# Interaction of a Nonrelativistic Particle with a Scalar Field with Application to Slow Electrons in Polar Crystals*

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A general variational technique is developed to study the effect of recoil on the motion of a nonrelativistic particle in a scalar field. The ground-state energy is determined, and the results obtained are shown to be exact in the limit of both weak and strong field-particle coupling. This method is applied to investigate the low-lying energy levels of a conduction electron in a polar crystal. The ground-state energy and effective mass so obtained are shown to be in good agreement with the results of Lee, Low, and Pines for the intermediate coupling strengths occurring in real polar crystals.

## I

THE motion of a nonrelativistic particle in a scalar field serves as a prototype for a wide variety of problems. Amongst these are the interaction between low-energy nucleons and scalar mesons, and the electron-lattice interaction in polar crystals, semiconductors, and metals. In these cases the field-particle interaction is frequently not weak so that the usual perturbation-theoretic methods are inapplicable. For such cases in which the coupling is not weak and in which the recoil of the source particle may be neglected, Tomonaga[1] has recently introduced a very useful method of approximation which has acquired the sobriquet, "intermediate coupling" approximation.

The Tomonaga approximation consists in a variational technique based on the physical assumption that successive virtual quanta (mesons or phonons) in the field around the source particle (nucleon or electron) are emitted independently, and hence that there is no correlation between different quanta. It is essentially a Hartree-Fock approximation, in that all identical quanta associated with the ground state of the system are assumed to be in the same physical state. The number of quanta in the field around the source is not limited. The probability amplitude for finding a given number of quanta and the particular functional form for their momentum distribution are found by a Rayleigh-Ritz variational calculation. This method for the case of the interaction of a charged meson with a fixed nucleon leads to the correct answer in the limit of both weak and strong coupling.

However, when the source particle is not fixed, it is easy to see that correlations will be introduced between successive field quanta since the recoil kinetic energy of the source will then come into play. Such correlations are indeed favored, especially when the field-particle coupling is strong, because they will act to reduce the momentum fluctuation of the source particle. Thus it is necessary to extend Tomonaga's formulation in such a way as to allow correlation between quanta to enter into the problem. This can be done by introducing additional degrees of freedom for the field quanta, such that a quantum can be emitted into any one of several states. Our generalization of Tomonaga's formulation is rendered easier by the introduction of certain formal techniques which are developed in Appendix I.

We shall show that for the case of zero total momentum of the system (source plus quanta) it is sufficient to introduce four possible states for the field quanta corresponding to one "$s$" and three "$p$" states. Indeed, the introduction of these extra degrees of freedom makes possible an *exact* solution in both the weak and strong coupling limits of the field-particle interaction. In the strong coupling limit the importance of correlations between successive quanta is reflected in the fact that the mean value of the source recoil kinetic energy turns out to be proportional to the square root of the total number of field quanta, in contrast to the linear dependence predicted by both weak coupling theory and the simple Tomonaga model neglecting such correlations.

Our variational technique is applied to the problem of a slow conduction electron (polaron) moving through a polar crystal, and both the ground-state energy and the polaron effective mass are calculated. For this latter case, in which the total system momentum is not zero, it is necessary to introduce somewhat more complicated trial functions than those required for zero system momentum. For the intermediate coupling strengths ($g^2 \lesssim 6$) encountered in real crystals, we find that the ground state energy differs very slightly from that calculated by Lee, Low, and Pines[2] using the simple Tomonaga approximation. The effective mass correction is somewhat larger and may be as appreciable as twenty percent for $g^2 \sim 5$.

## II

The Hamiltonian for a nonrelativistic particle interacting with a scalar field may be written as

$$H = p^2/2m + g\Sigma_k (V_k \alpha_k e^{i\mathbf{k}\cdot\mathbf{r}} + V_k^* \alpha_k^* e^{-i\mathbf{k}\cdot\mathbf{r}}) + \Sigma_k \omega(k) \alpha_k^* \alpha_k, \quad (1)$$

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[1] S. Tomonaga, Prog. Theoret. Phys. **2**, 6 (1947).

[2] T. D. Lee and D. Pines, Phys. Rev. **88**, 960 (1952); Lee, Low, and Pines, Phys. Rev. **90**, 297 (1953), hereafter referred to as LLP. See also M. Gurari, Phil. Mag. **44**, 329 (1953).

where $(\mathbf{r}, \mathbf{p})$ are the position and momentum of the particle, $\alpha_k^*$ and $\alpha_k$ are the creation and annihilation operators for the scalar field, $\omega(k)$ is the frequency of the $k$th normal mode of this field, and $g$ is the appropriate dimensionless coupling constant characterizing the strength of the field-particle interaction.[3] We find it convenient to take advantage of the fact that the total momentum of the system is a constant of the motion. The total momentum operator is $\Sigma_k \mathbf{k}\alpha_k^*\alpha_k + \mathbf{p}$ and commutes with the Hamiltonian, (1). It is therefore possible to transform to a representation in which the total momentum operator is diagonal and in which the Hamiltonian no longer contains the particle coordinates. The unitary transformation required is generated by

$$S = \exp i[(\mathbf{P} - \Sigma_k \alpha_k^* \alpha_k \mathbf{k}) \cdot \mathbf{r}],$$

which transforms

$$H \rightarrow S^{-1}HS = (\mathbf{P} - \Sigma_k \mathbf{k}\alpha_k^*\alpha_k)^2/2m + \Sigma_k \omega(k)\alpha_k^*\alpha_k + g\Sigma_k(V_k\alpha_k + V_k^*\alpha_k^*), \quad (2)$$

where $\mathbf{P}$ is a "$c$" number representing the total system momentum.

Let us first consider the case in which $P=0$. We shall use a variational technique and work in a representation in which the Schrödinger function $\Psi$ of our system is described by a set of functions corresponding respectively to states of no quanta, one quantum, two quanta, etc. Let $\langle \mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N/\Psi\rangle$ be the probability amplitude of finding $N$ quanta of momenta $\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N$ respectively in the field around the source particle, assuming these quanta are distinguishable. A trial function which corresponds to allowing field quantum emission into one of four possible states is

$$\langle k_1\cdots k_N/\Psi\rangle = C_{n,m_1,m_2,m_3}(n!\prod_i m_i!/N!)^{\frac{1}{2}} \times S[\prod_{i=1}^{n} f(k_i) \prod_{j_1=n+1}^{n+m_1} g_x(k_{j_1}) \prod_{j_2=n+m_1+1}^{n+m_1+m_2} g_y(k_{j_2}) \times \prod_{j=n+m_1+m_2+1}^{N} g_z(k_{j_3})], \quad (3)$$

where $f(k)$ is a normalized "$s$" wave function for the field quanta, and the $g_x(k)$, etc., are the three normalized "$p$" wave functions. $C_{n,m_1,m_2,m_3}$ is the probability amplitude for finding $n$ "$s$" quanta, and $m_1$, $m_2$, and $m_3$ of the three kinds of "$p$" quanta, respectively. $S$ is the symmetrization operator with respect to all quanta, and we also have

$$n + m_1 + m_2 + m_3 = N,$$

where $N$ may vary from zero to infinity. The functional form of $f(k)$ and $g_i(\mathbf{k})$, together with the numerical value of the $C_{n,m_1,m_2,m_3}$, are to be determined in such a way as to minimize the system energy. It is clear that since no preferred direction exists (for $P=0$), our three "$p$" state wave functions must have the same radial dependence. Thus we have

$$g_i = (k_i\sqrt{3}/k)g(k), \quad (i = x, y, z), \quad (4)$$

where $g(k)$ is a normalized "$s$" wave function.

The calculation of this mean energy for a trial function of the form (3) is quite complicated. However, the manipulations in such mean value calculations may be simplified considerably by going over to a suitable reduced space for the operators $\alpha_k$ and $\alpha_k^*$. In Appendix I, we show that if the Hamiltonian is ordered in such a way that *annihilation operators always appear on the right of creation operators*, then these operators may be formally replaced by

$$\alpha_k \rightarrow \alpha f(k) + \Sigma_i \beta_i k_i[\sqrt{3}g(k)/k], \quad (5)$$

with a corresponding expression for $\alpha_k^*$. $\alpha$ and $\beta_i$ are the annihilation operators for "$s$" and "$p$" wave quanta and are independent of $k$. The problem of finding the minimum energy for the Hamiltonian (2) then reduces to solving the equivalent minimum value problem in the reduced space,

$$\delta E = \delta\langle\Phi|\mathfrak{IC}|\Phi\rangle = 0, \quad (6)$$

where $\Phi$ is a normalized reduced space wave vector, and $\mathfrak{IC}$ is given by

$$\mathfrak{IC} = \omega_1\alpha^*\alpha + \omega_2 \sum_{i=x}^{z} \beta_i^*\beta_i + g(V\alpha + V^*\alpha^*) + M\sum_{i=x}^{z}[(\beta_i^*)^2\alpha^2 + (\alpha^*)^2\beta_i^2 + 2\alpha^*\beta_i^*\alpha\beta_i], \quad (7)$$

where[4]

$$\omega_1 = \Sigma_k(\omega + k^2/2m)|f(k)|^2, \quad (8a)$$

$$\omega_2 = \Sigma_k(\omega + k^2/2m)|g(k)|^2, \quad (8b)$$

$$V = \Sigma_k V(k)f(k), \quad (8c)$$

$$M = [\Sigma_k f^*(k)g(k)k]^2/6m. \quad (8d)$$

In carrying out the variation of $E$ with respect to $\Phi$, we shall restrict our trial function to the form

$$\Phi = [\exp(\alpha^* u)]F(\beta_i^*)|0\rangle, \quad (9)$$

where $u$ is an arbitrary real numerical constant (to be determined variationally) and $F$ is an arbitrary function of $\beta_i$. $|0\rangle$ is the state vector corresponding to no quanta in the field. This choice will be seen to be sufficiently general to enable us to obtain an exact solution in the limit of both strong and weak coupling. Using (9), we see that

$$\alpha\Phi = u\Phi,$$

and thus

$$\mathfrak{IC}\Phi = [(\omega_1 - 3M)u^2 + 2guV + \omega_2\Sigma_i\beta_i^*\beta_i + Mu^2\Sigma_i(\beta_i + \beta_i^*)^2]\Phi. \quad (10)$$

The ground-state energy corresponding to (10) may

[3] Both $\hbar$ and the system volume will be taken $=1$ throughout this paper.

[4] It will be seen that $V$ and $M$ are both real.

readily be obtained, since the eigenvalue problem is just that of three simple harmonic oscillators. We find

$$E=(\omega_1-3M)u^2+2guV+\tfrac{3}{2}\omega_2[(1+4Mu^2/\omega_2)^{\frac{1}{2}}-1]. \quad (11)$$

Thus our minimum value problem becomes one of minimizing $E$ with respect to the parameter $u$ and the arbitrary functional form of $f(k)$ and $g(k)$.

We now wish to examine the solution of our minimum value problem in the limit of both weak and strong coupling. For both these limits, on differentiating (11) with respect to $u$ it may easily be seen that $u$ will be proportional to $g$. In the weak coupling case, $(g\ll 1)$, we find on expanding in a power series in $g$,

$$E=\omega_1u^2+2guV+O(g^3)+\cdots, \quad (12)$$

so that the minimum value of the energy with respect to $u$ is

$$E=-g^2V^2/\omega_1. \quad (13)$$

In this limit, $E$ depends only on $f(k)$. This follows from the fact that in our Hamiltonian the interaction term between the source particle and the field quanta directly excites only "$s$" waves, and hence just involves $f(k)$. The "$p$" waves are coupled to the source indirectly through their coupling with the "$s$" waves via the recoil term. Consequently in the limit of weak coupling these will only influence the energy for higher power of $g$.

Upon minimizing $E$ with respect to an arbitrary functional variation of $f(k)$ we find the best form of $f(k)$ is

$$f(k)=\frac{N_1V^*(k)}{\omega+k^2/2m}, \quad (14)$$

where $N_1$ is a normalization constant. The corresponding minimum value for the energy is

$$E_0=-g^2\sum_k\frac{|V(k)|^2}{\omega+k^2/2m}. \quad (15)$$

This is precisely the familiar expression derivable from second-order perturbation theory.

For the strong coupling limit $(g\gg 1)$, we find on expanding in a power series in $(1/g)$.

$$E=[(\omega_1-3M)u^2+2guV][1+O(1/g)], \quad (16)$$

so that minimum value of the energy with respect to $u$ is

$$E=-g^2V^2/(\omega_1-3M). \quad (17)$$

Upon minimizing $E$ with respect to an arbitrary functional variation of $f(k)$ and $g(k)$ we find these take the following optimum forms:

$$f(k)=N_1V(k)/\omega(k), \quad (18a)$$

$$g(k)=N_2f(k)k, \quad (18b)$$

where $N_1$ and $N_2$ are normalization constants. The corresponding minimum value for the energy is

$$E_0=-g^2\sum_k\frac{|V(k)|^2}{\omega(k)}. \quad (19)$$

To show that this is indeed the exact solution in the strong coupling limit, we return to our original Hamiltonian, (2). We note that if the recoil terms, $(\Sigma_k\mathbf{k}\alpha_k^*\alpha_k)^2/2m$, were absent, the minimum value of the energy would be just (19). The recoil term is, however, always positive, so that (19) constitutes a lower bound for the energy. On the other hand, $E_0$ is the result of a variational calculation and is hence an upper bound for the ground-state energy. Since the upper and lower bounds here coincide, $E_0$ must be the exact ground-state energy.

The magnitude of the recoil term can be obtained by carrying out the expansion of (16) in powers of $(1/g)$ to the next order, and one finds that it is of order $g$. Since the total number of quanta $(N=\alpha^*\alpha+\Sigma_i\beta_i^*\beta_i)$ is on the average proportional to $g^2$, this result indicates that the mean square momentum fluctuation of the source particle, $\langle p^2\rangle_{\text{Av}}$, is proportional to $\langle N\rangle_{\text{Av}}^{\frac{1}{2}}$. If there were no correlation between the direction of emission of successive quanta by the source particle, $\langle p^2\rangle_{\text{Av}}$ would be proportional to $\langle N\rangle_{\text{Av}}$. Consequently in the strong coupling limit these correlations are seen to play a very important role by acting in such a way as to limit the recoil kinetic energy to order $g$.[5]

It is perhaps surprising that one can obtain an exact solution in the strong coupling case by using a simple trial function of the form (3) and (9). This may be understood in the following way. As we have remarked, in the general Hamiltonian (2), the source is directly coupled only to "$s$" waves. This coupling is linear in the amplitude of the "$s$" waves, and thus its main effect is to produce a simple displacement in the "$s$" wave amplitude, as reflected in our restricted trial wave function (9). The number of "$s$" quanta in the field is then proportional to $g^2$. On the other hand, the recoil term may be regarded as giving rise to a dipole-type coupling between the field quanta, i.e., "$s$" waves are coupled only with "$p$" waves, which in turn are coupled in addition just to "$d$" waves, etc. In virtue of this coupling, which according to (10) gives rise to a change in frequency for the "$p$" waves, the number of "$p$" wave quanta is proportional to the square root of the number of "$s$" wave quanta and hence to $g$. Since the "$d$" wave couples to the "$p$" wave in similar fashion, the total number of "$d$" wave quanta will be of still higher order in $1/g$, and their influence may be neglected, corresponding to our trial function (3).

For intermediate coupling strengths, the ground-

[5] A direct calculation of the strong coupling limit in this problem is also possible, provided one introduces creation and annihilation operators for spherical waves, rather than the plane waves used in (1). Similar results concerning the ground-state energy and the role of the source recoil can be obtained.

state energy depends on the specific form of $V(k)$, and we shall not enter on a general discussion of this here. In the following section we shall consider the detailed solution in this range of coupling for the polaron problem. It may be of interest to note here that the general form of $f(k)$ and $g(k)$ can be obtained by minimizing $E$ with respect to arbitrary functional variations of $f(k)$ and $g(k)$, under the constraint that these functions are normalized. We find these may be written as

$$f(k)=\frac{N_1 V_k^*(k^2+2m\omega+\lambda)}{(k^2+2m\omega)^2+\mu(k^2+2m\omega)+\gamma+\eta k^2}, \tag{20}$$

$$g(k)=\frac{N_2 fk}{k^2+2m\omega+\lambda}, \tag{21}$$

where $N_1$ and $N_2$ are normalization constants, and $\lambda$, $\mu$, $\gamma$, $\eta$ are numerical constants to be determined by our variational calculation.

## III

We now wish to apply the above considerations to a determination of the ground state energy of the polaron. In this case, we have from LLP,

$$V_k=-\frac{\omega i}{k}\left(\frac{8\pi^2}{m\omega}\right)^{\frac{1}{4}}, \tag{22}$$

$$g^2=\frac{e^2}{2c}\left(\frac{2mc^2}{\omega}\right)^{\frac{1}{2}}\left(\frac{1}{n^2}-\frac{1}{\epsilon}\right), \tag{23}$$

where $n$ and $\epsilon$ are the optical index of refraction and the static dielectric constant, respectively, and $\omega$ is the constant frequency of the longitudinal optical mode of the lattice vibrations.[6] There exists a natural cutoff for our interaction in $k$ space, $k_0$, due to the discrete nature of the crystal structure, and we shall understand that in this section $k$ is always considered to be less than $k_0$. For the continuum theory of lattice vibrations, $k_0$ is the usual Debye limit.

For the case of the polaron, our weak coupling solution, (15), becomes, on substituting (22),

$$E_0=-g^2\omega, \tag{24}$$

a solution first obtained by Frohlich, Pelzer, and Zienau.[7] In the strong coupling limit, in contrast to weak coupling, the cutoff $k_0$, plays an important role, and we find from (19) and (22)

$$E_0=-\frac{2}{\pi}\left(\frac{k_0^2}{2m\omega}\right)^{\frac{1}{2}}g^2\omega. \tag{25}$$

It is of some interest to investigate the region of validity of our strong coupling solution, (25). This can be estimated by a consideration of the importance of the terms neglected in (16), and one finds that the strong coupling limit is valid when

$$g\gg\tfrac{3}{2}(M\omega_2/V^2)^{\frac{1}{4}}. \tag{26}$$

On substituting (8) and (18) into (26) we find

$$g^2\gg(3/40\pi)(k_0^2/2m\omega)^{\frac{1}{2}}. \tag{27}$$

For typical polar crystals $k_0^2/2m\omega\sim100$, and hence the criterion for the validity of the strong coupling solution is

$$g^2\gg25.$$

For real polar crystals, the coupling constant $g^2$ is generally of the order of 3 to 6, so that neither the weak nor strong coupling solutions are valid. Thus it is necessary to find the minimum value of $E$, (11), more precisely. The calculation is straightforward, albeit somewhat complicated, and the details are given in Appendix II. The results of a numerical calculation for three values of the coupling constant $g^2$ are given in Table I. We note that $-E_0/\omega$ is always greater than

TABLE I. Ground-state energy and polaron effective mass for three values of the coupling constant.

| $g^2$ | $-E_0/\omega$ | $m_{\text{eff}}/m$ | $1+g^2/6$ |
|---|---|---|---|
| 5.2 | 5.52 | 2.21 | 1.86 |
| 10 | 11.17 | 3.96 | 2.67 |
| 15 | 17.56 | 6.35 | 3.50 |

$g^2$, the result obtained by perturbation theory and also by the simple one-phenon state Tomonaga approximation of LLP. However, as anticipated by LLP, for the case of NaCl, where $g^2=5.2$, the correction is quite small, being of the order of five percent.

## IV

In this section we consider the calculation of the effective mass of the source particle for the general Hamiltonian, (2). In order to do this, we must consider the case in which our Hamiltonian (2) describes a system for which $P\neq0$. We will however confine our attention to very small system momenta, such that $(P^2/2m\omega)\ll1$. For the effective mass is defined by the relation,

$$\frac{1}{2m_{\text{eff}}}=\left(\frac{\partial E}{\partial P^2}\right)_{P^2=0}, \tag{28}$$

and hence it is sufficient to calculate $E$ to order $P^2$.

When $P\neq0$ it is necessary to adopt a somewhat more general trial function than that given in (3). This may be done by introducing in place of the spherically symmetric $f(k)$ an arbitrary function $F(k)$ which is normalized and orthogonal to the $g_i(k)$. The functional forms of $F(k)$ and $g_i(k)$ again are determined by the variational principle. Since we are only interested in

[6] Here $g^2$ denotes the coupling constant instead of $\alpha$ as used by LLP.

[7] Frohlich, Pelzer, and Zienau, Phil. Mag. 41, 221 (1950).

calculating $E$ to order $P^2$, it will be sufficient to use a wave function which is accurate to order $P$. To this order, the $g_i(k)$ are found to be unchanged. However, $F(k)$ differs from the spherically symmetric $f(k)$ by the addition of a "$p_z$" wave, i.e.,

$$F(k)=f(k)+(dk_z\sqrt{3}/k)h(k)P+O(P^2),$$

where $d$ is a constant, $h(k)$ is a spherically symmetric function, and we have taken $\mathbf{P}$ in the $z$ direction. The presence of a "$p_z$" wave in $F(k)$ thus corresponds to a removal of the symmetry among the "$p$" waves and is to be expected since for $P\neq 0$ a preferred direction exists, namely that of $\mathbf{P}$.

The effective mass calculation is similar to that for the ground-state energy and is given in Appendix III, where we derive the following expression for the source particle effective mass,

$$m_{\text{eff}}/m=1+(4/3)\Sigma_k|f(k)|^2\{k^2/[k^2+2m\omega(k)]\}u^2, \quad (29)$$

where $u$ and $f(k)$ are determined by the $P=0$ calculation. It may be seen directly that this expression reduces to the appropriate perturbation theory value in the limit of weak coupling. However, in contrast to the $P=0$ calculation, our expression (29) cannot be regarded as yielding the correct strong coupling limit, since the latter expression is not yet known.

For the polaron, we utilize the numerical results following from Appendix II, and the results of our calculation for three values of the coupling constant are given in Table I. There we have compared these new results with that obtained by LLP

$$m_{\text{eff}}/m=1+\tfrac{1}{6}g^2.$$

We remark that in general the change in effective mass due to our consideration of additional "$p$" wave phonon excitation is in the direction of increasing $m_{\text{eff}}$. Percentage-wise this correction is considerably large for $m_{\text{eff}}$ than for the corresponding ground state energy calculation. For $g^2=5.2$, we find an increase of $\sim$twenty percent in $m_{\text{eff}}$ over the LLP value, which is in good agreement with their estimate of the accuracy of their method. This leads us to believe that the present calculation is quite reliable for such intermediate coupling strengths.

We should like to thank Professors J. Bardeen, M. Gell-Mann, and F. Low for pleasant discussions on these and related matters.

## APPENDIX I

In this appendix we should like to establish some elementary theorems concerning the use of Tomonaga-type wave functions. For simplicity we confine our attention to a trial function which corresponds to allowing field quantum emission into one of two possible states, which are described by any two orthonormal functions $f(k)$ and $g(k)$. Thus

$$\langle k_1\cdots k_n|\Psi\rangle=C_{n-m,m}\left(\frac{(n-m)!m!}{n!}\right)^{\frac{1}{2}}\times\mathcal{S}[\prod_{i=1}^{n-m}f(k_i)\prod_{j=n-m+1}g(k_i)],$$

where $\mathcal{S}$ is the symmetrization operator with respect to all quanta. The system wave function $\Psi$ may then be expressed in terms of the vacuum state as

$$\Psi=\sum_{n=0}^{\infty}\sum_{m=0}^{n}C_{n-m,m}\frac{1}{[(n-m)!m!]^{\frac{1}{2}}}\times(\sum_k f(k)\alpha_k^*)^{n-m}(\sum_k g(k)\alpha_k^*)^m|0\rangle,$$

where $|0\rangle$ denotes the vacuum state. Consider now a reduced space wave vector defined by

$$\Phi=\sum_{n=0}^{\infty}\sum_{m=0}^{n}D_{n-m,m}\frac{1}{[(n-m)!(m!)]^{\frac{1}{2}}}(\alpha^*)^{n-m}(\beta^*)^m|0\rangle,$$

where $\alpha^*$ and $\beta^*$ are two independent creation operators which are not related to $k$. $\Phi$ and $\Psi$ will be considered to describe equivalent physical situations if and only if $D_{n-m,m}=C_{n-m,m}$.

Theorem 1: If $\Psi\leftrightarrow\Phi$ and $\Psi'\leftrightarrow\Phi'$ then $\langle\Psi'|\Psi\rangle=\langle\Phi'|\Phi\rangle$. Proof:

$$\langle\Psi'|\Psi\rangle=\sum_{n=0}^{\infty}\sum_{m=0}^{n}(C'_{n-m,m})^*(C_{n-m,m})$$

is by definition the same as $\langle\Phi'|\Phi\rangle$.

Theorem 2: If $\Psi\leftrightarrow\Phi$, then $\alpha_k\Psi\leftrightarrow[\alpha f(k)+\beta g(k)]\Phi$. Proof: The coefficient of the term $(\Sigma_k f(k)\alpha_k^*)^{n-m}\times(\Sigma_k g(k)\alpha_k^*)^m|0\rangle$ in $\alpha_k\Psi$ is

$$[C_{n-m+1,m}(n-m+1)^{\frac{1}{2}}f(k)+C_{n-m,m+1}(m+1)^{\frac{1}{2}}g(k)]\times\frac{1}{[(n-m)!m!]^{\frac{1}{2}}},$$

which is the same as the corresponding coefficient of the term $(\alpha^*)^{n-m}(\beta^*)^m|0\rangle$ in $[\alpha f(k)+\beta g(k)]\Phi$. We remark that $\alpha_k^*\Psi$ is by no means equivalent to $[\alpha^* f(k)+\beta^* g(k)]\Phi$.

Theorem 3: If $\Psi\leftrightarrow\Phi$, and $\Psi'\leftrightarrow\Phi'$, then

$$\langle\Psi'|\prod_{i=1}^{N}\alpha_{k_i}^*\prod_{j=1}^{M}\alpha_{k_j}|\Psi\rangle=\langle\Phi'|\prod_{i=1}^{N}[\alpha^*f^*(k_i)+\beta^*g^*(k_i)]\prod_{j=1}^{M}[\alpha f(k_j)+\beta g(k_j)]|\Phi\rangle.$$

Proof: From Theorem 2, one has

$$\prod_{j=1}^{M}\alpha_{k_j}\Psi\leftrightarrow\prod_{j=1}^{M}[\alpha f(k_j)+\beta g(k_j)]\Phi.$$

and

$$\prod_{i=1}^{N}\alpha_{k_i}\Psi'\leftrightarrow\prod_{i=1}^{N}[\alpha f(k_i)+\beta g(k_i)]\Phi'.$$

Thus on using Theorem 1, one sees that Theorem 3 follows immediately.

These theorems can obviously be generalized to trial functions which allow quantum emission into one of any number of possible states.

## APPENDIX II

For the case of the polaron for which $\omega$ is a constant, our general trial functions, (20) and (21), may be written as

$$f(k)=\frac{N_1 V_k^*(k^2+a^2)}{(k^2-b^2)^2+c^2k^2},$$

$$g(k)=\frac{N_2 k V_k^*}{(k^2-b^2)^2+c^2k^2},$$

where $a$, $b$, $c$ are numerical constants to be determined. On substituting these expressions into (8a)–(8d), together with our expression (22) for $V_k$, we find, on changing the summation over $k$ to an integral, and carrying out the indicated integrations,[8]

$$\omega_1=\omega\left\{1+\frac{c^2+(1+a^2/b^2)^2b^2}{(1+a^2/b^2)^2+a^4c^2/b^6}\right\},$$

$$\omega_2=\omega(1+b^2),$$

$$M=-\frac{\omega}{3}\frac{b^2[1+(a^2/b^2)^2]}{(1+a^2/b^2)^2+a^4c^2/b^6},$$

$$V^2=6Mc\omega/b^2.$$

In obtaining these expressions, we have introduced dimensionless variables, in that all momenta ($k$, $a$, $b$, $c$) are measured in units of $(2m\omega)^{\frac{1}{2}}$. We then find that our general expression for $E$, (11) may be written as

$$\frac{E}{\omega}=\left[\frac{(1+a^2/b^2)^2+a^4c^2/b^6+c^2}{b^2(1+a^2/b^2)^2}\right][1+b^2]x^2+\frac{2g[(1+b^2)(2c)]^{\frac{1}{2}}x}{b}+\tfrac{3}{2}(1+b^2)\times\{[1+(4x^2/3)]^{\frac{1}{2}}-1\},\quad\text{(A1)}$$

where we have found it convenient to introduce

$$x^2=\frac{b^2(1+a^2/b^2)^2u^2}{(1+b^2)[(1+a^2/b^2)^2+a^4c^2/b^6]}$$

as a new independent variable in place of $u^2$. Thus our minimum value problem is reduced to minimizing (A1) with respect to the four parameters $a$, $b$, $c$, and $x$.

On varying (A1) with respect to $a$, one finds the simple result:

$$a^2=b^4.\quad\text{(A2)}$$

On minimizing (A1) with respect to $c$, one finds

$$c=[g^2b^2(1+b^2)/2x^2]^{\frac{1}{3}}.\quad\text{(A3)}$$

Using these relationships, and minimizing with respect to $x$ and $b$, one finds, after considerable simplification,

$$b^2=1+[1+(4/3)x^2]^{\frac{1}{2}},\quad\text{(A4)}$$

$$x^2=\frac{g^2b^2}{2(1+b^2)^{\frac{1}{2}}}\left(\frac{b^2-1}{2b^2-1}\right)^{\frac{3}{2}}.\quad\text{(A5)}$$

The corresponding value for the energy, (A1), is

$$\frac{E}{\omega}=-\frac{(1+b^2)(5b^2-2)x^2}{b^2(b^2-1)}+\tfrac{3}{2}(1-b^2)(b^2-2).\quad\text{(A6)}$$

Equations (A4) and (A5) may then be solved numerically to obtain the optimum values of $b$ and $x$, which on substitution into (A6) yield the minimum value of the ground state energy $E_0$. The results for three values of the coupling constant are given in Table I.

## APPENDIX III

As we have remarked, it is necessary to adopt a somewhat more general trial function than (3) for the case of $\mathbf{P}\neq 0$. This may be done by introducing an arbitrary function $F(\mathbf{k})$ in place of the "$s$" wave function $f(k)$. $F(\mathbf{k})$ is normalized and orthogonal to the $g_i(k)$. For small $P$, we may expand $F(\mathbf{k})$ as

$$F(\mathbf{k})=f(k)+d(k_z\sqrt{3}/k)h(k)P+O(P^2)+\cdots,$$

where $h(k)$ is symmetric. This form of $F(\mathbf{k})$ is just that adopted by LLP in the simple Tomonaga case. Thus we may regard our trial function in this case, just as was true for $P=0$, as a generalization of the LLP treatment in that we have simply added three "$p$" waves to take the correlation between quanta into account. One may then proceed to calculate the dependence of $E$ on $P^2$ in a completely analogous manner to our $P=0$ calculation, with the difference that the energy should now be varied with regard to $d$ and the functional form of $h(k)$ in addition to the other indicated variations. One finds that

$$E=(\omega_1-3M)u^2+2gVu+\tfrac{3}{2}\omega_2[(1+4Mu^2/\omega^2)^{\frac{1}{2}}-1]+\frac{P^2}{2m}-P^2\left\{\frac{[(M/m)^{\frac{1}{2}}u-\frac{1}{2}\omega_4 ud-2(2MN)^{\frac{1}{2}}u^3d]^2}{\frac{1}{2}\omega_2+2Mu^2}+(4Nu^2+\omega_3)u^2d^2-2(2N/m)^{\frac{1}{2}}u^2d\right\},\quad\text{(A7)}$$

where $M$, $\omega_1$, $\omega_2$, and $V$ are defined in (8a)–(8d) and $N$, $\omega_3$, $\omega_4$ are

$$N=(\Sigma_k h^*gk)^2/6m,$$

$$\omega_3=\Sigma_k|h|^2(\omega+k^2/2m),$$

$$\omega_4=\Sigma_k h^*g(\omega+k^2/2m).$$

[8] The upper limit of integration may be taken as $\infty$ to a good degree of approximation as long as $g^2<15$.

By inspection, we note that the optimum values for $f(k)$, $g(k)$, and $u$ will differ from those obtained for $P=0$ only to order $P^2$. Consequently, this difference will contribute a change in the energy of order $P^4$ which may be neglected in our approximation of small $P$. Thus the determination of the effective mass reduces to finding that form of $d$ and $h(k)$ which minimize (A7). This problem can, however, be simplified further by introducing an equivalent variational problem. This equivalent problem is obtained by regarding the operator $\beta_z$ as a numerical constant. It may be readily verified that although this replacement yields a different value for $E_0$, the $P^2$ coefficient in the energy is unchanged, and it is this latter value which we seek to determine. Thus we write for our equivalent problem

$$\alpha_k \rightarrow \alpha[f(k)+\eta P\varphi(k)(k_z/k)\sqrt{3}] + (\beta_x k_x+\beta_y k_y)\sqrt{3}g(k)/k, \quad \text{(A8)}$$

instead of

$$\alpha_k \rightarrow \alpha F(k)+\sum_{i=x}^{z}\beta_i k_i\sqrt{3}g(k)/k.$$

In (A8), $\eta$ is an arbitrary parameter and $\varphi(k)$ is a symmetric function which may be regarded as a linear combination of $g(k)$ and $h(k)$. Using (A8), we find that the $P^2$ terms in the energy may be written as

$$E_{\mathrm{I}}(P)=P^2\left(\frac{1}{2m}+\eta^2u^2\omega'-4\eta u^2\left(\frac{M'}{2m}\right)^{\frac{1}{2}}+4M'u^4\eta^2\right), \quad \text{(A9)}$$

where

$$M'=[\Sigma_k\varphi^*(k)f(k)k]^2/6m,$$
$$\omega'=\Sigma_k(\omega+k^2/2m)\,|\,\varphi(k)\,|^2.$$

Upon minimizing (A9) with respect to $\eta$, we find

$$E_{\mathrm{I}}=\frac{P^2}{2m}\frac{1}{1+4M'u^2/\omega'}. \quad \text{(A10)}$$

The variation with respect to $\varphi(k)$ is elementary and gives

$$\varphi(k)=N_3\frac{f(k)k}{k^2+2m\omega(k)}, \quad \text{(A11)}$$

where $N_3$ is a normalization constant. It is of interest to note that the corresponding best form of $h(k)$ is

$$h(k)=N_4\{\varphi(k)-[\Sigma_k\varphi(k)g^*(k)]g(k)\}.$$

On substituting (A11) into (A10), we obtain the effective mass,

$$\frac{m_{\mathrm{eff}}}{m}=1+u^2(4/3)\sum_k\frac{|f(k)|^2k^2}{(k^2+2m\omega(k))}.$$