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Large polaron in bilocal field theory

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The formalism of bilocal field theory was applied to the calculation of the ground-state energy and the effective mass of the large polaron. This calculation illustrates the bilocal field method using a relatively realistic model of a physical system. In bilocal theory the fermion field is dependent on two spatial points (nonrelativistically). Fermi particles can then be described in terms of a center of mass and internal wave function, and field operators can be expanded in functions related to the exact one-fermion Green's function, thereby eliminating self-energy terms from the S matrix and related operators. Similarities and differences between calculated large-polaron properties using the bilocal treatment and the customary local treatment are discussed. In particular, it is found that, within the approximations made, the bilocal and local methods give the same leading term in powers of the coupling constant for the ground-state energy and effective mass in the strongcoupling limit. For weak coupling, the bilocal energy is larger (more positive) and the effective mass smaller than in the local case due to an additional kinetic energy of internal motion.

I. INTRODUCTION

The large-polaron problem¹ has been of importance both for its intrinsic interest and as a testing ground for new field-theoretic formalisms. In the present paper, our primary purpose will be to display the technique of bilocal field theory using the comparatively transparent polaron problem as a vehicle. In this respect, the paper should be regarded as a possible step toward the development of a finite relativistic field theory whose content is equivalent to that of local theory. Though useful here for its simplicity, the polaron problem is not ideally suited to the objective of illustrating this theory for several reasons. It is nonrelativistic and does not require renormalization or regularization procedures for dealing with divergences. More important, unlike "fundamental" field theories such as quantum electrodynamics, the "bare" polaron, i.e., the physical electron, exists as a valid entity independent of the physical polaron with its attendant phonon cloud. However, a suitable relativistic problem would be many times more complicated without adding to the understanding of the procedure. Because the bilocal formalism does not permit the existence of bare Fermi particles, our picture of the polaron will be somewhat different from the standard (within the order of approximation used), particularly for weak coupling. The procedures that will be described are straightforward, explicitly momentum conserving at every step, and intrinsically divergence free. While they lend themselves easily to the study of excited states, the inclusion of electromagnetic effects, and similar matters, only the ground-state energy and polaron effective mass will be considered here.

Much of the formalism that will be used has been described previously both in general terms² and by the detailed example of a bilocal Lee model.³ Briefly, in the present formulation the Bose fields are taken as local, but Fermi fields are assumed to depend on two space-time points; they are bilocal. The qualitative picture of the physical Fermi particle is the conventional one of a bare Fermi particle, described by one of the two coordinates, surrounded by its self-generated virtual boson cloud. Here, this cloud is assumed to have mass and to behave like a point particle, described by the second coordinate, with which the bare fermion interacts. These two components are assumed to be inseparable, so only bound states can exist permanently, and there are no bare Fermi particles in the usual sense. Before general calculations can be made in this theory, it is necessary to at least approximately solve the one-fermion problem. This can be done by relating the interaction between the bare fermion and its boson cloud to the irreducible self-energy components of the fermion. The result is a system of non-

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linear Hartree-like equations for the internal motion of the physical Fermi particle. In accordance with the construction, the Green's function for these equations is identical to the one-fermion Green's function of the exact bilocal field theory.² Using the solutions of these equations to expand the bilocal field operator, the S matrix will no longer contain any explicit fermion self-energy components but will now contain form factors related to the solutions of the one-fermion equations. These form factors will render S-matrix perturbation integrals finite for Yukawa and other simple polynominal interactions.⁴

The mass of the virtual boson cloud associated with the physical fermion can be defined in a consistent way in terms of the expectation value of the boson portion of the total momentum operator with respect to the physical one-fermion state function. An equivalent kinetic energy increment will appear in the ground-state energy of the physical fermion and must be subtracted out to prevent double counting.

In Sec. II, the procedures outlined above will be applied to the Fröhlich-Feynman polaron problem and equations derived for the ground-state energy and effective mass. The treatment will be in the Schrödinger picture as a matter of convenience. Superficially, the present work has similarities to the Green's function approach to the polaron problem of Matz and Burkey,⁵ and some procedures used by these authors and earlier by Gross⁶ will be used again here. However, the ideas on which the present work is based are fundamentally different from simply an application of Green's-function techniques to a local field theory, and similarities stem from the fact that the bilocal formalism can be viewed as a transformation of a Green's function usage into a consistent field theory in its own right.

The large and small electron-phonon coupling limits of the ground-state polaron equations obtained in Sec. II are discussed in the third section of this paper. While bounds on the ground-state energy and effective mass for strong coupling are the same here as found in other works,⁷ the weak-coupling limits are different due to a necessity for bound-state solutions in the present theory. This will be discussed in greater detail. In addition, numerical results for small to moderate coupling will be considered. Some summary remarks and a speculative discussion about further applications of bilocal field methods to other physical systems and about a number of as yet unstudied questions will be given in Sec. IV.

II. BILOCAL FORMALISM

In the notation that will be used, the local polaron Hamiltonian takes the form

$$H = \int d^{3}x \psi^{\dagger}(\mathbf{x}) \left[-\frac{\hbar^{2}}{2m_{0}} \nabla^{2} \right] \psi(\mathbf{x}) + \hbar\omega \int d^{3}k a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$$
$$+ i\hbar\omega \left[2\pi\sqrt{2} \left[\frac{\hbar}{m_{0}\omega} \right]^{1/2} \right]^{1/2} \frac{g}{(2\pi)^{3/2}}$$
$$\times \int d^{3}x \psi^{\dagger}(\mathbf{x}) \psi(\mathbf{x}) \int \frac{d^{3}k}{k} (a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}} - a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}) .$$
(1)

Here $\psi(\mathbf{x})$ is the operator for a spinless "electron" field obeying anticommutation relations

$$\{\psi(\mathbf{x}),\psi^{\dagger}(\mathbf{x}')\}=\delta(\mathbf{x}-\mathbf{x}'), \quad \{\psi(\mathbf{x}),\psi(\mathbf{x}')\}=0,$$

 $a_{\mathbf{k}}$ is an annihilation operator for a longitudinal optical phonon of momentum $\hbar \mathbf{k}$ and constant frequency ω obeying commutation relations

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta(\mathbf{k} - \mathbf{k}'), \ [a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0,$$

and g is related to the usual polaron coupling constant α by

$$g^{2} = \alpha = \frac{e^{2}}{2\hbar\omega} \left[\frac{\hbar}{2m_{0}\omega}\right]^{1/2} \left[\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_{0}}\right],$$

with ϵ_0 the static dielectric constant of the medium (our vacuum) and ϵ_{∞} the high-frequency dielectric constant. Hereafter, units which make

$$\hbar = 1, m_0 = 1, \omega = 1$$

will be used.

The corresponding bilocal Hamiltonian is obtained from Eq. (1) by the replacements

$$\psi(\mathbf{x}) \rightarrow F(\mathbf{x}, \mathbf{y}), \quad \int d^3x \rightarrow \int d^3x \int d^3y$$

and

$$\frac{1}{m_0}\nabla^2 \rightarrow \frac{1}{m_0}\nabla_x^2 + \frac{1}{M}\nabla_y^2$$

to give (in the "natural" units)

$$H = \int d^{3}x \int d^{3}y F^{\dagger}(\mathbf{x}, \mathbf{y}) \left[-\frac{1}{2m_{0}} \nabla_{x}^{2} - \frac{1}{2M} \nabla_{y}^{2} \right] F(\mathbf{x}, \mathbf{y})$$
$$+ \int d^{3}k a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + i(2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{3/2}} \int d^{3}x \int d^{3}y F^{\dagger}(\mathbf{x}, \mathbf{y}) F(\mathbf{x}, \mathbf{y}) \int \frac{d^{3}k}{k} (a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}} - a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}) , \qquad (2)$$

where the bilocal field operators obey the anticommunication relations

$$\{F(\mathbf{x},\mathbf{y}),F^{\dagger}(\mathbf{x}',\mathbf{y}')\} = \delta(\mathbf{x}-\mathbf{x}')\delta(\mathbf{y}-\mathbf{y}'),$$

$$\{F(\mathbf{x},\mathbf{y}),F(\mathbf{x}',\mathbf{y}')\} = 0.$$
 (3)

The x coordinate is that of the bare electron (fermion) which is the source of interaction with the phonon (boson) field; coordinate y can be regarded as that of the center of mass of the virtual phonon cloud surrounding the bare electron. Again, only the bare electron interacts with the phonon field here.⁸ Transforming to center-ofmass and relative coordinates in the bilocal variables, and adding and subtracting a nonlocal potential term to the Hamiltonian, Eq. (2) can be rewritten in two parts as follows:

$$\mathbf{R} = \alpha \mathbf{x} + \beta \mathbf{y}, \quad \mathbf{r} = \mathbf{x} - \mathbf{y} ,$$

$$\alpha = 1/\mathcal{M}, \quad \beta = \mathcal{M}/\mathcal{M}, \quad \mathcal{M} = 1 + \mathcal{M} ,$$
 (4)

and

$$H = H_0 + H_I$$

where

$$H_{0} = \int d^{3}R \int d^{3}r F^{\dagger}(\mathbf{R},\mathbf{r}) \left[-\frac{1}{2\mathcal{M}} \nabla_{R}^{2} - \frac{1}{2m_{r}} \nabla_{r}^{2} \right] F(\mathbf{R},\mathbf{r}) + \int d^{3}k a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \int d^{3}R \int d^{3}r \int d^{3}R' \int d^{3}r' F^{\dagger}(\mathbf{R},\mathbf{r}) \mathcal{V}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}') ,$$
(5)

and where

 $H_I = H_I^{(1)} + H_I^{(2)}$,

with

$$H_{I}^{(1)} = i(2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{3/2}} \\ \times \int d^{3}R \int d^{3}r F^{\dagger}(\mathbf{R},\mathbf{r})F(\mathbf{R},\mathbf{r}) \\ \times \int \frac{d^{3}k}{k} (a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{R}-i\beta\mathbf{k}\cdot\mathbf{r}} \\ -a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}+i\beta\mathbf{k}\cdot\mathbf{r}})$$
(6)

and

$$H_{I}^{(2)} = -\int d^{3}R \int d^{3}r \int d^{3}R' \times \int d^{3}r' F^{\dagger}(\mathbf{R},\mathbf{r})\mathcal{V}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}') .$$
(7)

In the present units, the reduced mass $m_r = m_0 M / (m_0 + M)$ is equal to β , but we will continue to use the explicit notation m_r .

Our objective will be to choose the potential operator $\mathcal{V}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}')$ in such a way that the one electron Green's function of the "unperturbed" Hamiltonian H_0 is the same as that of the full Hamiltonian H. In terms of Feynman diagrams, this can be done by taking \mathcal{V} so as to cancel appropriate irreducible self-energy terms generated by $H_I^{(1)}$, Eq. (6), when a perturbation solution of the single electron states of H is constructed. We begin by making an expansion of the operator $F(\mathbf{R},\mathbf{r})$ in terms of center of mass and internal wave functions of the electron portion of H_0 :

$$F(\mathbf{R},\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int d^3 P \sum_{\sigma} e^{i\mathbf{P}\cdot\mathbf{R}} \chi_{\sigma,\mathbf{P}}(\mathbf{r}) b_{\sigma,\mathbf{P}} , \qquad (8)$$

where $b_{\sigma,\mathbf{P}}$ is the annihilation operator for an electron in state $[1/(2\pi)^{3/2}]e^{i\mathbf{P}\cdot\mathbf{R}}\chi_{\sigma,\mathbf{P}}(\mathbf{r})$ and satisfies anticommutation relations

$$\{b_{\sigma,\mathbf{P}}, b_{\sigma',\mathbf{P}'}^{\dagger}\} = \delta_{\sigma,\sigma'} \delta(\mathbf{P} - \mathbf{P}'), \quad \{b_{\sigma,\mathbf{P}}, b_{\sigma,\mathbf{P}'}\} = 0.$$
(9)

The index σ represents the set of quantum numbers which characterizes the function $\chi_{\sigma,\mathbf{p}}(\mathbf{r})$ describing the motion of the bare electron relative to its virtual phonon cloud. Similarly, we will expand $\mathcal{V}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}')$ as

$$\mathcal{V}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}') = \frac{1}{(2\pi)^{3/2}} \int d^{3}P \sum_{\sigma} V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}')e^{i\mathbf{P}\cdot\mathbf{R}'} \times \chi_{\sigma,\mathbf{P}}(\mathbf{r}')b_{\sigma,\mathbf{P}} .$$
(10)

To explicitly illustrate the construction of the potentials $V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}')$ and the derivation of the equations for the functions $\chi_{\sigma,\mathbf{P}}(\mathbf{r})$, we will develop the perturbation solution of the one-electron states of the Hamiltonian *H*. For this purpose, we will write the Hamiltonian as

$$H = H_0 + \lambda H_I^{(1)} + \lambda^2 H_I^{(2)}$$
,

where $\lambda = 1$ will be used as an ordering parameter. The interaction $H_I^{(2)}$ should be regarded as a power series in λ^2 , but only the zero-power term will be used here. Proceeding in the standard manner, we write the state vector of H and its eigenvalue as

$$\Psi = \Psi_0 + \lambda \Psi_1 + \lambda^2 \Psi_2 + \cdot$$

and

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots$$

The Schrödinger equation $H\Psi = E\Psi$ then decomposes into the set of successive approximation equations

$$H_{0}\Psi_{0} = E_{0}\Psi_{0} ,$$

$$H_{0}\Psi_{1} + H_{I}^{(1)}\Psi_{0} = E_{0}\Psi_{1} + E_{1}\Psi_{0} ,$$

$$H_{0}\Psi_{2} + H_{I}^{(1)}\Psi_{1} + H_{I}^{(2)}\Psi_{0} = E_{0}\Psi_{2} + E_{1}\Psi_{1} + E_{2}\Psi_{2} ,$$
(11)

etc. Restriction to the one-electron problem is accomplished by setting

$$\Psi_0 = b_{\sigma,\mathbf{P}}^{\dagger} |0\rangle \equiv |\sigma,\mathbf{P}\rangle$$
,

where $|0\rangle$ is the electron-phonon vacuum state.

The factor $\mathcal{V}(\mathbf{R}, \mathbf{r} | \mathbf{R}', \mathbf{r})$ occurring in $H_I^{(2)}$ will be determined by the requirement that the zero-order energy be the exact energy of the one-electron problem:

$$E_0 = E, E_n = 0 (n > 0).$$

This is equivalent to the elimination of self-energy terms. Using the expansion, Eq. (8), for $F(\mathbf{R},\mathbf{r})$ and Eq. (10), the zeroth-order equation of the perturbation set can now be written as

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$$H_{0}|\sigma,\mathbf{P}\rangle = \int d^{3}r \sum_{\sigma'} \chi_{\sigma',\mathbf{P}}^{*}(\mathbf{r}) \left[\frac{\mathbf{P}^{2}}{2\mathcal{M}} - \frac{1}{2m_{r}} \nabla_{r}^{2} \right] \chi_{\sigma,\mathbf{P}}(\mathbf{r}) |\sigma',\mathbf{P}\rangle + \int d^{3}R \int d^{3}r \int d^{3}R' \int d^{3}r' \int d^{3}P' \sum_{\sigma'} \frac{e^{i\mathbf{P}\cdot\mathbf{R}}}{(2\pi)^{3/2}} \chi_{\sigma',\mathbf{P}'}^{*}(\mathbf{r}) V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R},\mathbf{r}') \times \frac{e^{i\mathbf{P}\cdot\mathbf{R}'}}{(2\pi)^{3/2}} \chi_{\sigma,\mathbf{P}}(\mathbf{r}') |\sigma',\mathbf{P}'\rangle = E_{\sigma,\mathbf{P}}|\sigma,\mathbf{P}\rangle .$$
(12)

Because Ψ_1 represents the state vector increment in which the interaction term $H_I^{(1)}$ has acted once, and Ψ_2 that for which $H_I^{(1)}$ has acted twice, these perturbation increments will take the respective forms

$$\Psi_{1} = \int d^{3}Q \sum_{\sigma' \neq \sigma} \mathcal{C}(\sigma', \mathbf{Q}; \sigma, \mathbf{P}) b_{\sigma', \mathbf{Q}}^{\dagger} | 0 \rangle + \frac{g}{(2\pi)^{3/2}} \int d^{3}Q \sum_{\sigma'} \int d^{3}k h(\sigma', \mathbf{Q}; \mathbf{k}) b_{\sigma', \mathbf{Q}}^{\dagger} a_{\mathbf{k}}^{\dagger} | 0 \rangle$$
(13)

and

$$\Psi_{2} = \int d^{3}Q \sum_{\sigma' \neq \sigma} \mathcal{C}^{(2)}(\sigma', \mathbf{Q}; \sigma, \mathbf{P}) b^{\dagger}_{\sigma', \mathbf{Q}} |0\rangle + \frac{g^{2}}{(2\pi)^{3}} \int d^{3}Q \sum_{\sigma'} \int d^{3}k h^{(2)}(\sigma', \mathbf{Q}; \mathbf{k}) b^{\dagger}_{\sigma'; \mathbf{Q}} a^{\dagger}_{\mathbf{k}} |0\rangle + \frac{g^{2}}{(2\pi)^{3}} \int d^{3}Q \sum_{\sigma'} \int d^{3}k \int d^{3}k' f^{(2)}(\sigma', \mathbf{Q}; \mathbf{k}, \mathbf{k}') b^{\dagger}_{\sigma', \mathbf{Q}} a^{\dagger}_{\mathbf{k}} a^{\dagger}_{\mathbf{k}'} |0\rangle .$$

$$(14)$$

Insertion of these expressions into the second and third equation of the sequence, Eq. (11), results in the following relations for the as yet unspecified coefficients of Ψ_1 and Ψ_2 . For simplicity, we assume no degeneracies of internal states, set to zero certain generally vanishing terms when made indeterminate due to an intermediate energy summing to zero, and usually suppress the index (σ, \mathbf{P}) of the eigenstate under consideration. Then (a) the matrix element of the first-order perturbation equation with state $|\sigma, \mathbf{P}\rangle$ gives

 $E_1 = 0$,

and equating coefficients of the like states in this equation gives

$$\mathscr{C}(\sigma',\mathbf{Q};\sigma,\mathbf{P})=0$$

and

$$h(\sigma',\mathbf{Q};\mathbf{k}) = \frac{-i(2\pi\sqrt{2})^{1/2}}{(E_{\sigma',\mathbf{Q}} - E_{\sigma,\mathbf{P}} + \hbar\omega)} \times \frac{1}{k} \delta(\mathbf{Q} - \mathbf{P} + \mathbf{k}) d(\sigma',\mathbf{Q};\sigma,\mathbf{P};\mathbf{k}) , \quad (15)$$

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where

$$d(\sigma',\mathbf{Q};\sigma,\mathbf{P};\mathbf{k}) \equiv \int d^{3}r e^{-i\beta\mathbf{k}\cdot\mathbf{r}} \chi^{*}_{\sigma',\mathbf{Q}}(\mathbf{r})\chi_{\sigma,\mathbf{P}}(\mathbf{r}) ; \quad (16)$$

(b) similarly, from the second-order perturbation equation we obtain

$$E_{2} = \frac{1}{(2\pi)^{3}} \int d^{3}R \int d^{3}r \int d^{3}r' e^{-i\mathbf{P}\cdot\mathbf{R}} \chi^{*}_{\sigma,\mathbf{P}}(\mathbf{r}) \left[-2\pi\sqrt{2} \frac{g^{2}}{(2\pi)^{6}} \sum_{\sigma'} \int d^{3}Q \int \frac{d^{3}k}{k^{2}} e^{i\mathbf{R}\cdot(\mathbf{Q}+\mathbf{k})} \chi_{\sigma',\mathbf{Q}}(\mathbf{r}) \right] \\ \times e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} e^{-i\mathbf{R}'\cdot(\mathbf{Q}+\mathbf{k})} \frac{1}{E_{\sigma',\mathbf{Q}} - E_{\sigma,\mathbf{P}} + \hbar\omega} \chi^{*}_{\sigma',\mathbf{Q}}(\mathbf{r}') \\ - V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}') e^{i\mathbf{P}\cdot\mathbf{R}'} \chi_{\sigma,\mathbf{P}}(\mathbf{r}')$$
(17)

and

$$\mathcal{C}^{(2)}(\sigma',\mathbf{Q};\sigma,\mathbf{P})=0,$$

$$h^{(2)}(\sigma',\mathbf{Q};\mathbf{k})=0,$$

$$f^{(2)}(\sigma',\mathbf{Q};\mathbf{k},\mathbf{k}')=\frac{2\pi\sqrt{2}}{(E_{\sigma',\mathbf{Q}}-E_{\sigma,\mathbf{P}}+2\hbar\omega)}\frac{1}{k^{2}}\delta(\mathbf{Q}+\mathbf{k}+\mathbf{k}'-\mathbf{P})$$

$$\times\sum_{\sigma_{1}}\frac{1}{(E_{\sigma_{1},\mathbf{Q}+\mathbf{k}}-E_{\sigma,\mathbf{P}}+\hbar\omega)}d(\sigma',\mathbf{Q};\sigma_{1},\mathbf{Q}+\mathbf{k};\mathbf{k})d(\sigma_{1},\mathbf{Q}+\mathbf{k};\sigma,\mathbf{P};\mathbf{k}').$$
(18)

To make perturbation energy E_2 vanish, we set

$$V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}') = -2\pi\sqrt{2}\frac{g^2}{(2\pi)^6}\sum_{\sigma'}\int d^3Q\int \frac{d^3k}{k^2}e^{i\mathbf{R}\cdot(\mathbf{Q}+\mathbf{k})}\chi_{\sigma',\mathbf{Q}}(\mathbf{r})\frac{1}{E_{\sigma',\mathbf{Q}}-E_{\sigma,\mathbf{P}}+\hbar\omega}e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\chi_{\sigma',\mathbf{Q}}^*(\mathbf{r}')e^{-i\mathbf{k}\cdot(\mathbf{Q}+\mathbf{k})}.$$
(10)

In terms of Feynman diagrams, what has been done is to cancel the second-order self-energy term with a component of $H_I^{(2)}$ thereby defining $V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}')$ to order g^2 . This is shown diagramatically in Fig. 1. Rules for constructing higher-order components of $V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r},|\mathbf{R}',\mathbf{r}')$ from appropriate irreducible self-energy diagrams are given in the Appendix.

Inserting the potential, Eq. (19), into Eq. (12) for $H_0|\sigma, \mathbf{P}\rangle$ and carrying out the $\int d^3R$ and $\int d^3R'$ integrals gives, to order g^2 ,

$$H_{0}|\sigma,\mathbf{P}\rangle = \int d^{3}r \sum_{\sigma'} \chi_{\sigma',\mathbf{P}}^{*}(\mathbf{r}) \left[\left[\frac{\mathbf{P}^{2}}{2\mathcal{M}} - \frac{1}{2m_{r}} \nabla_{r}^{2} \right] \chi_{\sigma,\mathbf{P}}(\mathbf{r}) - 2\pi\sqrt{2} \frac{g^{2}}{(2\pi)^{3}} \int d^{3}r' \sum_{\sigma_{1}} \int \frac{d^{3}k}{k^{2}} \frac{e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{E_{\sigma_{1},\mathbf{P}-\mathbf{k}} - E_{\sigma,\mathbf{P}} + \hbar\omega} \chi_{\sigma_{1},\mathbf{P}-\mathbf{k}}(\mathbf{r}) + \chi_{\sigma_{1},\mathbf{P}-\mathbf{k}}^{*}(\mathbf{r}') \chi_{\sigma,\mathbf{P}}(\mathbf{r}') \right] |\sigma',\mathbf{P}\rangle = E_{\sigma,\mathbf{P}}|\sigma,\mathbf{P}\rangle .$$

$$(20)$$

The off-diagonal matrix elements of H_0 are $\langle \sigma', \mathbf{Q} | H_0 | \sigma, \mathbf{P} \rangle$

$$=\delta(\mathbf{Q}-\mathbf{P})\int d^{3}r \chi_{\sigma',\mathbf{P}}^{*}(\mathbf{r}) \left[\left[\frac{\mathbf{P}^{2}}{2\mathcal{M}} - \frac{1}{2m_{r}} \nabla_{r}^{2} \right] \chi_{\sigma,\mathbf{P}}(\mathbf{r}) -2\pi\sqrt{2} \frac{g^{2}}{(2\pi)^{3}} \int d^{3}r' \sum_{\sigma_{1}} \int \frac{d^{3}k}{k^{2}} \frac{e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{E_{\sigma_{1},\mathbf{P}-\mathbf{k}} - E_{\sigma,\mathbf{P}} + \hbar\omega} \times \chi_{\sigma_{1},\mathbf{P}-\mathbf{k}}(\mathbf{r}) \chi_{\sigma_{1},\mathbf{P}-\mathbf{k}}^{*}(\mathbf{r}') \chi_{\sigma,\mathbf{P}}(\mathbf{r}') \right], \quad \sigma' \neq \sigma .$$
(21)

In order that the right-hand side of this relation be zero and be consistent with the diagonal matrix elements as well as with the orthonormality of the internal wave functions $\chi_{\sigma,\mathbf{P}}(\mathbf{r})$ required for the original expansion of the field operator $F(\mathbf{R},\mathbf{r})$, it is necessary that the equation for $\chi_{\sigma,\mathbf{P}}(\mathbf{r})$ be

$$\left[\frac{\mathbf{p}^{2}}{2\mathcal{M}}-\frac{1}{2m_{r}}\nabla_{r}^{2}\right]\chi_{\sigma,\mathbf{P}}(\mathbf{r})-2\pi\sqrt{2}\frac{g^{2}}{(2\pi)^{3}}\int d^{3}r'\sum_{\sigma'}\int \frac{d^{3}k}{k^{2}}\frac{e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{E_{\sigma',\mathbf{P}-\mathbf{k}}-E_{\sigma,\mathbf{P}}+\hbar\omega}\chi_{\sigma',\mathbf{P}-\mathbf{k}}(\mathbf{r})\chi_{\sigma',\mathbf{P}-\mathbf{k}}^{*}(\mathbf{r}')\chi_{\sigma,\mathbf{P}}(\mathbf{r}')$$

$$=E_{\sigma,\mathbf{P}}\chi_{\sigma,\mathbf{P}}(\mathbf{r}) . \quad (22)$$

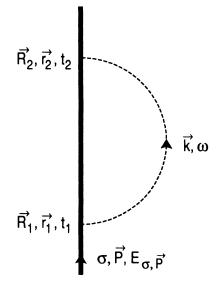


FIG. 1. Second-order polaron self-energy diagram used to obtain the internal state polaron potential considered in this paper. The dashed line represents a virtual longitudinal phonon and the heavy solid line represents a physical polaron.

Equation (22) represents a doubly infinite system of coupled eigenvalue equations enumerated by the internal quantum numbers σ and the polaron momentum **P**. Since only the order g^2 self-energy potential has been used in Eq. (22), it is the lowest-order equation set and corresponds to the approximation often employed for the polaron ground state. To make the equation for internal wave functions more tractable, the following approximations will be made: (a) the internal wave functions will be assumed to be independent of the total momentum,

$$\chi_{\sigma,\mathbf{P}}(\mathbf{r}) \longrightarrow \chi_{\sigma}(\mathbf{r}) ; \qquad (23a)$$

(b) the polaron energy will be assumed to be the sum of an internal energy and the center-of-mass kinetic energy,

$$E_{\sigma,\mathbf{p}} \simeq E_{\sigma} + \frac{\mathbf{P}^2}{2\mathcal{M}} \ . \tag{23b}$$

If we were to now let M go to infinity in the resultant equation, we would obtain the local Green's-functionrelated equation used by Matz and Burkey⁵ in their polaron study, except for the units employed. However, with the approximations of Eqs. (23a) and (23b), it is possible to carry out the $d^{3}k$ integration for a polaron of zero momentum, $\mathbf{P}=0$, giving MARVIN RICH

$$-\frac{1}{2m_{r}}\nabla_{r}^{2}\chi_{\sigma}(\mathbf{r})-2\pi\sqrt{2}\frac{g^{2}}{(2\pi)^{3}}\int d^{3}r'\sum_{\sigma'}\frac{2\pi^{2}}{\beta(E_{\sigma'}-E_{\sigma}+\hbar\omega)}\frac{1}{|\mathbf{r}-\mathbf{r}'|}(1-\exp\{-\beta|\mathbf{r}-\mathbf{r}'|[2\mathcal{M}(E_{\sigma'}-E_{\sigma}+\hbar\omega)]^{1/2}\})\times\chi_{\sigma'}(\mathbf{r})\chi_{\sigma'}(\mathbf{r}')\chi_{\sigma}(\mathbf{r}')=E_{\sigma}\chi_{\sigma}(\mathbf{r}).$$
(24)

In terms of Eq. (24), the Matz and Burkey⁵ equation again corresponds to letting $M \to \infty$ which replaces β by 1 and deletes the exponential term within the bold parentheses. Compared to the Matz and Burkey work, Eq. (24) tends to underestimate the potential and the value of $|E_{\sigma}|$, despite the factor of β in the denominator. If only the ground-state term is retained in the σ' sum of Eq. (24) and this is assumed to be an *s* state, so

$$\chi_0(\mathbf{r}) = \frac{1}{\sqrt{4\pi}} \frac{\psi(\mathbf{r})}{r} ,$$

we obtain a numerically tractible equation for $\psi(r)$, which might be expected to apply when $g^2 < 1$:

$$-\frac{1}{2m_{r}}\frac{d^{2}}{dr^{2}}\psi(r)-2\pi\sqrt{2}\frac{g^{2}}{(2\pi)^{3}}\frac{\pi^{2}}{\beta}\frac{\psi(r)}{r}\int_{0}^{\infty}dr'\frac{|\psi(r')|^{2}}{r'}\left[(r+r')-|r-r'|+\frac{1}{\beta\sqrt{2M}}(e^{-\beta\sqrt{2M}(r+r')}-e^{-\beta\sqrt{2M}|r-r'|})\right]=E_{0}\psi(r). \quad (25)$$

Before a solution of the equations for $\chi_0(\mathbf{r})$ and E_0 can be found (except in the limiting case $M \to \infty$), it is necessary to obtain an expression for the mass M of the phonon cloud associated with the bare electron. This can be done by considering the total momentum operator

$$\mathbf{P}_{op} = \mathbf{P}_{f} + \mathbf{P}_{b} ,$$

$$\mathbf{P}_{f} \equiv \int d^{3}R \int d^{3}r F^{\dagger}(\mathbf{R}, \mathbf{r}) \frac{1}{i} \nabla_{R} F(\mathbf{R}, \mathbf{r}) .$$
 (26)

$$\mathbf{P}_{b} \equiv \int d^{3}k \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$$

The first term \mathbf{P}_f corresponds to the momentum of the "bare" polaron, and contains no explicit information about the virtual phonons which form part of the physical polaron. The term \mathbf{P}_b provides the latter information as well as information about free phonons. Because the present formalism conserves momentum explicitly, one has for the bare polaron and the physical polaron, respectively,

$$\langle \sigma, \mathbf{P} | \mathbf{P}_f | \sigma, \mathbf{P} \rangle / \langle \sigma, \mathbf{P} | \sigma, \mathbf{P} \rangle = \mathbf{P}$$

and

$$\langle \Psi(\sigma,\mathbf{P})|\mathbf{P}_{op}|\Psi(\sigma,\mathbf{P})\rangle/\langle \Psi(\sigma,\mathbf{P})|\Psi(\sigma,\mathbf{P})\rangle = \mathbf{P}$$
.

In terms of the perturbative expansion of the state function, the expectation value of the momentum operator is

$$\begin{split} \langle \Psi(\sigma,\mathbf{P}) | \mathbf{P}_{op} | \Psi(\sigma,\mathbf{P}) \rangle \\ &= \langle \Psi_0(\sigma,\mathbf{P}) | \mathbf{P}_{op} | \Psi_0(\sigma,\mathbf{P}) \rangle \\ &+ \lambda^2 \langle \Psi_1(\sigma,\mathbf{P}) | \mathbf{P}_{op} | \Psi_1(\sigma,\mathbf{P}) \rangle + \cdots , \end{split}$$

with a similar expansion for $\langle \Psi(\sigma, \mathbf{P}) | \Psi(\sigma, \mathbf{P}) \rangle$. Confining the discussion to the ground state $\sigma = 0$, and making use of the explicit form of Ψ_1 , Eq. (13), in conjunction with Eqs. (15) and (16) we have to second order

$$\langle \Psi(0,\mathbf{P})|\mathbf{P}_{f}|\Psi(0,\mathbf{P})\rangle = \mathbf{P}\langle 0,\mathbf{P}|0,\mathbf{P}\rangle + \frac{g^{2}}{(2\pi)^{3}}\int d^{3}Q\sum_{\sigma'}\int d^{3}k(\mathbf{P}-\mathbf{k})|h(\sigma',\mathbf{Q},\mathbf{k})|^{2},$$
(27)

$$\langle \Psi(0,\mathbf{P})|\mathbf{P}_{b}|\Psi(0,\mathbf{P})\rangle = \frac{g^{2}}{(2\pi)^{3}} \int d^{3}Q \sum_{\sigma'} \int d^{3}k \,\mathbf{k} |h(\sigma',\mathbf{Q};\mathbf{k})|^{2} , \quad (28)$$

and

$$\langle \Psi(0,\mathbf{P}) | \Psi(0,\mathbf{P}) \rangle$$

$$= \langle 0, \mathbf{P} | 0, \mathbf{P} \rangle + \frac{g^2}{(2\pi)^3} \int d^3 Q \sum_{\sigma'} \int d^3 k |h(\sigma', \mathbf{Q}; \mathbf{k})|^2 , \qquad (29)$$

where, within the present approximations,

$$h(\sigma',\mathbf{Q};\mathbf{k}) = \frac{-i(2\pi\sqrt{2})^{1/2}}{E_{\sigma'} - E_0 + \mathbf{k}^2/2\mathcal{M} - \mathbf{k}\cdot\mathbf{P}/\mathcal{M} + \hbar\omega} \times \frac{1}{k}\delta(\mathbf{Q} - \mathbf{P} + \mathbf{k})\int d^3r \ e^{-i\beta\mathbf{k}\cdot\mathbf{r}}\chi_{\sigma'}(\mathbf{r})\chi_0(\mathbf{r}) \ .$$

The velocity v of a freely moving polaron of momentum **P** and mass \mathcal{M} is defined by the relation $\mathcal{M}v = P$. The portion of the total polaron momentum provided by its virtual phonon cloud will be the expectation value of the boson part of the total momentum operator, Eq. (26). Therefore we will define the mass \mathcal{M} by the relation⁹

$$M\mathbf{v} = \lim_{\mathbf{P} \to 0} \langle \Psi(0, \mathbf{P}) | \mathbf{P}_b | \Psi(0, \mathbf{P}) \rangle / \langle 0, \mathbf{P} | 0, \mathbf{P} \rangle .$$
(30)

This expectation value can be simplified for small momenta **P** by expanding the energy denominator of $|h(\sigma', \mathbf{Q}; \mathbf{k})|^2$ in powers of $(\mathbf{k} \cdot \mathbf{P})/\mathcal{M}$. Since there is no preferred spatial direction for the total momentum, its magnitude will be independent of direction. Therefore,

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taking the scalar product of Eq. (30) with \mathbf{P} and averaging over direction gives, to lowest order in $|\mathbf{P}|$,

$$M = \frac{2}{3} \frac{g^2}{(2\pi)^3} 2\pi \sqrt{2} \sum_{\sigma'} \int d^3k \frac{|d(\sigma', \mathbf{k})|^2}{(E_{\sigma'} - E_0 + k^2/2\mathcal{M} + \hbar\omega)^3} ,$$
(31)

where now, in approximation,

$$d(\sigma',\mathbf{k}) \equiv d(\sigma',-\mathbf{k};\mathbf{0},\mathbf{0};\mathbf{k})$$

= $\int d^3 r e^{-i\beta\mathbf{k}\cdot\mathbf{r}} \chi_{\sigma'}^*(\mathbf{r})\chi_0(\mathbf{r})$.

If we let $M \rightarrow \infty$ on the right-hand side of Eq. (31) and limit the σ' sum to the ground-state term $\sigma'=0$, we obtain

$$M \cong \frac{2}{3} \frac{g^2}{(2\pi)^3} 2\pi \sqrt{2} \int d^3k \frac{|d(0,\mathbf{k})|^2}{(\hbar\omega)^3}$$

which is the polaron mass increment approximation obtained by Gross^{10} and by Bolsterli^{11} and which was used by Matz and Burkey.⁵ If, instead, we carry out the d^3k integration in Eq. (31) we get

$$M = \frac{2}{3} \frac{g^2}{(2\pi)^3} \frac{\pi^3 \sqrt{2}}{2} (2\mathcal{M})^{3/2} \sum_{\sigma'} \frac{1}{(E_{\sigma'} - E_0 + \hbar\omega)^3} \int d^3 r \chi_0^*(\mathbf{r}) \chi_{\sigma'}(\mathbf{r}) \times \int d^3 r' \chi_{\sigma'}^*(\mathbf{r}') \chi_0(\mathbf{r}') \{1 + \beta | \mathbf{r} - \mathbf{r}' | [2\mathcal{M}(E_{\sigma'} - E_0 + \hbar\omega)]^{1/2} \} \times \exp\{-\beta |\mathbf{r} - \mathbf{r}| [2\mathcal{M}(E_{\sigma'} - E_0 + \hbar\omega)]^{1/2} \}.$$
(32)

As with Eq. (25), if we assume $\chi_0(\mathbf{r})$ to be an s state so $\chi_0(\mathbf{r}) = (1/\sqrt{4\pi})\psi(\mathbf{r})/r$ and keep only the first term $\sigma' = 0$ in the σ' sum, we can carry out the integrations over the angular parts of \mathbf{r} and \mathbf{r}' giving

$$M = \frac{g^2}{24} \frac{\sqrt{2}}{2} (2\mathcal{M})^{3/2} \int_0^\infty dr |\psi(r)|^2 \int_0^\infty dr' |\psi(r')|^2 \frac{1}{2\mathcal{M}\beta^2 rr'} \times \{ (2\mathcal{M}\beta^2 |r-r'|^2 + 3\beta\sqrt{2\mathcal{M}} |r-r'| + 3)e^{-\beta\sqrt{2\mathcal{M}} |r-r'|} - [2\mathcal{M}\beta^2 (r+r')^2 + 3\beta\sqrt{2\mathcal{M}} (r+r') + 3]e^{-\beta\sqrt{2\mathcal{M}} (r+r')} \} .$$
(33)

The equations for the ground-state quantities E_0 and $\chi_0(\mathbf{r})$ and for the mass increment M are highly nonlinear both in the explicit multiplicity of the appearance of χ_0 and indirectly through the mass M. In general, the equations must be solved numerically by iteration. There is the added complication of the need for knowledge of the entire excitation spectrum for proper characterization of the ground state.

Returning to the ground-state energy, within the present approximations we have from Eq. (22)

$$E_{0,\mathbf{P}} = \int d^{3}r \,\chi_{0}^{*}(\mathbf{r}) \left[\frac{\mathbf{P}^{2}}{2\mathcal{M}} - \frac{1}{2m_{r}} \nabla_{r}^{2} \right] \chi_{0}(\mathbf{r}) \\ -2\pi\sqrt{2} \frac{g^{2}}{(2\pi)^{3}} \int d^{3}r \,\chi_{0}^{*}(\mathbf{r}) \int d^{3}r' \chi_{0}(\mathbf{r}') \sum_{\sigma'} \int \frac{d^{3}k}{k^{2}} \chi_{\sigma'}(\mathbf{r}) \chi_{\sigma'}^{*}(\mathbf{r}') \frac{e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{E_{\sigma'} - E_{0} + \mathbf{k}^{2}/2\mathcal{M} - \mathbf{k}\cdot\mathbf{P}/\mathcal{M} + \hbar\omega} .$$
(34)

If we expand the energy denominator of Eq. (34) in powers of $(\mathbf{k} \cdot \mathbf{P}) / \mathcal{M}$ and proceed in a manner similar to that leading to Eq. (31), we obtain an energy increment to lowest order in the momentum of

$$-2\pi\sqrt{2}\frac{g^2}{(2\pi)^3}\frac{\mathbf{P}^2}{3\mathcal{M}^2}\int d^3r \int d^3r' \sum_{\sigma'}\int d^3k \frac{e^{i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{(E_{\sigma'}-E_0+k^2/2\mathcal{M}+\hbar\omega)^3}\chi_0^*(\mathbf{r})\chi_{\sigma'}(\mathbf{r})\chi_{\sigma'}^*(\mathbf{r}')\chi_0(\mathbf{r}') \ .$$

Referring to Eq. (31), this is just $-M\mathbf{P}^2/2\mathcal{M}^2$. If this were added to the term $\mathbf{P}^2/2\mathcal{M}$ on the right-hand side of Eq. (34), and it were assumed that the total kinetic energy should have the form $\mathbf{P}^2/2(\mathcal{M} + \Delta)$, then making the formal expansion

$$\frac{\mathbf{P}^2}{2(\mathcal{M}+\Delta)} = \frac{\mathbf{P}^2}{2\mathcal{M}} - \frac{\Delta \mathbf{P}^2}{2\mathcal{M}^2} + \cdots$$

leads to the identification $\Delta = M$. However, the total mass $\mathcal{M} = m_0 + M$ already includes the phonon mass increment M because the original Hamiltonian was so formulated that the physical or "renormalized" polaron mass was employed from the beginning. Therefore it is

necessary that the redundant appearance of mass M be subtracted from the energy to prevent multiple counting of mass increments and inconsistency with the total momentum. Here and in the following, these redundant mass increments will just be ignored. The redundancy can be eliminated formally by adding a term

$$H_{M} \equiv \mathcal{P} \frac{M}{2\mathcal{M}^{2}} \int d^{3}R \int d^{3}r F^{\dagger}(\mathbf{R},\mathbf{r}) \nabla_{R}^{2} F(\mathbf{R},\mathbf{r})$$
(35)

to the zero-order Hamiltonian, Eq. (5), where \mathcal{P} is the no boson projection operator

$$\mathcal{P} \equiv \Theta \left[1 - \epsilon - \int d^3 k \ a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \right], \quad \epsilon = 0 +$$

with $\Theta(x)$ the step function

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases}$$

III. DISCUSSION AND RESULTS

A. Small-coupling limit

The present theory does not have a perturbation limit in the usual sense. If the bilocal polaron problem under consideration were viewed as a fundamental field theory rather than as a model for a physical electron in interaction with a polar medium, it would be essential that the equation for the ground-state internal wave function have a stable bound solution. Otherwise the virtual boson cloud surrounding the bare fermion could escape to infinity. This would not be acceptable physically. If there were no bound solution, one would have to conclude that the field particle in question cannot exist freely, and barring the existence of some other stable entity associated with this field, that the field theory itself would not be physically valid. It will be shown numerically that Eq. (25) continues to have bound ground-state solutions for the polaron ground state as the coupling constant approaches zero. Therefore the interaction potential corresponding to the self-energy diagram of Fig. 1 will be iterated an infinite number of times in producing the ground-state energy of the bilocal polaron. There is also a non-negligible positive kinetic energy contribution due to the relative motion of the electron and its virtual phonon cloud. Both iteration of the interaction potential and the kinetic energy affect the spatial extension of the polaron wave function which, in turn, acts to modify the interaction potential.

Despite the qualifications implied above, it is possible to obtain the leading terms for the expansions of the polaron ground-state interaction energy and effective mass increment in powers of g^2 in the weak-coupling limit. In Eq. (32) and Eq. (36) below,

$$E_{0} = -\frac{1}{2m_{r}} \int d^{3}r \, \chi_{0}^{*}(\mathbf{r}) \nabla_{r}^{2} \chi_{0}(\mathbf{r}) -2\pi \sqrt{2} \frac{g^{2}}{(2\pi)^{3}} \frac{2\pi^{2}}{\beta} \sum_{\sigma'} \frac{1}{(E_{\sigma'} - E_{0} + 1)} \int d^{3}r \, \chi_{0}^{*}(\mathbf{r}) \chi_{\sigma'}(\mathbf{r}) \int d^{3}r' \chi_{\sigma'}^{*}(\mathbf{r}') \chi_{0}(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \times (1 - \exp\{-\beta |\mathbf{r} - \mathbf{r}'| [2\mathcal{M}(E_{\sigma'} - E_{0} + 1)]^{1/2}\}), \quad (36)$$

all powers of the coupling g^2 are present implicitly in the internal wave functions $\chi_{\sigma}(\mathbf{r})$, the energies E_{σ} , and the mass ratio $\beta = M/(m_0 + M)$ occurring in the intergrands. If Taylor expansions of the exponentials in these integrands are made, ignoring the validity of such expansions, one obtains

$$M = \frac{2}{3} \frac{g^2}{(2\pi)^3} \frac{\pi^3 \sqrt{2}}{2} (2\mathcal{M})^{3/2}$$

$$\times \sum_{\sigma'} \frac{1}{(E_{\sigma'} - E_0 + 1)^3} \int d^3 r \, \chi_0^*(\mathbf{r}) \chi_{\sigma'}(\mathbf{r}) \int d^3 \mathbf{r}' \chi_{\sigma'}^*(\mathbf{r}') \chi_0(\mathbf{r}) [1 - \beta^2 (\mathbf{r} - \mathbf{r}')^2 \mathcal{M}(E_{\sigma'} - E_0 + 1) + \cdots]$$

and

$$E_{0} = -\frac{1}{2m_{r}} \int d^{3}r \, \chi_{0}^{*}(\mathbf{r}) \nabla_{r}^{2} \chi_{0}(\mathbf{r})$$

$$-2\pi \sqrt{2} \frac{g^{2}}{(2\pi)^{3}} \frac{2\pi^{2}}{\beta} \sum_{\sigma'} \frac{1}{(E_{\sigma'} - E_{0} + 1)} \int d^{3}r \, \chi_{0}^{*}(\mathbf{r}) \chi_{\sigma'}(\mathbf{r}) \int d^{3}r' \chi_{\sigma'}^{*}(\mathbf{r}') \chi_{0}(\mathbf{r}) \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

$$\times \{\beta |\mathbf{r} - \mathbf{r}'| [2\mathcal{M}(E_{\sigma'} - E_{0} + 1)]^{1/2}$$

$$-\beta^{2} |\mathbf{r} - \mathbf{r}'|^{2} \mathcal{M}(E_{\sigma'} - E_{0} + 1) \cdots \}.$$

Using the orthonormality for the internal wave functions and the fact that for $g^2 \ll 1$ $\mathcal{M} = 1 + \mathcal{M} \cong 1$ then gives

$$M=\frac{g^2}{6}+\cdots$$

and

$$E_0 = -\frac{1}{2m_r} \int d^3r \, \chi_0^*(\mathbf{r}) \nabla_r^2 \chi_0(\mathbf{r}) - (g^2 + \cdots) \, .$$

Though the leading terms for M and the potential part

of E_0 obtained above have the usual weak-coupling values¹ found in the perturbative treatment of the local theory, what has been done is, in fact, misleading. This is because the root-mean-square radii $r_{\rm rms} \equiv (\langle r^2 \rangle_0)^{1/2}$ of the ground-state internal wave functions of the bilocal theory increase in such a manner that the quantity $\beta r_{\rm rms}$ remains large and approximately constant as g^2 goes to zero. Therefore expansion of the exponentials is not permissible. This behavior is due to the internal kinetic energy, absent in the local theory. Only by going to the local

cal field-theoretic limit in which excited internal states are omitted and the ground-state internal wave function collapsed to a point at the origin

$$\chi_0(\mathbf{r}) \rightarrow \sqrt{\delta(\mathbf{r})}$$

do we validly obtain the small coupling interaction energy and mass increment. However, in going to the local field limit of the bilocal formalism, it is necessary to disregard an infinite internal kinetic energy that arises.

B. Strong-coupling limit

We obtain the standard results for the leading term in powers of g^2 for both the ground-state energy and effective mass in the strong-coupling limit. For the sake of completeness, we will outline this calculation following procedures employed previously by Gross⁶ and by Matz and Burkey.⁵ Here, one makes a variational calculation, replacing the true internal wave functions $\chi_{\sigma}(\mathbf{r})$, by harmonic oscillator functions $\psi_{\eta}(\mathbf{r})$, $\eta = \{n, l, m\}$ with *n* the number of radial modes, *l* the orbited angular momentum, and *m* its projection on the *z* axis, which satisfy the equation

$$-\frac{1}{2m_r}\nabla_r^2\psi_\eta(\mathbf{r})+\frac{1}{2}m_r\widetilde{\omega}^2r^2\psi_\eta(\mathbf{r})=\mathcal{E}_\eta\psi_\eta(\mathbf{r}),$$

with

$$\mathcal{E}_n = \widetilde{\omega}(2n + l + \frac{3}{2})$$
.

The oscillator frequency $\tilde{\omega}$ will be used as the variational parameter. Since the polaron effective mass is expected to become infinitely large as the coupling g^2 goes to infinity, we will begin by making the approxiations

$$\mathcal{M} = 1 + M \simeq M, \quad \beta = M/(M+1) \simeq 1,$$

 $m_r = M/(M+1) \simeq 1,$

and setting the kinetic energy terms in the energy denominators of Eqs. (31) and (34) to zero. These approximations will be justified by consistency with the final results. The variational equations for the ground-state energy and effective mass in the strong-coupling limit may then be written as

$$E_{0} = -\frac{1}{2} \int d^{3}r \,\psi_{0}^{*}(\mathbf{r}) \nabla_{r}^{2} \psi_{0}(\mathbf{r}) - 2\pi \sqrt{2} \frac{g^{2}}{(2\pi)^{3}} \int d^{3}r \,\psi_{0}^{*}(\mathbf{r}) \int d^{3}r' \psi_{0}(\mathbf{r}') \int \frac{d^{3}k}{k^{2}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \sum_{\eta} \psi_{\eta}^{*}(\mathbf{r}) \psi_{\eta}(\mathbf{r}') \int_{0}^{\infty} d\tau \, e^{-(\mathcal{E}_{\eta}-\mathcal{E}_{0}+1)\tau} d\tau \, d\tau \, e^{-(\mathcal{E}_{\eta}-\mathcal{E}_{0}+1)\tau}$$

and

$$\mathcal{M} = \frac{2}{3} 2\pi \sqrt{2} \frac{g^2}{(2\pi)^3} \int d^3 r \,\psi_0^* \mathbf{r} \int d^3 r' \psi_0(\mathbf{r}') \int d^3 k \, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \sum_{\eta} \psi_{\eta}(\mathbf{r}) \psi_{\eta}^*(\mathbf{r}') \frac{1}{2} \frac{\partial^2}{\partial\omega^2} \int_0^\infty d\tau \, e^{-(\mathcal{E}_{\eta}-\mathcal{E}_0+\omega)\tau} \big|_{\omega=1} \,,$$

where the relation $(\mathcal{E}_{\eta} - \mathcal{E}_{0} + \omega)^{-1} = \int_{0}^{\infty} d\tau e^{-(\mathcal{E}_{\eta} - \mathcal{E}_{0} + \omega)\tau}$ has been used. Using the Green's function for the spherical harmonic oscillator¹² in the present units

$$G(\mathbf{r},\mathbf{r}';-i\tau) = \sum_{\eta} \psi_{\eta}(\mathbf{r})\psi_{\eta}^{*}(\mathbf{r}')e^{-E_{\eta}\tau}$$
$$= \left[\frac{\widetilde{\omega}}{2\pi\sinh\widetilde{\omega}\tau}\right]^{3/2} \exp\left[-\frac{\widetilde{\omega}}{4}\left[(\mathbf{r}+\mathbf{r}')^{2}\tanh\frac{\widetilde{\omega}\tau}{2} + (\mathbf{r}-\mathbf{r}')^{2}\coth\frac{\widetilde{\omega}\tau}{2}\right]\right]$$

and the explicit expressions

$$\psi_0(\mathbf{r}) = (4\pi)^{-1/2} 2\pi^{-1/4} \widetilde{\omega}^{3/4} e^{-(1/2)\widetilde{\omega}r^2}, \quad \mathcal{E}_0 = \frac{3}{2} \widetilde{\omega} ,$$

all but the $d\tau$ integral may be done easily to give

$$E_0 = \frac{3\widetilde{\omega}}{4} - \frac{g^2}{\sqrt{\pi}} \widetilde{\omega}^{1/2} \int_0^\infty dx \ e^{-x} (1 - e^{-\widetilde{\omega}x})^{-1/2}$$

and

$$\mathcal{M} = \frac{g^2}{3\sqrt{\pi}} \tilde{\omega}^{3/2} \int_0^\infty x^2 dx \ e^{-x} (1 - e^{-\tilde{\omega}x})^{-3/2}$$

If it is now assumed that $\tilde{\omega} \to \infty$ as $g^2 \to \infty$, the terms in parentheses in the above integrals can be expanded and the dx integrals performed giving

$$E_0 = \frac{3\widetilde{\omega}}{4} - \frac{g^2}{\sqrt{\pi}} \widetilde{\omega}^{1/2} [1 + O(\widetilde{\omega}^{-1})]$$

$$\mathcal{M} = \frac{g^2 \tilde{\omega}^{3/2}}{3\sqrt{\pi}} [2 + O(\tilde{\omega}^{-3})] .$$

Finally, minimizing this last expression for E_0 with respect to $\tilde{\omega}$ results in

$$\widetilde{\omega} = \left[\frac{2g^2}{3\sqrt{\pi}}\right]^2,$$

and so, to leading order,

$$E_0 = -\frac{g^4}{3\sqrt{\pi}}, \quad \mathcal{M} = \frac{16g^8}{81\pi^2}$$

These final strong-coupling results validate the prior assumptions of large M and $\tilde{\omega}$.

C. Infinite-M and zero-M limits

If the polaron mass increment M were regarded as a free parameter rather than a quantity to be calculated

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self-consistently within the theory, there are two limits which are worth considering briefly. The first is the $M = \infty$ limit which was mentioned earlier in connection with the Matz and Burkey paper. In this limit, polaron kinetic energies vanish for finite momenta. The bilocal coordinates become

$$\mathbf{R} = \mathbf{y}, \mathbf{r} = \mathbf{x} - \mathbf{R}$$

so the physical picture becomes that of a bare fermion moving in the potential of an infinite mass virtual boson cloud. This is not the limit of local field theory despite the fact that Eq. (22) for the bilocal internal wave function reduces to a similar equation derived from the single-particle Green's function for the corresponding local field theory.¹³ The fundamental difference between the local theory and the $M = \infty$ bilocal limit, which is not apparent in the ground-state energy and effective mass calculations, is that S-matrix elements evaluated within the bilocal theory will, in general, contain internal fermion wave functions explicitly. No similar appearance of anything corresponding to an internal fermion wave function occurs in standard S-matrix calculations within local field-theoretic frameworks which center about the usage of free fermion fields. It might be added that while it is possible to let $M = \infty$ in the bilocal theory and thereby obtain the same results for polaron quantities as, say, Matz and Burkey,⁵ doing so would be inherently inconsistent with a later calculation of a finite effective mass.

In a sense, the strict M = 0 limit may be regarded as the local field limit of the bilocal theory. The bilocal coordinates are now

$$\mathbf{R} = \mathbf{x}, \mathbf{r} = \mathbf{R} - \mathbf{y}$$

so the bare fermion coordinate and the center-of-mass coordinate coincide. The relative kinetic energy operator in the Hamiltonian, Eq. (5), becomes infinite, ¹⁴ and all exponential factors of the form $\exp(i\beta \mathbf{k} \cdot \mathbf{r})$ containing the relative coordinate become unity. If we ignore the overall infinite energy shift due to the relative kinetic energy and insert the expansion for the bilocal field operator explicitly, then as *M* approaches zero, the total bilocal Hamiltonian, Eq. (5) plus (6) and (7), becomes

$$H = \int d^{3}R \int d^{3}r \left[(2\pi)^{-3/2} \sum_{\sigma} \int d^{3}P \chi_{\sigma,\mathbf{P}}^{*}(\mathbf{r}) \frac{e^{-i\mathbf{P}\cdot\mathbf{R}}}{(2\pi)^{3/2}} b_{\sigma,\mathbf{P}}^{\dagger} \right] \left[-\frac{1}{2m_{0}} \nabla_{R}^{2} \right]$$

$$\times \left[(2\pi)^{-3/2} \sum_{\sigma'} \int d^{3}P' \chi_{\sigma',\mathbf{P}}(\mathbf{r}) e^{i\mathbf{P}\cdot\mathbf{R}} b_{\sigma',\mathbf{P}'} \right]$$

$$+ i(2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{3/2}} \int d^{3}R \int d^{3}r \int \frac{d^{3}k}{k} \left[(2\pi)^{-3/2} \sum_{\sigma} \int d^{3}P \chi_{\sigma,\mathbf{P}}^{*}(\mathbf{r}) e^{-i\mathbf{P}\cdot\mathbf{R}} b_{\sigma,\mathbf{P}}^{\dagger} \right]$$

$$\times (a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{R}} - a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}}) \left[(2\pi)^{-3/2} \sum_{\sigma'} \int d^{3}P' \chi_{\sigma',\mathbf{P}'}(\mathbf{r}) e^{i\mathbf{P}'\cdot\mathbf{R}} b_{\sigma',\mathbf{P}'} \right]$$

$$+ \int d^{3}k a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} .$$

If we assume, further, that the internal wave functions $\chi_{\sigma,\mathbf{P}}(\mathbf{r})$ are independent of center-of-mass momentum in the M=0 limit, then performing the d^3r integrations and applying the orthonormality of the internal wave functions reduces the above Hamiltonian to

$$H = \sum_{\sigma} \left[\int d^3 R \ F_{\sigma}^{\dagger}(\mathbf{R}) \left[-\frac{1}{2m_0} \nabla_R^2 \right] F_{\sigma}(\mathbf{R}) + i (2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{3/2}} \int d^3 R \ \int \frac{d^3 k}{k} F_{\sigma}^{\dagger}(\mathbf{R}) F_{\sigma}(\mathbf{R}) (a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{R}} - a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}}) \right] + \int d^3 k \ a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} ,$$

where the operator $F_{\sigma}(\mathbf{R})$ is

$$F_{\sigma}(\mathbf{R}) \equiv (2\pi)^{-3/2} \int d^{3}P \, e^{i\mathbf{P}\cdot\mathbf{R}} b_{\sigma,\mathbf{P}}$$

Except for the redundancy in the electron field term of the Hamiltonian involving the σ index, which can be ignored since excited internal states no longer have relevancy, this is just the local polaron Hamiltonian, Eq. (1), with which we started.

Finally, it might be noted that if we set M=0 in the right-hand sides of Eqs. (36) and (32) for the polaron energy (omitting the kinetic energy) and mass increment, respectively, we will obtain the weak-coupling values of $E_0 = -g^2$ and $M = g^2/6$.

D. Some numerical calculations

Simultaneous numerical solutions of Eqs. (25) and (33) for the polaron ground-state energy and mass increment have been obtained for values of g^2 between 0.0 and 3.0. These should have validity here only for $g^2 \leq 1$ since excited-state contributions are not included in these equations. (The validity of these and other polaron calculations for $g^2 > 1$ can also be questioned if they do not include contributions from irreducible self-energy terms of order g^4 and higher.) In addition, an estimate of the contribution of the first excited state to the ground-state energy and effective mass has been obtained by approximating it with the lowest excited state of a spherical harmon-

ic oscillator and adjusting the oscillator frequency $\tilde{\omega}$ variationally to minimize the ground-state energy. Contributions of additional excited states could be included straightforwardly in a similar manner, and, in principle, the entire excited oscillator spectrum could be included in a like manner to that used in Sec. III B for the strong-coupling limit, though this would be considerably more difficult numerically.

To include the contribution of the first excited polaron state approximately in the ground-state calculation, we start with Eqs. (24) and (32), taking the lowest internal wave function, as before, to be

$$\chi(\mathbf{r}) = \frac{1}{\sqrt{4\pi}} \frac{\psi(r)}{r}$$

and the first excited function to be that of the 1p oscillator state

$$\chi_{1,m}(\mathbf{r}) = Y_{1,m}(\theta,\phi) \frac{1}{r} R_{0,1}(r) ,$$

with

$$R_{0,1}(r) = \left[\left(\frac{\tilde{\omega}^3}{\pi} \right)^{1/2} \frac{2^3}{3} \right]^{1/2} \tilde{\omega}^{-1/2} r^2 e^{-(1/2)\tilde{\omega}r^2}$$

Omitting the higher excited states in Eqs. (24) and (32), and making use of the spherical harmonic composition relation

$$Y_{l,0}(\theta_{12},\phi_{12}) = \left(\frac{4\pi}{2l+1}\right)^{1/2} \sum_{m=-l}^{l} Y_{l,m}(\theta_{1},\phi_{1}) Y_{l,m}^{*}(\theta_{2},\phi_{2})$$

all angular integrals can be performed to give

$$-\frac{1}{2m_{r}}\frac{d^{2}\psi(r)}{dr^{2}}-2\pi\sqrt{2}\frac{g^{2}}{(2\pi)^{3}}\frac{\pi^{2}}{\beta}\frac{1}{r}\psi(r)\int_{0}^{\infty}dr'\frac{1}{r'}|\psi(r')|^{2} \times \left[(r+r')-|r-r'|+\frac{1}{\beta\sqrt{2M}}(e^{-\beta\sqrt{2M}(r+r')}-e^{-\beta\sqrt{2M}|r-r'|})\right]+U(r)=E_{0}\psi(r) \quad (37)$$

and

$$M = \frac{2}{3} \frac{g^2}{(2\pi)^3} \frac{\pi^3 \sqrt{2}}{4} (2\mathcal{M})^{3/2} \int_0^\infty dr |\psi(r)|^2 \int_0^\infty dr' |\psi(r')|^2 \times \frac{1}{rr'} \left[\left[|r - r'|^2 + \frac{3}{\beta\sqrt{2\mathcal{M}}} |r - r'| + \frac{3}{2\mathcal{M}\beta^2} \right] e^{-\beta\sqrt{2\mathcal{M}}|r - r'|} - \left[(r + r')^2 + \frac{3}{\beta\sqrt{2\mathcal{M}}} (r + r') + \frac{3}{2\mathcal{M}\beta^2} \right] e^{-\beta\sqrt{2\mathcal{M}}(r + r')} \right] + \frac{2}{3} \frac{g^2}{(2\pi)^3} \frac{3\pi^3\sqrt{2}}{4} (2\mathcal{M})^{3/2} \frac{1}{(\bar{\omega} + 1)^3} \int_0^\infty dr \,\psi^*(r) R_{0,1}(r) \int_0^\infty dr' \psi(r') R_{0,1}(r') \frac{1}{rr'} \Lambda(r, r') , \qquad (38)$$

where

$$U(r) = -2\pi\sqrt{2} \frac{g^2}{(2\pi)^3} \frac{3\pi^2}{\beta(\tilde{\omega}+1)} \frac{1}{r} R_{0,1}(r) \int_0^\infty dr' \psi(r') R_{0,1}(r') \\ \times \frac{1}{r'} \left\{ -(r+r') - |r-r'| + \frac{1}{a\beta} (e^{-a\beta(r+r')} + e^{-a\beta|r-r'|}) \right. \\ \left. -\frac{1}{rr'a^2\beta^2} \left[\left[r+r' + \frac{1}{a\beta} \right] e^{-a\beta(r+r')} - \left[|r-r'| + \frac{1}{a\beta} \right] e^{-a\beta|r-r'|} \right] \\ \left. +\frac{1}{3rr'} [(r+r')^3 - |r-r'|^3] \right\}$$
(39)

and

$$\Lambda(\mathbf{r},\mathbf{r}') = \left[(\mathbf{r}+\mathbf{r}')^2 + \frac{3}{a\beta}(\mathbf{r}+\mathbf{r}') + \frac{3}{a^2\beta^2} \right] \left[1 + \frac{3}{rr'a^2\beta^2} \right] e^{-a\beta(\mathbf{r}+\mathbf{r}')} \\ + \left[|\mathbf{r}-\mathbf{r}'|^2 + \frac{3}{a\beta}|\mathbf{r}-\mathbf{r}'| + \frac{3}{a^2\beta^2} \right] \left[1 - \frac{3}{rr'a^2\beta^2} \right] e^{-a\beta|\mathbf{r}-\mathbf{r}'|} \\ - \frac{1}{rr'a\beta} \left[(\mathbf{r}+\mathbf{r}')^3 + \frac{3}{a\beta}(\mathbf{r}+\mathbf{r}')^2 + \frac{6}{a^2\beta^2}(\mathbf{r}+\mathbf{r}') + \frac{6}{a^3\beta^3} \right] e^{-a\beta(\mathbf{r}+\mathbf{r}')} \\ + \frac{1}{rr'a\beta} \left[|\mathbf{r}-\mathbf{r}'|^3 + \frac{3}{a\beta}|\mathbf{r}-\mathbf{r}'|^2 + \frac{6}{a^2\beta^2}|\mathbf{r}-\mathbf{r}'| + \frac{6}{a^3\beta^3} \right] e^{-a\beta|-\mathbf{r}-\mathbf{r}'|} .$$
(40)

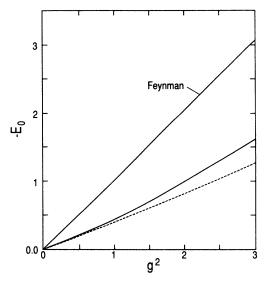


FIG. 2. Bilocal ground-state energy for $g^2 \leq 3$ using only the ground-state wave function in the internal potential (dashed curve) and with the contribution from the first excited state (solid curve). The Feynman ground-state energies are shown for comparison.

The energy difference between the ground and first excited state has been taken equal to that of the harmonic oscillator

$$E_1 - E_0 = \hbar \tilde{\omega}$$

so that parameter a is

$$a = [2\mathcal{M}(E_1 - E_0 + 1)]^{1/2} = \sqrt{2\mathcal{M}(\tilde{\omega} + 1)} \; .$$

Equations (37) and (38) have been solved iteratively using a modified Numerov integration scheme. Simpson's rule was used to perform integrals. The results of these numerical calculations are shown in Figs. 2–6. The bilocal

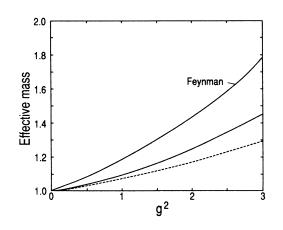


FIG. 3. Bilocal polaron effective mass $\mathcal{M} = 1 + M$ for $g^2 \leq 3$ using only the ground-state internal wave function (dashed curve) and including the contribution from the first excited state (solid curve). The Feynman effective masses are shown for comparison.

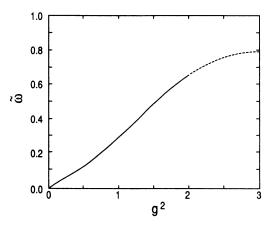


FIG. 4. Values of the harmonic oscillator frequency $\tilde{\omega}$ which minimize the polaron ground-state energy when the first excited internal state is included variationally, shown as a function of the coupling constant for $g^2 \leq 3$. The dashed portion of this curve shows approximately where the next higher excited states are expected to be of importance.

ground-state energies with and without the first excitedstate contribution are given in Fig. 2 as a function of g^2 . For comparison, the Feynman values for the ground-state energy as given by Schultz¹⁵ are also shown. A corresponding plot of the polaron effective mass $\mathcal{M}=1+M$ is given in Fig. 3. For small values of g^2 , both the bilocal energy and mass increment are roughly half of the local field results. The values of the oscillator frequency $\tilde{\omega}$ which minimize E_0 are given in Fig. 4 as a function of g^2 . These may be regarded as approximations to the excita-

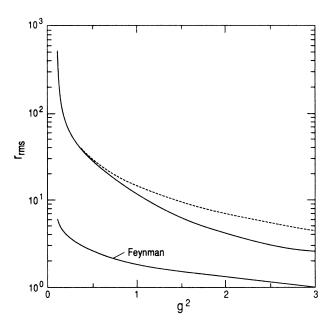


FIG. 5. Root-mean-square radii of the ground-state internal wave functions with (solid curve) and without (dashed curve) the contribution from the first excited state to the internal potentials. Feynman rms radii are shown for comparison.

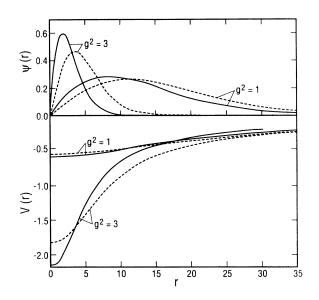


FIG. 6. Internal ground-state wave functions $\psi(r)=r\chi(r)$ and ground-state potentials for $g^2=1.0$ and 3.0 with (solid curves) and without (dashed curves) first excited-state contributions. The solid curves are what would constitute the "local" potentials of Eq. (37) and do not include the nonlocal term U(r).

tion energy of the first excited polaron state relative to E_0 . The sudden decrease in the slope of the $\tilde{\omega}$ versus g^2 curve for $g^2 \gtrsim 2$ suggests the necessity for inclusion of the next level of excited states in the calculation. Finally, root-mean-square radii for the polaron ground state

$$r_{\rm rms} \equiv \left(\int_0^\infty dr \, r^2 |\psi(r)|^2\right)^{1/2}$$

are given in Fig. 5, and ground-state wave functions $\psi(r)$ and potentials (not including all effects of the first excited state for the latter) are shown in Fig. 6 as a function of radius for several values of the coupling constant.

IV. SUMMARY AND SPECULATIONS

In the preceding sections, we have demonstrated the use of the bilocal field formalism by applying it to the large-polaron problem. Only the lowest-order approximation to the self-energy (Fig. 1) was used to obtain the internal state potential which determines the polaron properties in this theory. Within this framework, it was shown that the bilocal formalism gives the usual Feynman expressions for the leading term in powers of the coupling constant for the upper bound of the strongcoupling ground-state energy and for the polaron effective mass. In the weak-coupling limit, the theory gives a higher energy for the polaron ground state than obtained from local field theory, and a smaller effective mass. This is due to the kinetic energy of internal motion in the bilocal theory which leads to bound-state polaron solutions for all values of the coupling, with internal wave functions that expand uniformly over all space as g^2 approaches zero (a stable bound internal state being a necessity for the bilocal formulation). On the other hand, making a formal expansion of the ground-state interaction energy and mass increment in powers of the coupling (although here this expansion is not legitimate mathematically), or collapsing the internal wave function to the origin to recover the local limit, results in the usual leading term for each as $g^2 \rightarrow 0$. In large measure, though not entirely for the polaron example, the bilocal field procedures discussed here give results equivalent to those of local field theory.

In the bilocal formalism, nonrelativistic or relativistic, all Fermion self-energy effects transform into the characteristics of potentials which determine the internal spatial motion of the composite system consisting of the bare fermion and its virtual boson (etc.) cloud. In terms of Fevnman diagrams, single fermion self-energy inclusions no longer occur in the S matrix, for instance, but the fermion propagator is now altered to take into account virtual transitions to the various internal states¹⁶ of the spatially extended physical particle. Only pure vertex corrections, possible boson self-energy terms, and graphs which couple more than one vertex through virtual boson emission and reabsorption (related to multiparticle Green's functions), as in Fig. 7, remain as complications in the S matrix. Because of the spatially extended nature of the physical fermion, we expect that all Feynman diagram terms will now be finite, but this has not yet been proved in general. As a speculation, all of the complications with ultraviolet divergences may now rest on the behavior of the fermion internal (i.e., self-energy) potentials at the origin. Extending this speculation, it may be that bilocal fields with renormalizable local field counterparts produce potentials with at most weak singularities at the origin from all relevant self-energy contributions

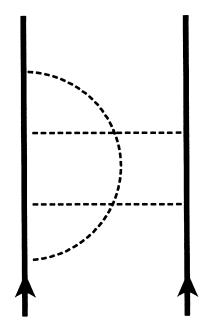


FIG. 7. Example of a Feynman diagram in which several vertices are coupled by the emission and reabsorption of a virtual boson.

and so could permit bound-state solutions, while for nonrenormalizable local counterparts potentials are too singular. Here, if the fermion self-energy potentials do not permit a stable bound internal state solution, the free physical particle in question does not exist.

With regard to renormalizations, since we expect all Feynman diagrams to be finite in suitable bilocal theories, mass renormalization consists of just calculating a mass increment from a formula similar to Eq. (32) obtained from the expectation value in the one-fermion state of the boson contribution to the total momentum operator, and state function renormalizaton is just ordinary normalization. Only finite-coupling-constant renormalizations remains to be done in a manner similar to that in local field theory.

Focusing further on purely formal aspects of bilocal theory, the question arises as to whether this theory is really distinct from its local counterpart. Though no investigation of this matter has been made, we suspect that the answer is no, at least for "fundamental" fields, where no bare fermion exists independent of its surrounding virtual cloud. If so, what has been done is just a restructuring of the formalism which places initial emphasis on the characteristics of the physical Fermi particle. If physical Fermi particles have such an internal bound-state structure, then at least some of the difficulties that have occurred in local field theories result from attempting to obtain bound solutions by perturbation methods using plane-wave expansions.

Aside from the speculations discussed above, there are a large number of technical questions that could be asked concerning internal consistency and how to develop and deal with the bilocal formalism mathematically. For example, can path-integral techniques be applied here profitably? However, the primary question is still that of the applicability of the bilocal formalism to basic physical problems. Two such problems that may be tractable are the calculation of the electromagnetic contribution to the mass of the electron and a possible explanation for the lack of occurrence of free quarks. The electromagnetic mass problem should involve a fourth-order calculation of the internal potentials since the second-order potential is expected to be repulsive, with attractive components coming from the fourth-order vacuum polarization term. Unlike the polaron calculations considered in this paper, the electron problem will require the use of charge renormalization since only the renormalized charge is known while the bare charge is required for the calculation of the internal potentials. Similarly, the bare mass of the electron would be a parameter to be determined by the coupled calculation of the electromagnetic mass, the unrenormalized coupling constant, and the internal wave functions. In accordance with bilocal theory, the determination of the nonexistence of free quarks would result by showing that a bare quark cannot bind to its accompanying virtual gluon cloud. Analogous ideas to those discussed in this paper may also be applicable to the study of hadronic structure.

APPENDIX

Use of the interaction picture (here nonrelativistic) rather than the Schrödinger picture provides a simpler and more systematic method for calculating potential terms from irreducible Fermi particle self-energy diagrams and for obtaining single fermion state functions. It is also more appropriate for relativistic calculations. Derivation of all interaction picture relations follow in the same manner as in local field theory, and only a listing of some useful equations and rules will be given below.

In the interaction picture the "unperturbed" bilocal Hamiltonian and the bilocal interaction Hamiltonian for the large polaron may be written as

$$H_{0} = \int d^{3}R \int d^{3}r F^{\dagger}(\mathbf{R},\mathbf{r},t) \left[-\frac{1}{2\mathcal{M}} \nabla_{R}^{2} - \frac{1}{2m_{r}} \nabla_{r}^{2} \right] F(\mathbf{R},\mathbf{r},t) + \omega \int d^{3}k a_{k}^{\dagger}a_{k} + \int d^{3}R \int d^{3}r \int d^{3}r' \int d^{3}r' \int_{-\infty}^{\infty} dt' F^{\dagger}(\mathbf{R},\mathbf{r},t) V(\mathbf{R},\mathbf{r},t|\mathbf{R}',\mathbf{r}',t') F(\mathbf{R}',\mathbf{r}',t')$$
(A1)

and $H_I(t) = H_I^{(1)}(t) + H_I^{(2)}(t)$, with

$$H_{I}^{(1)}(t) = i(2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{3/2}} \int d^{3}R \int d^{3}r \ F^{\dagger}(\mathbf{R},\mathbf{r},t) F(\mathbf{R},\mathbf{r},t) \int \frac{d^{3}k}{k} (a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot(\mathbf{R}+\beta\mathbf{r})+i\omega t} - a_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}+\beta\mathbf{r})-i\omega t}) , \quad (A2)$$

$$H_{I}^{(2)}(t) = -\int d^{3}R \int d^{3}r \int d^{3}r' \int d^{3}r' \int_{-\infty}^{\infty} dt' F^{\dagger}(\mathbf{R},\mathbf{r},t) V(\mathbf{R},\mathbf{r},t|\mathbf{R}',\mathbf{r}',t') F(\mathbf{R}',\mathbf{r}',t') .$$
(A3)

The expansion of the Fermion field function is now $F(\mathbf{R}, \mathbf{r}, t) \equiv e^{iH_0 t} F(\mathbf{R}, \mathbf{r}) e^{-iH_0 t}$

$$=(2\pi)^{-3/2}\sum_{\sigma}\int d^{3}P \,\chi_{\sigma,\mathbf{P}}(\mathbf{r})e^{i\mathbf{P}\cdot\mathbf{R}-iE_{\sigma,\mathbf{P}}t}b_{\sigma,\mathbf{P}}.$$
(A4)

The equations which determine the internal wave functions $\chi_{\sigma,\mathbf{P}}(\mathbf{r})$ are the same as before, Eq. (23) in second order, with the relation between the potential $V(\mathbf{R}, \mathbf{r}, t | \mathbf{R}', \mathbf{r}', t')$ and potentials $V_{\sigma, \mathbf{P}}(\mathbf{R}, \mathbf{r} | \mathbf{R}', \mathbf{r}')$ specified in Eq. (10) given by

$$V_{\sigma,\mathbf{P}}(\mathbf{R},\mathbf{r}|\mathbf{R}',\mathbf{r}') = e^{iE_{\sigma,\mathbf{P}}t} \int_{-\infty}^{\infty} dt' V(\mathbf{R},\mathbf{r},t|\mathbf{R}',\mathbf{r}',t') e^{iE_{\sigma,\mathbf{P}}t'} .$$
(A5)

We can now use standard S-matrix procedures in conjunction with Feynman diagrams to obtain the potential $V(\mathbf{R}, \mathbf{r}, t | \mathbf{R}', \mathbf{r}', \mathbf{t}')$ and, similarly, calculate the onefermion state function by operating on the state $|\sigma, \mathbf{P}\rangle$ of H_0 with the time evolution operator $U(0, -\infty)$. In series form, these operators are

$$S = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \left[\int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \right]$$
$$\times T[H_I(t_1) \cdots H_I(t_n)]$$
(A6)

and

$$U(0, -\infty) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \left[\int_{-\infty}^0 dt_1 \cdots \int_{-\infty}^0 dt_n \right]$$
$$\times T[H_I(t_1) \cdots H_I(t_n)], \qquad (A7)$$

where T is the Wick time-ordering operator. In the following, we will use notation similar to that of Schweber's book¹⁷ and give rules for writing S-matrix terms from Feynman diagrams completely in a configuration space representation, leaving undone the center-of-mass coordinate and time integrals which lead to conservation of momentum and energy at each diagram vertex. The propagators for the electron and for the phonon in the polaron problem are then

$$S_{F}(\mathbf{R},\mathbf{r},t;\mathbf{R}',\mathbf{r}',t') \equiv -2\langle 0|T[F(\mathbf{R},\mathbf{r},t)F^{\dagger}(\mathbf{R}',\mathbf{r}',t')]|0\rangle$$

$$= \frac{-2i}{(2\pi)^{4}} \sum_{\eta} \int d^{3}Q \int_{-\infty}^{\infty} dE \frac{e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R}')-iE(t-t')}}{E-E_{\eta,\mathbf{Q}}+i\epsilon} \chi_{\eta,\mathbf{Q}}(\mathbf{r})\chi_{\eta,\mathbf{Q}}^{*}(\mathbf{r}')$$
(A8)

.

and

$$\Delta_F(\mathbf{x},t;\mathbf{x}'t') \equiv 2\langle 0 | T[\phi(\mathbf{x},t)\phi(\mathbf{x}',t')] | 0 \rangle$$

$$=\frac{4i\omega}{(2\pi)^4}\int \frac{d^3k}{k^2}\int_{-\infty}^{\infty} d\bar{\omega} \frac{e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')+i\beta\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')-i\bar{\omega}(t-t')}}{\bar{\omega}^2-\omega^2+i\epsilon},$$
(A9)

where we have defined $\phi(\mathbf{x}, t)$ to be

$$\phi(\mathbf{x},t) = \frac{i}{(2\pi)^{3/2}} \int \frac{d^3k}{k} (a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} - a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t}) .$$

Using the abbreviations

$$S_F(1,2) \equiv S_F(\mathbf{R}_1,\mathbf{r}_1,t_1;\mathbf{R}_2,\mathbf{r}_2,t_2)$$

and

$$\Delta_F(1,2) \equiv \Delta_F(\mathbf{x}_1,t_1;\mathbf{x}_2,t_2) ,$$

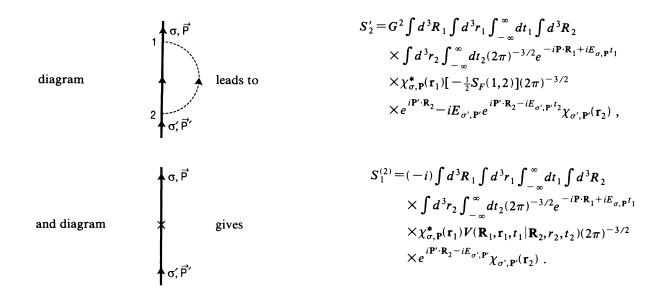
the rules for constructing S-matrix elements for irreducible fermion self-energy diagrams using $H_I^{(1)}(t)$ are as follows:

Source of factor	Factor
nth-order diagram	$(-i)^{n}$
Coupling factor for each $H_1^{(1)}$ vertex	$i(2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{3/2}}$
Incoming fermion (σ, \mathbf{P}) to vertex <i>i</i>	$\frac{(2\pi)^{-3/2}e^{i\mathbf{P}\cdot\mathbf{R}_{i}-i\boldsymbol{E}_{\sigma,\mathbf{P}}t_{i}}\chi_{\sigma,\mathbf{P}}(\mathbf{r}_{i})}{(2\pi)^{-3/2}e^{-i\mathbf{P}\cdot\mathbf{R}_{j}+i\boldsymbol{E}_{\sigma,\mathbf{P}}t_{j}}\chi_{\sigma,\mathbf{P}}(\mathbf{r}_{j})}$
Outgoing fermion (σ, \mathbf{P}) from vertex j	$(2\pi)^{-3/2}e^{-i\mathbf{P}\cdot\mathbf{R}_j+iE_{\sigma,\mathbf{P}}t_j}\chi_{\sigma,\mathbf{P}}(\mathbf{r}_j)$
Internal fermion line from vertex j to i	$-\frac{1}{2}S_F(i,j)$
Internal boson line for vertex j to i	$\frac{1}{2}\Delta_F(i,j)$
Space and time integrals	
at each vertex i	$\int d^3R_i \int d^3r_i \int_{-\infty}^{\infty} dt_i$

For the contribution of $H_I^{(2)}(t)$, which will be denoted by an "x" on a fermion line, the rightmost coordinates of $V(\mathbf{R}_i, \mathbf{r}_i, t_i | \mathbf{R}_j, \mathbf{r}_j, t_j)$ are treated as a vertex end point of an incoming fermion line and the leftmost as a vertex for an outgoing line for either interior or exterior lines of a Feynman diagram. Therefore, completing the above table, the contribution from $H_I^{(2)}(t)$ on a fermion line will be

$$\int d^3R_i \int d^3r_i \int_{-\infty}^{\infty} dt_i \int d^3R_j \int d^3r_j \int_{-\infty}^{\infty} dt_j V(\mathbf{R}_i, \mathbf{r}_i, t_i | \mathbf{R}_j, \mathbf{r}_j, t_j) \ .$$

With this prescription, and the requirement that $V(\mathbf{R}, \mathbf{r}, t | \mathbf{R}', \mathbf{r}', t')$ be chosen to cancel the irreducible self-energy terms of the S matrix for the one-fermion system, all fermion self-energy components are eliminated from the S matrix. As an example, for the second-order potential



Requiring that $S_2 + S_1^{(2)} = 0$ leads to the identification

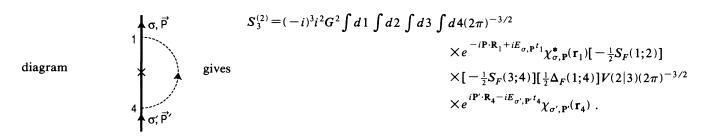
$$V(\mathbf{R}_1,\mathbf{r}_1,t_1|\mathbf{R}_2,\mathbf{r}_2,t_2) \equiv V(1|2) = -iG^2[-\frac{1}{2}S_F(\mathbf{R}_1,\mathbf{r}_1,t_1;\mathbf{R}_2,\mathbf{r}_2,t_2)][\frac{1}{2}\Delta_F(\mathbf{R}_1,\mathbf{r}_1,t_1;\mathbf{R}_2,\mathbf{r}_2,t_2)],$$

where

$$G \equiv (2\pi\sqrt{2})^{1/2} \frac{g}{(2\pi)^{-3/2}}$$
.

An example of a fourth-order cancellation is as follows:

where
$$\int d1 \equiv \int d^3R_1 \int d^3r_1 \int_{-\infty}^{\infty} dt_1$$
, etc., and



$$S_{3}^{(2)} = (-i)^{4} i^{2} G^{4} \int d1 \int d2 \int d3 \int d4(2\pi)^{-3/2} e^{-i\mathbf{P}\cdot\mathbf{R}_{1} + iE_{\sigma,\mathbf{P}}t_{1}} \chi_{\sigma,\mathbf{P}}^{*}(\mathbf{r}_{1})$$

$$\times [-\frac{1}{2}S_{F}(1;2)][-\frac{1}{2}S_{F}(2;3)][-\frac{1}{2}S_{F}(3;4)][\frac{1}{2}\Delta_{F}(1;4)][\frac{1}{2}\Delta_{F}(2;3)]$$

$$\times (2\pi)^{-3/2} e^{i\mathbf{P}'\cdot\mathbf{R}_{4} - iE_{\sigma',\mathbf{P}'}t_{4}} \chi_{\sigma',\mathbf{P}'}(\mathbf{r}_{4}) .$$

Therefore

 $S_4^{(1)} + S_3^{(2)} = 0$.

- ¹(a) H. Fröhlich, Adv. Phys. 3, 325 (1954); (b) R. P. Feynman, Phys. Rev. 97, 660 (1955); (c) J. Appel, in Solid State Physics, edited by Frederick Seitz, David Turnbull, and Henry Ehrenreich (Academic, New York, 1968), Vol. 21, pp. 193-391. This article contains extensive references and a comprehensive coverage of the state of polaron work up to the time of its publication.
- ²Marvin Rich, Los Alamos National Laboratory Report No. LA-4831-MS, 1972 (unpublished).
- ³M. Rich, Phys. Rev. D 8, 1091 (1973).
- ⁴Although the discussion of the present paper is in terms of a Yukawa-type interaction, similar procedures should be applicable, for instance, to the self-interacting $\lambda \phi^4$ field.
- ⁵D. Matz and B. C. Burkey, Phys. Rev. B 3, 3487 (1971).
- ⁶E. P. Gross, Ann. Phys. (N.Y.) 8, 78 (1959).
- ⁷For instance, Refs. 1(b), 1(c), 5, and 6.
- ⁸In a theory with direct boson-boson interactions, some modifications of the treatment given here may be necessary.
- ⁹The bilocal formalism discussed here assumes a single mass M associated with the virtual boson cloud accompanying the bare fermion of the physical free particle. The natural choice for M is that of Eq. (30) associated with the ground-state configuration. The question of the use of separate M values for each of the excited states in the approximate energy decomposition, Eq. (23b), has not been looked into fully, and the ground-state M value has been used for all states. This is not of consequence for the purpose of the present paper, but

does require further consideration.

- ¹⁰E. P. Gross, in *Mathematical Methods of Solid State and Superfluid Theory*, edited by R. C. Clark and G. H. Derrick (Plenum, New York, 1968), p. 94.
- ¹¹M. Bolsterli, Phys. Rev. D 7, 2967 (1973).
- ¹²See R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), p. 200, for the Green's function of the one-dimensional harmonic oscillator from which the three-dimensional Green's function is easily obtained.
- ¹³See D. Matz and B. C. Burkey, Phys. Rev. B 3, 3487 (1971), Eq. (18).
- ¹⁴In terms of the specifics of the polaron, the picture now would be that of infinitesimally weak correlated polarization waves whirling around a stationary electron. This does not seem reasonable physically, and is likely related to why the ground-state energy in the local theory is lower than in the bilocal theory.
- ¹⁵T. D. Schultz, Phys. Rev. **116**, 526 (1959).
- ¹⁶A question that could be asked is whether the divergent integrals of local field theory have merely been replaced by a sum over internal states which may be similarly divergent. A general answer is not known and requires investigation, though in the (nondivergent) example of the present paper, this does not appear to be so.
- ¹⁷Silvan S. Schweber, An Introduction to Relativistic Quantum Field Theory (Row, Peterson, Evanston, IL, 1961).