) = \begin{cases} V_0 & , \gamma \leq \lambda \\ 2 \chi (p-1)/\gamma & , \gamma \geq \lambda \end{cases} \]  \hspace{1cm} (1.37)

where \( \lambda = 2 \chi (p-1)/V_0 \) and where \( V_0 \) represents the approximated potential at \( \gamma = 0 \) and may be obtained from Eqs. (1.30), (1.31), (1.33), and (1.34). For later reference, the Fourier transform of Eq. (1.37) is

\[ \widetilde{\mathbf{V}}(k) = \frac{4 \pi V_0}{\zeta} \frac{\sin (L_i \lambda)}{R^2} \]  \hspace{1cm} (1.38)
1. Introduction

It is the purpose of this chapter to examine a lattice model for the low-lying states of the system of polarons interacting via an effective spin independent potential. This examination consists of a calculation of the energy of the system in a static lattice configuration and an investigation of the dynamic small deviations of the lattice from the static configuration by calculating the normal mode frequencies of the lattice. In order for the lattice to be a stable one it is necessary that the resulting normal mode frequencies be positive real numbers. As is usual in lattice calculations, the indistinguishability of lattice occupants is ignored.

2. The Static Lattice

Consider a lattice of particles at lattice points $\mathbf{R}_i$ and let the potential energy of two particles a distance $r$ apart be $\varphi(r)$. The total energy of the static lattice including the static uniform background of positive charge is then

$$V_o = \frac{\rho^2}{2} \int d\mathbf{r} \int d\mathbf{r}' \varphi(|\mathbf{r} - \mathbf{r}'|) + \frac{1}{2} \sum_i \sum_{j \neq i} \varphi(|\mathbf{R}_i - \mathbf{R}_j|)$$

$$- \rho \sum_j \int d^3 \mathbf{r} \varphi(|\mathbf{r} - \mathbf{R}_j|)$$

(2.1)
In Eq. (4.1) \( \rho \) is the number of particles per unit volume. The first term is the self-energy of the uniform positive charge. The second term is the energy of interaction of the lattice of point charges, and the third is the energy of interaction between the lattice and the uniform charge distribution.

The lattice energy \( V_0 \) has been calculated, using a Coulombic potential, for body-centered cubic, face-centered cubic, simple cubic, and hexagonal close-packed structures. It was found that, of these structure types, the body-centered cubic (bcc) lattice has the lowest energy, although the energy of the bcc lattice differs from that of the face-centered cubic lattice only in the fourth significant figure. For this reason, only the bcc structure will be examined.

In view of Eqs. (1.28), (1.33), and (1.34), the potential \( \varphi (r) \) may be separated into two parts: \( \varphi = \varphi_1 + \varphi_2 \), where \( \varphi_2 (r) = e^2 / r \epsilon_0 \), and \( \varphi_1 = \varphi - \varphi_2 \), where \( \varphi_1 \) is a short-range potential. The terms in Eq. (4.1) involving \( \varphi_2 \) may be calculated exactly to give

\[-1.79186/r_s \epsilon_0 \text{ rydbergs (ry) per particle, where } r_s \text{ is a measure of the particle density and is defined by}\]

\[
\rho = \frac{N}{a^3} = \frac{1}{\frac{4}{3} \pi r_s^3 \epsilon_0^2} \]

(2.2)

where \( a_0 \) is the Bohr radius. The remaining terms of Eq. (4.1) involve only the short-range potential \( \varphi_1 \) and may be calculated for a
given $\phi (r)$ by direct summation over lattice points.

3. The Dynamic Lattice

The units used in this section are atomic units: energy is measured in rydbergs and distances in Bohr radii. The potential $\phi (r)$ in these units is related to the potential $f(y)$ measured in ergs as a function of $y$, the separation in centimeters, by

$$\phi (r) = \frac{f}{\frac{a_0}{r}} \left( \frac{a_0}{r^2} \right) . \quad (2.3)$$

Let the position of the polaron near the lattice point $R_j$ be $x_j$. Then the potential energy of the dynamic lattice is

$$V_{xy} = V_0_{xy} - \frac{3}{4\pi r_0^3} \sum_{j} \left[ \int \phi (|r - R_i|) d^3 r - \int \phi (|r - R_j|) d^3 r \right]$$

$$+ \frac{1}{2} \sum_{i \neq j} \left[ \phi (|x_i - R_j|) - \phi (|x_j - R_i|) \right] \quad (2.4)$$

where $V_0_{xy}$ is the $V_0$ of Eq. (2.1) measured in rydbergs. For the bcc lattice, the lattice points, measured from an arbitrary site, are given by

$$R_j = (\pi / 3) \frac{1}{2} r_s n_j \quad (2.5)$$

where $n_j$ is a triple of integers, all even or all odd. Latin
summation indices \( i \) and \( j \) are used synonymously with the vectors \( \mathbf{R}_i \) and \( \mathbf{R}_j \). Let \( \mathbf{r}_j = \mathbf{R}_j + \mathbf{u}_j \), and assume that, for all lattice points \( j \), \(|\mathbf{u}_j| \ll \) the lattice spacing. An expansion in ascending powers of \( \mathbf{u}_j \) may then be made in Eq. (2.4). The result is

\[
V_{\mathbf{r}_j} = V_{0\mathbf{r}_j} + \sum_{\alpha, \beta} C_{\alpha \beta}^i \mathbf{u}_i \mathbf{u}_j \mathbf{u}_j \mathbf{u}_j \mathbf{u}_j \mathbf{u}_j ^{\beta} \quad (2.6)
\]

where

\[
C_{\alpha \beta}^i = (F + \epsilon_0^{-1} \mathbf{r}_s^{-3}) \delta_{\alpha \beta} \delta_{\mathbf{j} \mathbf{j}} + (\delta_{\mathbf{j} \mathbf{j}} - 1) D_{\alpha \beta}^i \quad (2.7)
\]

\[
F = \frac{1}{3} \sum_{i \neq 0} \left[ \Phi''(1 \mathbf{R}_i |) + 2 \Phi'(1 \mathbf{R}_i |) \mathbf{R}_i |^{-1} \right] \quad (2.8)
\]

\[
D_{\alpha \beta}^i = \frac{1}{2} \left( 1 - \delta_{\mathbf{j} \mathbf{j}} \right) \left\{ \alpha \beta r^{-3} \left[ \nabla \phi''(r) - \phi'(r) r^{-1} \right] + \delta_{\alpha \beta} \phi'(r) r^{-1} \right\} \quad (2.9)
\]

and a prime indicates differentiation. Here \( \alpha \) and \( \beta \) take on the values \( x, y, z \) and summations are indicated explicitly. In the derivation of Eqs. (2.7)-(2.9) the cubic symmetry of the lattice was used.

The total Hamiltonian is then
where

\[ \Delta = \sum_i \frac{1}{\xi_i} \frac{\partial}{\partial \xi_i} \cdot \frac{\partial}{\partial \xi_i} \quad (2.11) \]

The transformation which reduces Eq.(2.10) to a sum of one-dimensional simple harmonic oscillator Hamiltonians is given in Reference 10. Eq.(4.10) is reduced thereby to the form

\[ H_{r,s} = \sum_{k, l} \left[ -\left( \frac{\hbar^2}{2m^2} \right) \frac{\partial^2}{\partial k^2} + \omega^2 (k,s) \frac{q^2}{3} \right] \quad (2.12) \]

where \( k \) is a vector in the basic cell of the reciprocal lattice and \( s \) takes on the values 1,2,3.

Only a representative set of reciprocal lattice vectors \( k \) will be considered. The Cartesian components of the vectors in this set are given by

\[ 1 \leq k^\alpha = 2 \pi^{2/3} 3^{1/3} v_\alpha^{-1} q^\alpha \quad (2.13) \]

where \( q^\alpha \) runs in integral steps from -8 to +8 and \( q^x + q^y + q^z \) is even. For any given \( k \) and \( s \), the frequency \( \omega \) \((k,s)\) may be
calculated by solving the secular equation

\[ \sum_{\ell} G_{\alpha \beta}(\mathbf{r} \ell) - \left( \frac{\Omega_{\alpha \beta}}{m_e} \right) \omega^2 (2, \ell) \mathbf{J}_{\alpha \beta}(\mathbf{r} \ell) = 0 \]  

(2.14)

where

\[ G_{\alpha \beta}(n_{ij}) = \sum_{\ell} C_{\gamma \delta}(n_{ij}) \exp\left(i \frac{\pi}{2} \frac{\alpha}{\gamma \delta} \cdot \mathbf{r}_{ij} \right) \]  

(2.15)

and where \( C_{\alpha \beta}(n_{ij}) = C_{\alpha \beta}^{ij} \). If the polaron potential \( \varphi \) is separated into a long-range part, \( \varphi_L \), and a short-range part, \( \varphi_s \), as in Section 2, then the tensors \( C \) and \( G \) may be separated also, so that \( C = C_1 + C_2 \) and \( G = G_1 + G_2 \), where

\[ C_{1 \alpha \beta}^{ij} = \begin{cases} \frac{F}{2} \delta_{\alpha \beta}, & i = j \\ -\frac{1}{2} \left\{ \alpha_{\beta} r^{-3} \left[ r \varphi''_1(r) - \varphi'_1(r) - 6 r^{-2} \varepsilon_0^{-1} \right] + \delta_{\alpha \beta} \left[ (r - 2 r^{-3} \varepsilon_0^{-1}) \right]_{r = R_i - R_j} \right\}, & i \neq j \end{cases} \]  

(2.16)

\[ C_{2 \alpha \beta}^{ij} = \begin{cases} \frac{\varepsilon_0^{-1} r_s^{-3}}{2} \delta_{\alpha \beta}, & i = j \\ \frac{\varepsilon_0^{-1}}{2} \left[ \delta_{\alpha \beta} r^{-3} - 3 \alpha_{\beta} r^{-5} \right] \right|_{r = R_i - R_j}, & i \neq j \end{cases} \]  

(2.17)
\[ G_{1 \alpha \beta}(\mathbf{q}, \mathbf{e}) = \sum_{j} C_{1 \alpha \beta}(\mathbf{q}, j) e^{i \frac{q}{2} \cdot \mathbf{e} \cdot j} \]  

(2.18)

\[ G_{2 \alpha \beta}(\mathbf{q}, \mathbf{e}) = \frac{3}{4 \pi \varepsilon_{0} c^{3}} [d_{\alpha \beta} S_{3}(\mathbf{q}, \mathbf{e}) - 3S_{5}^{\alpha \beta}(\mathbf{q}, \mathbf{e})] \]  

(2.19)

The quantities \( S_{3} \) and \( S_{5}^{\alpha \beta} \) are defined as

\[ S_{3}(\mathbf{k}) = \rho^{-1} \sum_{j \neq 0} | \mathbf{R}_{j} |^{-3} e^{\cdot (i \mathbf{k} \cdot \mathbf{R}_{j})} \]  

(2.20)

and

\[ S_{5}^{\alpha \beta}(\mathbf{k}) = \rho^{-1} \sum_{j \neq 0} R_{j \alpha} R_{j \beta} | \mathbf{R}_{j} |^{-5} e^{\cdot (i \mathbf{k} \cdot \mathbf{R}_{j})} \]  

(2.21)

and are tabulated in Reference 10.

Eq. (2.14), for specified values of \( \mathbf{k} \) and \( s \), is a cubic equation in \( \Omega^{2} \), and, if \( \mathbf{k} \neq 0 \), may be solved by any of several methods.

The quantity \( G \) does not possess a limit as \( q \to 0 \), but if the determinant in Eq. (2.14) is evaluated before the limit is taken,
the unambiguous result is obtained that the equation

$$\lim_{|q| \to 0} \det \left[ G_{\alpha\beta} (q) - \frac{\hbar}{\omega_{\alpha\beta}} \omega^2 (q, s) \delta_{\alpha\beta} \right] = 0$$

becomes

$$\left[ \left[ G_{1,xx} (q) + F - \frac{\hbar}{m_e} \omega (q, s) \right] \right]$$

$$\times \left[ \left[ G_{1,xx} (q) + F' + \frac{3}{\varepsilon_0 Y_{e}} - \frac{\hbar}{m_e} \omega^2 (q, s) \right] \right] = 0 \quad (2.22)$$

Thus the calculation of normal mode frequencies is reduced to computational form. Discussion of the numerical results is postponed until Chapter 5.
The Hartree-Fock approximation is a variational method for calculating the ground-state wave function of a system of \( N \) fermions. The approximate trial variational wave function is

\[
\Psi_{\text{HF}} = \frac{1}{\sqrt{N!}} \left| \begin{array}{cccc}
U_1(1) & U_2(1) & U_3(1) & \ldots & U_N(1) \\
U_1(2) & U_2(2) & U_3(2) & \ldots & U_N(2) \\
U_1(3) & U_2(3) & U_3(3) & \ldots & U_N(3) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
U_1(N) & U_2(N) & U_3(N) & \ldots & U_N(N)
\end{array} \right|
\]

where the \( U_j(i) \) is a single particle wave function with label \( j \), and is a function of the coordinates of the \( i \)-th particle, and vertical lines bracketing a matrix represents the determinant of the matrix. If the single particle functions are orthonormal to each other, then \( \Psi_{\text{HF}} \) is normalized. The wave function \( \Psi_{\text{HF}} \) represents a system in which each particle moves in an effective potential which is an average of the potentials due to all the other particles. The only correlations which are included in this description are those implied by the permutation symmetry, i.e. the statistical correlations. Dynamical correlations, brought about by the nature of the interparticle potential, are ignored. If the expectation value of a system Hamiltonian (restricted for this discussion to a sum of one-and-two-particle operators) is taken with respect to \( \Psi_{\text{HF}} \) and the result varied with respect to
one of the single-particle functions \( \langle \phi_x \rangle \) remains normalized during the variation), the result is a set of \( N \) coupled integrodifferential equations for the single-particle functions. This set is called the Hartree-Fock equations. Little is known about the existence or uniqueness of solutions of these equations, although the equations are widely used in the literature. In particular, for any solution, it is possible that there exists a second with lower energy, in which case the second one is the better approximation to the exact ground-state wave function of the system.

There is one solution of the Hartree-Fock equations which is well known, namely the Hartree-Fock plane-wave gas. In this solution the single-particle functions are chosen to be plane wave states multiplied by spin eigenfunctions:

\[
U_{\frac{i}{j}}(\sigma_i) = S^{-\frac{1}{2}} e^{i k_j \cdot x_j} \chi_{\sigma_i} (\sigma_j) 
\]

where \( S \) is the normalization volume, where \( k_j \) is a vector each of whose Cartesian components is a positive or negative integral multiple of \( \pi S^{-\frac{1}{2}} \), where \( \chi_{\sigma_i} (\sigma_j) \) is a spin function for a particle of spin \( \frac{1}{2} \), and where \( \sigma_i \) and \( \sigma_j \) may take on the values \( \uparrow \) denoting spin up and \( \downarrow \) denoting spin down.

The energy associated with the "quasi-particle" state \( u_\uparrow \) is given by

\[
E_\uparrow = \langle \uparrow | T | \uparrow \rangle + \sum_{j=1}^{N} \left( \langle i_j | v | i_j \rangle - \langle i_{j} \uparrow | v | i_j \uparrow \rangle \right) 
\]

(3.3)
where $T$ is the kinetic energy operator and $v$ is the two-particle potential energy operator. The expectation value of $H$ with respect to the trial ground state of Eq. (3.1) is

$$E_0 = \sum_i \langle i | T | i \rangle + \frac{1}{2} \sum_{i,j} \left[ \langle i,j | v | i,j \rangle - \langle i,i | v | i,i \rangle \right], \quad (3.4)$$

where $i$ and $j$ each runs from 1 to $N$ and labels the occupied single-particle functions of Eq. (3.1). With the potential energy operator given by Eq. (1.32), Eq. (3.3) for the energy of a quasi-particle of wave vector $p$ becomes

$$\varepsilon_p = \langle p | T | p \rangle + \frac{\varepsilon}{8 \pi^3} \frac{1}{2} \int d^3 p \left[ \nabla_s (p^2 - p^2) - 3 \nabla_s (p^2 - p^2) \right], \quad (3.5)$$

independently of the spin of the quasi-particle, and Eq. (3.4) becomes

$$E_0 = \frac{3}{4} N \varepsilon_F + \frac{1}{4} \left( \frac{\varepsilon}{8 \pi^3} \right)^2 \int d^3 p d^3 q \left[ \nabla_s (p^2 - p^2) - 3 \nabla_s (p^2 - p^2) \right], \quad (3.6)$$

where the limit of Eq. (1.4) has been taken, where $\nabla_s (0)$ and $\nabla_t (0)$ have been set to zero to account for the positive background charge, where the integrals are over a sphere of radius $k_F = (3 \pi^2 N/S)^{1/3}$, and where $\varepsilon_F$ is the energy of a free particle at the Fermi surface.
In cases for which $V_s$ and $V_t$ may be approximated by the form of Eq. (1.38), the integrals in Eqs. (3.5) and (3.6) may be performed by the techniques of reduction of multifold integrals to single integral form developed in Appendix 3. The result for the Hartree-Fock ground-state energy per particle is a special case of a more general result obtained in the next chapter and is given by setting $\beta = 0$ in Eq. (4.14).
CHAPTER 4

THE HARTREE-FOCK GAS OF PLASMA-SHIELDED POLARONS

1. Introduction

The present chapter contains a description and investigation of another candidate for the ground state of the system of polarons with effective mass given by Eq. (1.13) and interaction potential energy given by Eq. (1.32).

The state considered is similar to one introduced by Pines for the description of the ground state of a high-density collection of electrons. This state describes a system with long-wavelength simple harmonic modes of electron density motion (called plasma modes) interacting with the electrons which interact among themselves with a modified, short range (shielded) interaction. The state of the electrons is described by a HF gas wave function like that of Chapter 2 and the state of the plasma modes is described by ground state simple harmonic oscillator wave functions. The product of these wave functions represents the wave function of the system.

In Section 2 the plasmon modes are introduced and in Section 3 the ground state energy of the system is calculated.

2. Introduction of Plasma Modes

The Hamiltonian for a system of polarons, interacting via the
potential given by Eq. (1.35) may be written as

$$H_{p.o} = \sum_i p_i^2 / 2 m_p + \frac{1}{4} \sum_i \left\{ \left[ \vec{V}_s(k) + \vec{V}_t(k) \right] \left[ \hat{\rho}_s^+(\sigma, \sigma') \rho_s(\sigma', \sigma') \right] \right\} \hbar^2 - 2 N_{\sigma_p} \right) \right\} \right\}$$

(4.1)

where

$$\rho_s^+(\sigma, \sigma') = \delta^{\sigma'} - \sum_i e^{-i \frac{\hbar}{\epsilon} \cdot r_i} \left| \sigma \right> \left< \sigma' \right|$$

(4.2)

$$N_{\sigma_p} = \sum_i \left| \sigma \right> \left< \sigma' \right|$$

(4.3)

where the summation convention applies for the indices $\sigma$ and $\sigma'$, where $\sigma$ takes on the two values $\uparrow$ and $\downarrow$, and where $\uparrow)$ is the spin-up state and $\downarrow)$ the spin-down state of a polaron of spin $\frac{1}{2}$. The operator $\rho_s = \rho_s^+(\sigma, \sigma)$ is the Fourier transform of the particle density operator for a system of point particles, that is,

$$\rho_s = \delta^{\sigma'} \int \rho(\vec{r}) e^{-i \frac{\hbar}{\epsilon} \cdot \vec{r}} d^3 \vec{r}$$

where

$$\rho(\vec{r}) = \sum_i \delta'(\vec{r} - \vec{r}_i) \left| \sigma \right> \left< \sigma' \right|$$

wherein $\delta'(\vec{r})$ is the Dirac delta function.

If the second time derivative, $\dot{\rho}_s$, of $\rho_s$ is evaluated using the Heisenberg equations of motion and the Hamiltonian $H_{pol}$,
one finds a term \(-\omega_{\pi}(k)^2\) plus other terms, where

\[
\omega_{\pi}(k) = \frac{N}{\beta} \left( \frac{2\pi}{\nu_e} \right)^{\frac{1}{2}} \left[ \nu_{oe} \sinh \left( \frac{\beta \omega_c}{2} \right) + \nu_{oe} \sinh \left( \frac{\beta \omega_c}{2} \right) \right] \frac{1}{\nu_e}
\]  

(4.4)

Pines has shown \(^{12}\) that, in the case of the electron system, the other terms are negligible for sufficiently small \(k\) so that the \(P_k\) will, for small \(k\), undergo undamped vibration with angular frequency \(\omega_{\pi}(k)\). This result is applicable to the polaron system due to the similarity of the forms of the interactions for large separations (small \(k\)). Pines' method of treating these collective modes, which is followed here, is to add terms describing the new modes to the original Hamiltonian. Thus the model Hamiltonian becomes

\[ H = H_{\pi \pi} + \sum_{k < k_c} \left\{ \frac{\Pi^+_k \Pi^-_k}{2} + \left( \frac{\mathcal{V}_e(k) + \mathcal{V}_e(k)}{2} \right) \frac{1}{\Pi^+_k \Pi^-_k} \right\} \]  

(4.5)

where \(k_c\) is a cutoff parameter which will be determined later. The last sum in Eq. (4.5) is meant to describe a plasmon field and the interaction between plasmons and polarons. The plasmon momentum operators \(\Pi^\pm_k\) and the conjugate coordinate operators \(Q_k\) obey the Bosonic commutation relations

\[
\left[ \Pi^+_k, Q_{k'} \right] = -i k \delta_{k,k'}
\]  

(4.6)
and the condition
\[ Q^+_k = Q^-_{-k} \]  
ensures the reality of the plasmon field.

The Hamiltonian in Eq. (4.5) may be written, using the transformation \( \exp(iS/\hbar) \), where

\[
S' = -\sum_{k<k_c} \left[ \frac{\tilde{v}_s(k) + \tilde{v}_e(k)}{2} \right]^{1/2} Q_k \rho_k S
\]  

as

\[
H' = e^{-iS'/\hbar} H e^{iS'/\hbar} = \sum_i \frac{p_i^2}{2m_p} + H_{sr} + H_{int} + U
\]  

\[ + \sum_{k<k_c} \left[ \frac{\pi_p}{2} + \frac{\omega_p^2(k)}{2} \frac{Q_k^+ Q_k^-}{2} - \frac{i}{\hbar} (\tilde{v}_s(k) + \tilde{v}_e(k)) N_{op} \right],
\]

where

\[
H_{sr} = \frac{1}{4} \sum_{k>k_c} \left[ \tilde{v}_s(k) + \tilde{v}_e(k) \right] \left[ \rho^+_k (\sigma, \sigma') \rho_k (\sigma', \sigma') S^2 - N_{op} \right]
\]

\[ + \frac{1}{4} \sum_{k} \left[ \tilde{v}_e(k) - \tilde{v}_s(k) \right] \left[ \rho^+_k (\sigma, \sigma') \rho_k (\sigma', \sigma') S^2 - 2 N_{op} \right],
\]

\[
H_{int} = i \sum_{k<k_c} \left( \frac{F_i k_i^2}{m_p} + \frac{k_i k^2}{2m_p} \right) \left( \tilde{v}_s(k) + \tilde{v}_e(k) \right) \frac{1}{2} Q_k e^{-i k \cdot r}
\]

and
The Hamilton of Eqs. (4.9)-(4.12) describes a system of particles and a system of plasmons, $H_{sr}$ being a short-range particle-particle interaction (note that $V_t(0)=V_s(0)$ so that the second sum in Eq. (4.10) is a short-range potential), and $H_{int}$ and $U$ particle-plasmon interaction terms.

The cutoff parameter $k_c$ must satisfy the condition that $\tilde{V}_t(k) + \tilde{V}_s(k)$ be positive for all $k < k_c$, so that $S$ in Eq. (4.8) remains Hermitian.

As a result of adding the plasmon terms to the Hamiltonian, new degrees of freedom have been added. In order to recover a description with the proper number of degrees of freedom, it is necessary to impose upon the states of the Hamiltonian $H^i$ subsidiary conditions. It has been shown, however, that the energy of the ground-state of the original polaron Hamiltonian, $H_{pol}^i$, is equal to the ground-state energy of $H^i$. Thus the variational method may be applied to $H^i$ to obtain an upper bound approximation, $E_o$, to the ground state of $H_{pol}$ by ignoring the subsidiary conditions and minimizing $E_o$ with respect to $k_c$.
3. Ground-State Energy of the Plasmon-Polaron System

The trial ground state, \( \Psi'_{\text{plas}} \), of \( H' \) which will be investigated in this section is composed of ground state simple harmonic oscillator wave functions for the plasma modes and a H-F gas wave function for the N polarons. The contribution to 

\[
\langle \Psi'_\text{plas} | H' | \Psi'_\text{plas} \rangle
\]

from \( U \) and \( H_{\text{int}} \) is zero. The calculation of 

\[
\langle \Psi'_\text{plas} | H' | \Psi'_\text{plas} \rangle / N
\]

where \( H' \) is given by Eq. (4.9), is then straightforward except for the contribution from \( H_{\text{sr}} \). This contribution may be obtained by comparing Eq. (4.10) with (4.1) and using Eq. (3.6). The result is

\[
\langle \Psi'_\text{plas} | H' | \Psi'_\text{plas} \rangle = \frac{3}{8} \varepsilon_F - \frac{1}{4N} \left( \frac{3\pi N}{8\mu} \right)^{1/2} \int_{\frac{3}{2}k_F}^{k_F} d^3k \left[ \tilde{\nu}_s(k) + \tilde{\nu}_t(k) \right]
\]

\[
+ \frac{1}{4N} \left( \frac{3\pi N}{8\mu} \right)^{1/2} \int_{\frac{3}{2}k_F}^{k_F} d^3k \left[ \tilde{\nu}_s(1p - 2l) + \tilde{\nu}_t(1p - 2l) \right]
\]

\[
+ \frac{1}{N} \left( \frac{3\pi N}{8\mu} \right)^{1/2} \int_{\frac{3}{2}k_F}^{k_F} d^3k \left[ \tilde{\nu}_s(1p - 2l) - \tilde{\nu}_t(1p - 2l) \right]
\]

\[
+ \frac{1}{2N} \left( \frac{3\pi N}{8\mu} \right)^{1/2} \int_{\frac{3}{2}k_F}^{k_F} d^3k \left[ \omega_p(k) \right]
\]

\[(4.13)\]

where \( k_F = (3\pi^2 N / S)^{1/3}, \varepsilon_F = \frac{2}{3} k_F^2 / \mu \), and where \( \omega_p(k) \) is given by Eq. (4.4).

In cases for which \( \tilde{\nu}_s \) and \( \tilde{\nu}_t \) may be approximated by the form of Eq. (1.38), the integrals in Eq. (4.13) may be performed by use of Appendix 3. The result is
\[
\langle \psi_{\text{plas}} | \frac{H}{\hbar^2} | \psi_{\text{plas}} \rangle = \frac{3}{8} \frac{\hbar^2 k_F^2}{m_p} - \frac{1}{2\pi} \left[ V_{\omega e} S_c (\beta \lambda k_F) + V_{\omega e} S_c (\beta \lambda k_F) \right] \\
+ \left[ \frac{5}{3\pi^2} \left( \frac{a_0}{\lambda_c} \right)^2 V_{\omega e} \left( \frac{\hbar^2}{2 m_p a_0^2} \right) \right] \frac{1}{2} \int_0^{\frac{k_F}{\lambda_c}} \sin x + \frac{V_{\omega e}}{\omega e} \sin (\lambda_c / \lambda_c) x^{3/2} d x \\
- \left[ f_{\pm} (2) + f_{\pm} (\beta) - f_{\pm} (\beta) \right] \left\{ \frac{1}{\beta^2} \right\} - 2 \left[ f_{\pm} (2) - f_{\pm} (2) - f_{\pm} (0) + f_{\pm} (0) \right]
\]

(4.14)

where \( \beta \equiv k_c / k_F = (\pi / 4)^{1/2} a_0 \), and

\[
f_{\pm} (x) = V_{\omega e} \cdot F (x, \lambda_c, k_F) / 2\pi
\]

(4.15)

where

\[
F (x, z) = \frac{3 \cos (x z)}{4 z^2} + \frac{1}{16 z^3} \left[ 2x z \sin (x z) + (2 - \kappa z^2) \cos (x z) + 6 \kappa z \right]
\]

(4.16)

Equation (4.14) gives an upper bound approximation to the ground state energy per particle of the polaron system for any value of the parameter \( \beta \) subject to the restriction that the integrand of Eq. (4.14) remains real throughout the region of integration. It remains to minimise the result with respect to \( \beta \) subject to this restriction. Such a numerical treatment occurs in the following chapter for a particular application.

The number, \( N' \), of plasma modes may be expressed as \( \beta / 6 \). The ratio of \( N' \) to the number of degrees of freedom, \( 3N \), of the polarons is of interest because if \( N' / 3N \ll 1 \), then the polaron-plasmon interaction, not accounted for in this model, is expected to be unimportant.\(^{13}\)
1. Choice of Parameters

To determine which of the proposed models yields the least ground state energy, values must be chosen for the parameters which describe the polaron and the density of polarons. In this chapter a test set of parameters is chosen to represent polarons in an ionic crystal with a hypothetically strong polaron coupling constant. For this test case the Bloch mass, \( m_B \), of the electron is taken to be equal to the free electron mass, \( m_e \). The values \( \epsilon_0 = 12 \), \( \epsilon_{\infty} = 2.0 \) and \( \omega = 2.5 \times 10^{13} \) \( \text{sec}^{-1} \) are chosen not atypically for ionic crystals\(^{14,15}\), but so that they combine to yield a polaron coupling constant \( \alpha = 12 \) which is sufficiently large so that the Landau-Pekar approximation is expected to be applicable\(^6\). Equation (1.15) then gives \( p = 1.2 \). For this pair of values of \( \alpha \) and \( p \), the approximation, Eq.(1.37), for the effective potential may be employed to within the limits of accuracy described in Section 3 of Chapter 1. The numerical values of the parameters defined in connection with Eq.(1.37) are \( V_{os} = 11 \), \( V_{ot} = 10 \), \( \lambda_s = 0.44 \), and \( \lambda_c = 0.47 \). The final independent parameter, \( r_s \), defined by Eq.(2.2), characterizes the polaron density in terms of the Bohr radius whose value in polaron units is given by \( a_0 = .035 \) for the parameter values being used.
2. Results

The equations which were developed in Chapter 2 for calculating the ground state energy per particle and the phonon dispersion curves of a polaron lattice involve a spin-independent interaction potential \( \phi \). The singlet and triplet parts of the effective interpolaron potential developed in Chapter 1 are asymptotically equivalent and differ by at most 10%. If the triplet potential is approximated by the singlet potential, then the interaction potential becomes spin independent and the expressions of Chapter 2 may be employed. Since the secular equation for the phonon dispersion curves then involves derivatives of \( V_s(y) \), it is preferable to use the exact equations for \( V_s(y) \), namely Eqs. (1.25), (1.26), and (1.32)-(1.34), rather than the approximate form \( V_1(y) \) since the derivative of \( V_1(y) \) might not represent the derivative of \( V_s(y) \) with sufficient accuracy. The values of the square of the phonon frequencies, \( \omega(\lambda_0, \eta) \), were calculated from Eq. (2.14) with \( \phi = V_s \). The calculation was done for values of \( r_s \) ranging from 0.5 to 100. It was found that the polaron lattice was dynamically unstable at each of the corresponding densities.

The ground-state energy per particle of the Hartree Fock gas, \( E_{HF}/N \), was calculated from Eq. (4.14) with \( \xi = 0 \) for values of \( r_s \) ranging from 0.5 to 100. Several of these values are shown in Table 1.
To compare these energies with the polaron-plasmon model ground-state energy per polaron, \( E_{pp}/N \); for each value of \( r_s \) in Table 1, \( \langle \psi_{\text{plas}} | H'_{N} | \psi_{\text{plas}} \rangle \) was calculated from Eq. (4.14) as a function of \( \beta \) (subject to the restriction on \( \beta \) that the outcome be real). The result for \( E_{pp}/N \) was then determined numerically as the minimum value of \( \langle \psi_{\text{plas}} | H'_{N} | \psi_{\text{plas}} \rangle \) with respect to \( \beta \). The results are given in Table 1, where \( \beta_m \) represents the minimizing value of \( \beta \).

<table>
<thead>
<tr>
<th>( r_s )</th>
<th>( E_{H-F}/N )</th>
<th>( E_{pp}/N )</th>
<th>( \beta_m \equiv k_c/k_F )</th>
<th>( r_s a_0/\lambda )</th>
<th>( k_c \lambda /\pi )</th>
<th>( N'/3N = \beta^3/6 )</th>
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<td>0.39</td>
<td>0.95</td>
<td>0.29</td>
</tr>
<tr>
<td>20.</td>
<td>2.7</td>
<td>4.5</td>
<td>1.5</td>
<td>0.95</td>
<td>2.3</td>
<td></td>
</tr>
<tr>
<td>50.</td>
<td>1.2</td>
<td>4.5</td>
<td>4.5</td>
<td>3.9</td>
<td>0.71</td>
<td>15.</td>
</tr>
<tr>
<td>100.</td>
<td>0.61</td>
<td>3.3</td>
<td>6.3</td>
<td>7.7</td>
<td>0.50</td>
<td>42.</td>
</tr>
</tbody>
</table>

**TABLE 1**

For use in the interpretation of these results, Table 1 displays three additional quantities. The first is \( r_s a_0/\lambda \) where \( r_s a_0 \) is an average separation of the polarons and \( \lambda = 0.45 \) is an approximate distance such that the two-polaron interaction potential is flat for separations less than \( \lambda \) and is Coulombic for separations greater than \( \lambda \). The second quantity, \( k_c \lambda /\pi \), is proportional to \( k_c \), the maximum wave vector of plasma modes, with the constant of proportionality chosen so that this quantity takes on a value of about unity when \( k_c \) has the largest value allowed (by the restriction that \( E_{pp} \) be real). The
final quantity is the ratio of the number of plasma modes to the number of degrees of (translational) freedom described by the original polaron Hamiltonian.

3. Discussion

In summary, of the models examined and for the wide range of polaron densities investigated, the stable state of lowest energy was obtained for the polaron-plasmon model.

Other models may, of course, lead to superior results, even for the test case treated here. One obvious improvement would be a model which would take into account plasmon-phonon interaction (at least such interactions that are linear in plasma coordinates). An interesting possibility for an improved ground state of the polaron-plasmon Hamiltonian $H'$ is suggested by the following observations in the case $r_s = 5$ (for which the polaron-plasmon interaction is probably not very important since $N'/3N \ll 1$): Since $V_s \approx V_t$ and $k C \lambda \approx \pi$, it follows that the Fourier transform, $\tilde{V}_{sr}(k)$, of the short range plasma-shielded two-polaron interaction is zero for $k < \pi / \lambda$, is negative for $\pi / \lambda \leq k \leq 2 \pi / \lambda$, and damps out with oscillations for $k > 2 \pi / \lambda$. For this case, $k_F \approx 2 \pi / 3 \lambda$ where $\tilde{V}_{sr}(k)$ is a negative minimum. The condition that $\tilde{V}_{sr}$ is negative at the Fermi surface indicates the possibility that the plasma-shielded polarons may be superconductive.

The two-polaron potential obtained in Ch. 1 might be useful in contexts other than the description of conduction electrons in polar solids. For example, it may be useful in describing systems of solvated electrons in polarizable liquids, such as ammonia. In
such a context, however, the two-polaron interaction may require modification to take into account additional complexities which arise such as the formation of cavities in the liquid in the neighborhood of the electrons.
APPENDIX 1

Fröhlich's Hamiltonian may be straightforwardly extended to the case in which two electrons are present by adding the kinetic energy of the second electron, adding the Coulomb energy between electrons, and recognizing that the electric displacement is now due to two electrons:

\[ H = \frac{\gamma}{2} \int \left[ \nabla \cdot \mathbf{P}_{ir} (\mathbf{r}) + \omega^{2} \mathbf{P}_{ir} (\mathbf{r}) \right] d^{3} \mathbf{r} + \frac{\gamma}{2} \int \left[ \nabla \cdot \mathbf{P}_{o} (\mathbf{r}) + \omega_{o}^{2} \mathbf{P}_{o} (\mathbf{r}) \right] d^{3} \mathbf{r} 
- \int \mathbf{D} (\xi_{1}, \xi_{2}) \cdot \left[ \mathbf{P}_{ir} (\mathbf{r}) + \mathbf{P}_{o} (\mathbf{r}) \right] d^{3} \mathbf{r} 
+ \frac{1}{2} \mathbf{m}_{G} \mathbf{r}_{1}^{2} + \frac{1}{2} \mathbf{m}_{G} \mathbf{r}_{2}^{2} + \varepsilon^{2} |\xi_{1} - \xi_{2}|^{-1} \tag{A1.1} \]

The notation is that of Reference 1, except that the electron coordinates are now \( \xi_{1} \) and \( \xi_{2} \) and the high-frequency dielectric constant, called \( \varepsilon \) by Fröhlich, is now \( \varepsilon_{0} \). \( \mathbf{P}_{ir} (\mathbf{r}) \) is the low-frequency polarization field and \( \mathbf{P}_{o} (\mathbf{r}) \) is the high-frequency polarization field. In the presence of electrons 1 and 2, these fields satisfy the equations of motion

\[ \ddot{\mathbf{P}}_{ir} (\mathbf{r}) + \omega^{2} \mathbf{P}_{ir} (\mathbf{r}) = \mathbf{D} (\xi_{1}, \xi_{2}) / \gamma \tag{A1.2} \]

\[ \ddot{\mathbf{P}}_{o} (\mathbf{r}) + \omega_{o}^{2} \mathbf{P}_{o} (\mathbf{r}) = \mathbf{D} (\xi_{1}, \xi_{2}, \xi_{3}) / \delta \]
where \( \mathbf{D} \) is the electric displacement due to the two electrons and is given by

\[
\mathbf{D}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}) = -\frac{2}{\varepsilon_0} \left[ \frac{\varphi}{|\mathbf{r}_1-\mathbf{r}|} + \frac{\varphi}{|\mathbf{r}_2-\mathbf{r}|} \right]. \tag{A1.3}
\]

The parameters \( \gamma \) and \( \delta \) are given by

\[
\frac{1}{\gamma} = \frac{\omega_\pi^2}{\omega_0^2} \left( \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right) \tag{A1.4}
\]

\[
\frac{1}{\delta} = \frac{\omega_\pi^2}{\omega_0^2} \left( 1 - \frac{1}{\varepsilon_\infty} \right)
\]

where \( \omega_0 \) is the frequency at which \( \varepsilon_0 \) is measured. In the equations of motion (A1.2), \( \dot{\mathbf{P}}_o \) will be neglected in comparison with \( \omega_o^2 \mathbf{P}_o \), and therefore the term involving \( \dot{\mathbf{P}}_o \) will be omitted from Eq.(A1.1). Justification for this is given in Reference 1.

Consider the part of \( \mathbf{H}' \) which involves \( \mathbf{P}_o \):

\[
\mathbf{H}_{\mathbf{P}_o} = \int \left[ \frac{\delta \omega^2}{2} \mathbf{P}_o^2(\mathbf{r}) - \mathbf{D}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}) \cdot \mathbf{P}_o(\mathbf{r}) \right] d^3 \mathbf{r} \tag{A1.5}
\]

Equations (A1.3) and (A1.2), with \( \dot{\mathbf{P}}_o \) omitted, may be used to write this in the form

\[
\mathbf{H}_{\mathbf{P}_o} = -\frac{1}{2\delta \omega^2} \left\{ \text{self-energy terms} + 2 \varepsilon \int \left[ \frac{\partial^2}{\partial r^2} \left( |\mathbf{r}_1-\mathbf{r}_2|^2 \right) \right] d^3 \mathbf{r} \right\}
\]

\[
- |\mathbf{r}_1-\mathbf{r}_2|^2 \frac{\partial^2}{\partial \mathbf{r}_1^2} \left| \mathbf{r}_1-\mathbf{r}_2 \right|^2 \int d^3 \mathbf{r} \tag{A1.6}
\]
where $\partial^2 / \partial x^2$ is used to represent the Laplacian with respect to $x$.

The first integral is zero and the second may be evaluated to give

$$H_{P_o} = -\left(2\omega^2\right)^{-1} \int \frac{d^3 r}{(2\pi)^3} \phi^* \left(\frac{1}{k} + \frac{1}{\epsilon} \right) \phi \left(\frac{1}{k} - \frac{1}{\epsilon} \right).$$

The sum of $H_{P_o}$ and the Coulomb interaction energy is, if the self-energy terms are dropped,

$$\left[-\left(2\omega^2\right)^{-1} \frac{1}{\pi} + \frac{1}{\epsilon} \right] \phi^* \left(\frac{1}{k} - \frac{1}{\epsilon} \right) \phi = \epsilon^2 \phi^* \left(\frac{1}{k} - \frac{1}{\epsilon} \right) \phi$$

where Eq. (A1.4) was used to eliminate $\delta$. Equation (A1.8) may be used, along with the definitions

$$\mathcal{P}_{i, r}(\tau) = (\hbar / 2 \tau \omega) \frac{1}{2} \sum_y \frac{\nu}{\nu} \left[ b^+_y e^{-i\nu \cdot r} + b_y e^{i\nu \cdot r} \right]$$

and

$$\mathcal{P}_{i, r}(\tau) = (\hbar / 2 \tau \omega) \frac{1}{2} \sum_y \frac{\nu}{\nu} \left[ b^+_y e^{-i\nu \cdot r} - b_y e^{i\nu \cdot r} \right]$$

and the quantum correspondences

$$\mathcal{M}_p \frac{\partial}{\partial \tau} \rightarrow -i \hbar \frac{\partial}{\partial \tau} \quad \text{and} \quad \mathcal{M}_p \frac{\partial}{\partial \tau} \rightarrow -i \hbar \frac{\partial}{\partial \tau}$$

to write $H'$ in Eq. (A1.1) in the form given in Eq. (1.1).
The functions $E_1$ and $E_4$, defined by Eqs. (1.25) and (1.26), are not convenient for numerical work. Instead, with the aid of the following quantities:

$$F_1 = \frac{\xi(x)}{\xi(x/\alpha)} = \frac{\beta \gamma}{\gamma} \mathcal{E} \mathcal{H}^\gamma(x/\beta) ; \quad x^2 = \frac{\beta}{\gamma} \gamma^2$$

$$F_2 = \frac{\xi(x)}{\xi(x/\alpha)} = \frac{\beta \gamma}{\gamma} \mathcal{E} \mathcal{H}^\gamma(x) ; \quad \mathcal{E} = \sqrt{\frac{\beta}{\gamma}}$$

they may be written in the forms

$$E_1 = [3\beta + 2p \alpha \mathcal{E} F_2 \pm \mathcal{E}^{-2x^2} (3\beta - \rho x^2 + 2p \alpha \mathcal{E})] / (1 \pm \mathcal{E}^{-2x^2})$$

(A2.2)

and

$$E_4 = 2 \alpha \mathcal{E} \left[ 1 + F_2 \pm 2 \mathcal{E}^{-2x^2} \gamma \mathcal{E}^{-2x^2} F_1 / \mathcal{E} \mathcal{E}^{-2x^2} \right] / \mathcal{E}^{-2x^2} \mathcal{E}^{-2x^2} \mathcal{E}^{-2x^2}$$

(A2.3)

For small $x$, the above quantities, taken with positive signs, $E_1^+$ and $E_4^+$, are mathematically well behaved and may be calculated numerically from Eqs. (A2.2) and (A2.3) without modification. The corresponding quantities $E_1^-$ and $E_4^-$ are of the form $0/0$ for small $x$.
and are therefore not directly suitable for numerical calculation. To this end, the power series expressions for the error and exponential functions may be used and equal powers of $x$ divided out of numerator and denominator. The result of these operations is that $E_o(y, \beta)$ may be written

$$E_o(y, \beta) = \frac{\frac{2}{\gamma} S_1 + \frac{4}{\gamma} \sum_{k=2}^{n} \frac{k S_2 + S_3}{S_4}}{y}$$  \hspace{1cm} (A2.4)$$

where

$$S_1 = \sum_{j=0}^{\infty} \frac{x^{2 j}}{(2 j + 1) (2 j + 2) \lambda} \left[ \frac{(2 j + 5) 2^{j+2}}{(2 j + 2) \lambda} - 2(2 j + 3) \right] \right] / (j + 2)! \hspace{1cm} (A2.5)$$

$$S_2 = \sum_{j=0}^{\infty} \frac{x^{2 j} (-1)^{j} (2 j + 1) \lambda (2 j + 2) \lambda}{(2 j + 2) \lambda} \left[ \frac{b^{(2 j + 3) 2^{j+2}}}{(2 j + 2) \lambda} - b^{(2 j + 3) 2^{j+2}} \right] \right] / (j + 2)! \hspace{1cm} (A2.6)$$

$$S_3 = \sum_{j=0}^{\infty} \frac{x^{2 j} (-1)^{j} (2 j + 1) \lambda (2 j + 2) \lambda}{(2 j + 2) \lambda} \left[ \frac{b^{(2 j + 3) 2^{j+2} - 1}}{(2 j + 2) \lambda} - b^{(2 j + 3) 2^{j+2}} \right] \right] / (j + 2)! \hspace{1cm} (A2.7)$$

$$S_4 = \sum_{j=0}^{\infty} \frac{(-1)^{j} x^{2 j} (2 j + 2 - 2) \lambda}{(j + 2)!} \right] / (j + 2)! \hspace{1cm} (A2.8)$$
The coefficients \( b_0 \) and \( b_1 \) are defined by

\[
\begin{align*}
\sum_{k=0}^{j} \left[ \frac{(j-k)!}{k!} \left( \frac{2k+1}{2} \right)^{j-k} \right]^{-1} \quad (A2.9)
\end{align*}
\]

\[
\sum_{k=0}^{j} \left[ \frac{(j-k)!}{k!} \left( \frac{2k+1}{2} \right)^{j-k} \right]^{-1} \quad (A2.10)
\]

and appear in the expansions of

\[
\begin{align*}
\sum_{n=0}^{\infty} (-1)^n x^{2n+1} b_n 
\end{align*}
\]

and

\[
\begin{align*}
\sum_{n=0}^{\infty} (-1)^n x^{2n+1} b_n 
\end{align*}
\]

The coefficients \( b_0 \) and \( b_1 \) obey inequalities which are useful in proving the convergence of the series in Eqs. (A2.5)-(A2.8). Let

\[
\begin{align*}
\sum_{k=0}^{j} x^{2k+1} \left[ \frac{(n-k)!}{k! (2k+1)!} \right] \quad (A2.13)
\end{align*}
\]

Then

\[
\begin{align*}
b_{n} (1/2, 1) = b_n \quad j \quad f_n (1/2, 1) = b_n \quad (A2.14)
\end{align*}
\]
\[ \frac{\partial}{\partial x} \hat{f}_n (x, y) = \frac{1}{n!} \sum_{k=0}^{\infty} \frac{n!}{(n-k)!} \frac{z^k \cdot 2^{(n-k)}}{k!} = \left( \frac{x^2 + y^2}{\kappa^2} \right)^n \]  \hspace{1cm} (A2.15)

and so

\[ \hat{f}_n (x, y) = \frac{1}{n!} \int_0^\infty \left( \frac{z^2 + y^2}{\kappa^2} \right)^n \frac{d z}{z} \]  \hspace{1cm} (A2.16)

Thus

\[ b_n^0 = \frac{1}{n!} \int_0^1 \left( \frac{z^2 + 1}{\kappa^2} \right)^n \frac{d z}{z} \leq \frac{n}{\kappa^l} \]  \hspace{1cm} (A2.17)

\[ b_n^l = \frac{1}{n!} \int_0^{\frac{1}{2}} \left( \frac{z^2 + 1}{\kappa^2} \right)^n \frac{d z}{z} \leq \frac{2^{n-1}}{\kappa^l} \]  \hspace{1cm} (A2.18)
In this appendix it will be shown how the multi-dimensional integrals in Eqs. (3.9), (3.11), and (3.14) may be reduced to one-dimensional integrals.

A lemma will be useful. Let \( \rho \) be the radius of a sphere centered on point \( P \), let \( r \) be the radius of a sphere centered on point \( P' \), and let the distance between \( P \) and \( P' \) be \( q \). Let \( A(r, q, \rho) \) be the area of the \( \rho \)-sphere which is cut by and interior to the \( r \)-sphere, and let \( r+\rho > q > r-\rho \). Then

\[
A(r, q, \rho) = 2\pi \rho^2 \left[ q - \frac{q^2 + \rho^2 - r^2}{2\rho^2} \right]. \tag{A3.1}
\]

The first integral to be reduced is

\[
\mathcal{I}_1(q) = \int \mathcal{V}(p) A(k_F, q, \rho) \, dp. \tag{A3.2}
\]

The integral is over the volume of a sphere of radius \( k_F \).

Suppose \( q > k_F \). Then

\[
\mathcal{I}_1(q) = \int_{q - k_F}^{q + k_F} \mathcal{V}(p) A(k_F, q, \rho) \, dp
\]

\[
= \int_{q - k_F}^{q + k_F} \mathcal{V}(p) \frac{2\pi \rho^2}{2} \left[ q - \frac{q^2 + \rho^2 - k_F^2}{2\rho^2} \right]. \tag{A3.3}
\]
Introduce the notation  
\[ V_n \left| _a \right| = \int_a^l \rho \left( \theta \right) \rho ^n \] \tag{A3.4}

Then for \( q > k_F \),

\[ I_1 \left( q \right) = 2\pi \left[ V_2 \left| _{q-k_F} \right| + \left( \frac{k_F^2}{2} - \frac{a}{2} \right) V_1 \left| _{q-k_F} \right| - \frac{V_3}{2} \left| _{q-k_F} \right| \right] \] \tag{A3.5}

If \( q < k_F \), then by the same methods

\[ I_1 \left( q \right) = 2\pi \left[ V_2 \left| _{k_F-q} \right| + \left( \frac{k_F^2}{2} - \frac{a}{2} \right) V_1 \left| _{k_F-q} \right| - \frac{V_3}{2} \left| _{k_F-q} \right| \right] \] \tag{A3.6}

The second integral to be reduced is

\[ I_2 = \frac{1}{2} \int \int \phi \left( | r_1 - r_2 | \right) d^3 r_1 d^3 r_2 \] \tag{A3.7}

This represents the self-energy of a uniform spherical charge distribution in which \( \phi \left( r \right) \) is the potential energy at distance \( r \) from a unit charge. Let \( M\left( r \right) \) be the charge contained in a sphere of radius \( r \). The potential at the surface of the sphere is

\[ \Phi \left( r \right) = \frac{M\left( r \right)}{4 \pi r^3} \int \phi \left( \rho H_c \left( \rho \right) \right) d\rho \] \tag{A3.8}
where $A_c(p) \, d^3p = A(r, r, p) \, d\rho = 2 \pi p^2 \left[ \int_{p}^{\infty} \frac{1}{r^2} \, dr \right] \, d\rho$ is the element of volume. The work done in increasing the radius of the sphere from $r$ to $r+dr$ is $f(r) \, dM(r)$, so the total energy of the charge in a sphere of radius $R$ is

$$I_2 = \int_{R=0}^{R} \frac{f(r)}{r^2} \, dM(r). \quad (A3.9)$$

Since the charge is evenly distributed,

$$dM(r) = 4 \pi \rho^2 \, r^2 \, dr. \quad (A3.10)$$

where $\rho$ is the volume charge density. Substituting $A_c(p)$, Eq. (A3.8), and Eq. (A3.10) into Eq. (A3.9), one has

$$I_2 = 8 \pi^2 \rho^2 \int_{r=0}^{R} \left[ \int_{\rho=0}^{\rho} \varphi(\rho) \rho^2 \left( 1 - \frac{\rho}{2r} \right) \, d\rho \right] \rho^2 \, dr. \quad (A3.11)$$

With the substitution $2x = \rho$, the order of integrations may be interchanged to give

$$I_2 = 64 \pi^2 \rho^2 \int_{0}^{R} \frac{d^2x}{r^3} \varphi(2x) \left[ \frac{R^3}{3} - \frac{xR^2}{2} + \frac{x^3}{6} \right]. \quad (A3.12)$$

Equations (A3.12) and (A3.7) may be combined to give the result

$$\int \int_{r_2 < r_1^2} \varphi \left( (r_1^2 - r_2^2)^{1/2} \right) \, d^2r_1 \, d^2r_2 = 12 \pi^2 \int_{0}^{R} \frac{d^2x}{r^3} \varphi(2x) \left[ \frac{R^3}{3} - \frac{xR^2}{2} + \frac{x^3}{6} \right]. \quad (A3.13)$$
The last integral to be reduced is

\[ I_3 = \int d^2 r_2 \int d^3 \mathbf{r}_3 \phi (| \mathbf{r}_2 - \mathbf{r}_3 |) \]  

where the integral is over the volume of a spherical shell of interior radius \( r_a \) and exterior radius \( r_b \). By methods similar to those used in the reduction of \( I_2 \), one has

\[ I_3 = 4 \pi \int_{r_a}^{r_b} r^2 dr q(r) \]  

with

\[ q(r) = \int_{r_a}^{r} d \rho \phi (\rho) 2 \pi \rho^2 \left[ r - \frac{\rho^2 + r^2 - r^2}{2 r \rho} \right] + \int_{r}^{r_b} d \rho \phi (\rho) 2 \pi \rho^2 \left[ r - \frac{\rho^2 + r^2 - r^2}{2 r \rho} \right]. \]  

The first two integrals represent the contribution from the whole sphere of radius \( r_b \); the third is the contribution of the sphere of radius \( r_a \). The order of integrations may be interchanged and the notations

\[ \begin{bmatrix} r_n, r_j, b_j, v_3, r_4 \end{bmatrix} = \int_{r_2}^{r_1} d \rho \phi (\rho) \rho^2 \chi_b (\rho) \bigg|_{r_2}^{r_3} \]  

and
\[ x'_i(x) \bigg|_{r_{\theta}} = \int_{r_{\theta}}^{r_{\phi}} d\rho r^2 \left[ \rho^2 + \frac{r^2 - r_{\phi}^2}{2} \right] \quad (A3.18) \]

used to give

\[ I_3 = 8\pi \left\{ \left[ r_b - r_a, o; b, b, r_b, r_b - r_a \right] + \left[ r_b + r_a, r_a - r_a, b; b, r_b, r_b \right] \right\} + \frac{2}{3} \int_0^\infty \rho^2 \phi(x) [ (r_b - r_a)^3 - r_b^3 ] \quad (A3.19) \]

\[ \begin{cases} 
2 [ r_a, a; \rho + r_a, r_b ] + [ r_b - r_a, 2 r_a, a; r_b, \rho + r_a, \rho - r_a ] \\
[ r_b - r_a, o; a, a; r_b, r_b, \rho - r_a ] + [ r_b + r_a, r_b - r_a, a; r_b, \rho - r_a ] \quad \text{if} \quad r_b > 3 r_a \\
[ r_b - r_a, o; a, a; \rho + r_a, r_b ] + [ 2 r_a, r_b - r_a, a; r_b, r_b ] \quad \text{if} \quad r_b < 3 r_a 
\end{cases} \]
VITA

James Lloyd Edwards was born in Morgan City, Louisiana, on September 9, 1941. He attended Bolton High School, Alexandria, Louisiana. He received the degree of Bachelor of Science in physics from Louisiana State University in 1962. While a graduate student in physics at Louisiana State University, he was a National Defense Education Act Title IV Fellow and later served as instructor in the Department of Physics and Astronomy. During the summer of 1969 he was an Oak Ridge Associated Universities' Summer Research Participant in the Theory Section, Solid State Division, Oak Ridge National Laboratory and is at present Assistant Professor of Physics at East Tennessee State University.
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Candidate: James Lloyd Edwards

Major Field: Physics


Approved:

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Dean of the Graduate School

EXAMINING COMMITTEE:

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Date of Examination: 1/13/70