On the excitonic-polaron theory in angular variables

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The model of an electron bound to an impurity (or to a core hole) and interacting with a boson field is analyzed in terms of bosonic variables *symmetry adapted* to the spherical symmetry about the impurity center. It is shown that the use of this appropriate set of variables considerably simplifies the solution of the variational problem based on a Lee–Low–Pines-type of ansatz for the ground-state variational wave function.

I. INTRODUCTION

Quasiparticle excitations may sometimes be envisaged as built up by coupling a bare electron (or hole) to a boson field. Well-known examples are the polaron[1] and the plasmaron[2] where the "dressing" of the bare excitation is provided by the coupling to (optical) phonons and to plasmons, respectively. In all cases one starts by reducing the problem to the solution of a model Hamiltonian with a *linear coupling* between the bare particle and the boson field, and then proceeds to determine its ground state and lowest excited states by a variational procedure. Methods of solution differ at this stage, as they are based either on the use of the so-called "coherent states"[3] or on the Feynman path integral approach.[4]

In the problem above one can take full advantage of the conservation of the *total* linear momentum since the medium in which the bare particle is embedded is regarded as being homogeneous and isotropic. The presence of an impurity center (such as a localized core hole) spoils, however, the conservation of linear momentum and makes it apparently more difficult to solve the variational problem. In particular, if the additional interaction between the bare particle and the impurity center can sustain bound states, one is interested in determining the binding energy of the bound quasiparticle. Examples are the bound polaron in ionic insulators and (core) excitons in semiconductors.

Since the presence of an impurity center destroys the homogeneity but not the isotropy, the *total angular momentum* about the impurity center is still a conserved quantity and one may make use of this conservation explicitly to simplify the solution of the variational problem. As previous treatments of this problem based on the use of coherent states[5,6] do not seem to have fully exploited the conservation of angular momentum, we provide in this note the mathematical framework based on this conservation law. Possible applications (such as to the physics of the metallic rare earths) and extensions to systems with lower symmetry remain open.

II. ANGULAR VARIABLES FOR THE BOSON FIELD

For the sake of definiteness, we consider the problem of an electron and a core hole (or impurity) localized at $\mathbf{r} = 0$, which interact among themselves through a *spherically symmetric* bare potential $v_b(r)$. Both particles are also coupled to a plasmon field which provides the screening to $v_b(r)$. The total Hamiltonian can be written as[2,7,8] ($\hbar = 1$)

$$\hat{H} = \frac{\mathbf{p}^2}{2m^*} + v_b(r) + \sum_{\mathbf{k}} \omega_{|\mathbf{k}|} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \left(W_{\mathbf{k}}(\mathbf{r}) \hat{a}_{\mathbf{k}} + W^*_{\mathbf{k}}(\mathbf{r}) \hat{a}^\dagger_{\mathbf{k}} \right). \quad (2.1)$$

Here $\hat{a}_{\mathbf{k}}$ and $\hat{a}^\dagger_{\mathbf{k}}$ are annihilation and creation operators for plasmons with wave vector **k** that satisfy the usual commutation relation

$$[\hat{a}_{\mathbf{k}}, \hat{a}^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}; \quad (2.2)$$

$\omega_{|\mathbf{k}|}$ is the plasmon dispersion relation that we may conveniently take of the form[8]

$$\omega_{|\mathbf{k}|} = \omega_p + \mathbf{k}^2/2m, \quad (2.3)$$

where ω_p is the plasma frequency and m is the (bare) electronic mass; $W_{\mathbf{k}}(\mathbf{r})$ is the coupling between the electron (e) and the core hole (h) with the plasmons

$$W_{\mathbf{k}}(\mathbf{r}) = V^e_{\mathbf{k}}(\mathbf{r}) + V^h_{|\mathbf{k}|}, \quad (2.4)$$

where

$$V^e_{\mathbf{k}}(\mathbf{r}) = \bar{V}^e_{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{r}},$$
$$\bar{V}^e_{\mathbf{k}} = [v(\mathbf{k})\omega_p^2/2\Omega\omega_{|\mathbf{k}|}]^{1/2}, \quad (2.5)$$

and

$$V^h_{|\mathbf{k}|} = -S_c(|\mathbf{k}|)\bar{V}^e_{|\mathbf{k}|}, \quad (2.6)$$

$v(\mathbf{k}) = 4\pi e^2/k^2$ being the Fourier transform of the Coulomb potential, Ω the (quantization) volume, and $S_c(|\mathbf{k}|)$ the structure factor of the core hole. In Eq. (2.1) the effective electronic mass m^* includes possible band-structure effects.

The model Hamiltonian (2.1) treats the excitations of the (metallic) background, wherein the electron and the impurity center are embedded, in terms of "collective variables."[9] Other forms of the coupling (2.5) are possible when the background represents, e.g., electron-hole pair excitations in a semiconductor[10] or optical phonons in an ionic material.[1] In all cases the Hamiltonian can be cast in the form (2.1).

In the absence of the electron, the Hamiltonian that results from (2.1) describes the relaxation about the impurity and can be solved exactly in terms of "displaced" plasmon oscillators.[11] When the sole electron is present, on the other

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hand, the Hamiltonian that results from (2.1) commutes with the total linear momentum operator

$$\hat{\mathscr{P}} = -i\nabla + \sum_{\mathbf{k}} \mathbf{k}\, \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}, \tag{2.7}$$

because virtual creations or absorptions of plasmons are compensated by the recoil of the electron. This fact is indeed essential for the variational treatment in terms of coherent states[3] in order to obtain the effective mass of the electron due to "dressing" by the boson field, i.e., for obtaining not only the ground state but also the low-lying excited states of the Hamiltonian.

Since the medium about the impurity center is isotropic [cf., Eqs. (2.3) and (2.6)], the Hamiltonian (2.1) should not be affected by rotating the electron *and* the medium simultaneously about the center. To show this invariance explicitly, it is convenient first to rewrite Eq. (2.1) in an alternative form by transforming canonically the boson operators into the angular momentum representation:

$$\begin{aligned} \hat{\underset{\sim}{a}}(k\ell m) &= k\left[\frac{\Omega}{(2\pi)^3}\right]^{1/2} \int_{4\pi} d\hat{k}\, Y^*_{\ell m}(\hat{k}) \hat{a}_{\mathbf{k}}, \\ \hat{\underset{\sim}{a}}^{\dagger}(k\ell m) &= k\left[\frac{\Omega}{(2\pi)^3}\right]^{1/2} \int_{4\pi} d\hat{k}\, Y_{\ell m}(\hat{k}) \hat{a}^{\dagger}_{\mathbf{k}}, \end{aligned} \tag{2.8}$$

where the tilde signifies that taking the continuum limit is understood before performing the angular integration. One may readily verify that the new operators satisfy the commutation relation

$$[\hat{\underset{\sim}{a}}(k\ell m), \hat{\underset{\sim}{a}}^{\dagger}(k'\ell'm')] = \delta(k-k')\delta_{\ell\ell'}\delta_{mm'}. \tag{2.9}$$

Expanding the plane wave in Eq. (2.5) into spherical harmonics of $\hat{k}$ and $\hat{r}$ and using the orthonormality of the spherical harmonics, we can then rewrite the Hamiltonian (2.1) as follows:

$$\begin{aligned} \hat{H} &= \frac{\mathbf{p}^2}{2m^*} + v_b(r) + \int_0^{\infty} dk\, \omega_k \sum_{\ell m} \hat{\underset{\sim}{a}}^{\dagger}(k\ell m)\hat{\underset{\sim}{a}}(k\ell m) \\ &\quad + \int_0^{\infty} dk\, \mathscr{V}^h_{k0}(\hat{\underset{\sim}{a}}(k0) + \hat{\underset{\sim}{a}}^{\dagger}(k0)) \\ &\quad + \int_0^{\infty} dk \sum_{\ell m} (\mathscr{V}^e_{k\ell m}(\mathbf{r})\hat{\underset{\sim}{a}}(k\ell m) \\ &\quad + \mathscr{V}^e_{k\ell m}(\mathbf{r})^* \hat{\underset{\sim}{a}}^{\dagger}(k\ell m)), \end{aligned} \tag{2.10}$$

where we have introduced the notation

$$\begin{aligned} \mathscr{V}^e_{k\ell m}(\mathbf{r}) &= \mathscr{V}^e_{kl}(r) Y_{lm}(\hat{r}), \\ \mathscr{V}^e_{kl}(r) &= 4\pi k\left[\frac{\Omega}{(2\pi)^3}\right]^{1/2} \overline{V}^e_{|\mathbf{k}|}\, i^l j_l(kr), \end{aligned} \tag{2.11}$$

and

$$\mathscr{V}^h_{k0} = 4\pi k\,[\Omega/(2\pi)^3]^{1/2}\, V^h_{|\mathbf{k}|}\, Y_{00}(\hat{r}), \tag{2.12}$$

$j_l(kr)$ being the spherical Bessel function of order l and i the imaginary unit. Notice that Eq. (2.10) allows one to analyze the plasmon relaxation into *multipole components*. By the same token, one sees from Eq. (2.10) that only the "monopole" relaxation couples to the spherically symmetric core hole.

Simultaneous rotations of the electron and the plasmon background can now be achieved in terms of the total angular momentum operators

$$\begin{aligned} \hat{L}_+ &= \ell_+ + \int_0^{\infty} dk \sum_{lm} [\ell(\ell+1) - m(m+1)]^{1/2} \\ &\quad \times \hat{\underset{\sim}{a}}^{\dagger}(k\ell m+1)\hat{\underset{\sim}{a}}(k\ell m), \\ \hat{L}_- &= \ell_- + \int_0^{\infty} dk \sum_{\ell m} [\ell(\ell+1) - m(m-1)]^{1/2} \\ &\quad \times \hat{\underset{\sim}{a}}^{\dagger}(k\ell m-1)\hat{\underset{\sim}{a}}(k\ell m), \\ \hat{L}_z &= \ell_z + \int_0^{\infty} dk \sum_{\ell m} m \hat{\underset{\sim}{a}}^{\dagger}(k\ell m)\hat{\underset{\sim}{a}}(k\ell m), \end{aligned} \tag{2.13}$$

where $\ell = -i\mathbf{r}\times\nabla$ is the angular momentum operator for the electron and $\ell_{\pm} = \ell_x \pm i\ell_y$. It may be verified that the operators (2.13) correctly satisfy the usual commutation relations ($\hbar = 1$)

$$\begin{aligned} &[\hat{L}_z, \hat{L}_+] = \hat{L}_+, \quad [\hat{L}_z, \hat{L}_-] = -\hat{L}_-, \\ &[\hat{L}_+, \hat{L}_-] = 2\hat{L}_z, \end{aligned} \tag{2.14}$$

which justifies identifying them as angular momentum operators in the first place. It may also be verified that *the Hamiltonian (2.10) commutes with the operators (2.13)*, the angular momentum quanta absorbed or released by the plasmon field being exactly compensated by the recoil of the electron. How this conservation law can be exploited to simplify the solution to the variational problem will be considered in the next section.

III. SOLUTION TO THE VARIATIONAL PROBLEM IN ANGULAR VARIABLES

We look for a variational solution to the model Hamiltonian (2.10) based on the *ansatz*

$$|\Phi(\mathbf{r})\rangle_{LM} = \exp\{\hat{\underset{\sim}{S}}(\mathbf{r})\}|0\rangle \psi_{LM}(\mathbf{r}). \tag{3.1}$$

Here $|0\rangle$ denotes the ground state of the free-boson field, $\psi_{LM}(\mathbf{r})$ is a single-particle wave function to be specified below, and $\hat{\underset{\sim}{S}}(\mathbf{r})$ is taken to be linear in the bosons operators in analogy with the exact solution to the core-hole problem.[11] The symmetry labels LM for the rotation group are common to both sides of Eq. (3.1) since the operator $\hat{\underset{\sim}{S}}(\mathbf{r})$ is assumed to be an *invariant* of that group, namely, to satisfy the condition

$$[\hat{L}_{\alpha}, \hat{\underset{\sim}{S}}(\mathbf{r})] = 0, \tag{3.2}$$

where the label α distinguishes the three operators (2.13). The ansatz (3.1) is then understood to hold for the lowest state of each symmetry. It may be verified that the (anti-Hermitian) choice

$$\hat{\underset{\sim}{S}}(\mathbf{r}) = \int_0^{\infty} dk \sum_{\ell m} (\underset{\sim}{f}_{k\ell m}(\mathbf{r})\hat{\underset{\sim}{a}}(k\ell m) - \underset{\sim}{f}^*_{k\ell m}(\mathbf{r})\hat{\underset{\sim}{a}}^{\dagger}(k\ell m)) \tag{3.3}$$

satisfies the requirement (3.2) *provided* the functions $\underset{\sim}{f}_{k\ell m}(\mathbf{r})$ belong to the symmetry species ℓm of the rotation group:

$$\underset{\sim}{f}_{k\ell m}(\mathbf{r}) = \underset{\sim}{f}_{k\ell}(r) Y_{\ell m}(\hat{r}). \tag{3.4}$$

By minimizing the expectation value of the Hamiltonian (2.10) for the state (3.1) one obtains a set of coupled differential equations for the unknown functions $f_{k\ell m}(\mathbf{r})$ and $\psi_{LM}(\mathbf{r})$ which need to be solved self-consistently:

$$-\frac{1}{2m^*}\nabla^2 f_{k\ell m}(\mathbf{r}) + \omega_k f_{k\ell m}(\mathbf{r}) - \frac{1}{m^*}\nabla f_{k\ell m}(\mathbf{r})\cdot\frac{\nabla\psi^*_{LM}(\mathbf{r})}{\psi^*_{LM}(\mathbf{r})} + i\mathbf{j}(\mathbf{r})\cdot\nabla f_{k\ell m}(\mathbf{r}) + \frac{i}{2}f_{k\ell m}(\mathbf{r})\frac{\nabla\cdot(|\psi_{LM}(\mathbf{r})|^2\mathbf{j}(\mathbf{r}))}{|\psi_{LM}(\mathbf{r})|^2} + \frac{1}{4m^*}f_{k\ell m}(\mathbf{r}) \times\frac{\nabla\cdot(\psi^*_{LM}(\mathbf{r})\nabla\psi_{LM}(\mathbf{r}) - \psi_{LM}(\mathbf{r})\nabla\psi^*_{LM}(\mathbf{r}))}{|\psi_{LM}(\mathbf{r})|^2} = \mathscr{V}^e_{k\ell m}(\mathbf{r}) + \mathscr{V}^h_{k0}\delta_{l,0}, \tag{3.5a}$$

and

$$[(1/2m^*)(-i\nabla + m^*\mathbf{j}(\mathbf{r}))^2 + v_{\text{eff}}(r) - E]\psi_{LM}(\mathbf{r}) = 0. \tag{3.5b}$$

In Eqs. (3.5) $\mathbf{j}(\mathbf{r})$ has the form of a "plasmon current"

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2im^*}\int_0^\infty dk \sum_{\ell m}(f_{k\ell m}(\mathbf{r})\nabla f^*_{k\ell m}(\mathbf{r}) - f^*_{k\ell m}(\mathbf{r})\nabla f_{k\ell m}(\mathbf{r})), \tag{3.6}$$

while $v_{\text{eff}}(r)$ indicates the (spherically symmetric) *effective potential* seen by the electron

$$v_{\text{eff}}(r) = v_b(r) + \frac{1}{2m^*}\int_0^\infty dk \sum_{lm}\nabla f^*_{k\ell m}(\mathbf{r})\cdot\nabla f_{k\ell m}(\mathbf{r}) + \int_0^\infty dk\,\omega_k\sum_{lm} f^*_{k\ell m}(\mathbf{r}) f_{k\ell m}(\mathbf{r}) - \int_0^\infty dk\sum_{\ell m}[(\mathscr{V}^e_{k\ell m}(\mathbf{r}) + \mathscr{V}^h_{k0}\delta_{l,0})f^*_{k\ell m}(\mathbf{r}) + (\mathscr{V}^e_{k\ell m}(\mathbf{r}) + \mathscr{V}^h_{k0}\delta_{l,0})^* f_{k\ell m}(\mathbf{r})]. \tag{3.7}$$

Notice that Eq. (3.5a) is inhomogeneous owing to the presence of the coupling terms at its right-hand side. We shall specifically be concerned with finding a particular solution to this equation because we require on physical grounds the functions $f_{k\ell m}(\mathbf{r})$ to vanish if the coupling terms are allowed to vanish. Equation (3.5b), on the other hand, has the form of an ordinary single-particle Schrödinger equation where the energy parameter E originates from the subsidiary normalization condition of the trial eigenfunction (3.1).

The structure of Eq. (3.5a) can be simplified as follows. We notice at the outset that the last term at its left-hand side actually vanishes if we take

$$\psi_{LM}(\mathbf{r}) = R_L(r)Y_{LM}(\hat{r}) \tag{3.8}$$

with $R_L(r)$ real. The constant hole coupling term at the right-hand side of Eq. (3.5a) may also be eliminated by setting

$$f_{k\ell m}(\mathbf{r}) = f^e_{k\ell m}(\mathbf{r}) + (\mathscr{V}^h_{k0}/\omega_k)\delta_{l,0}, \tag{3.9}$$

whereby Eq. (3.5a) becomes an equation for the electronic part $f^e_{k\ell m}(\mathbf{r})$ only. The resulting equation is still quite complicated to solve, being apparently nonlinear in the set of functions $f^e_{k\ell m}(\mathbf{r})$ owing to the presence of the current (3.6). However, by exploiting the geometrical as well the dynamical symmetry of the problem at hand we can prove that both the transverse and the radial components of $\mathbf{j}(\mathbf{r})$ vanish identically, i.e.,

$$\mathbf{j}(\mathbf{r}) = 0. \tag{3.10}$$

The vanishing of the transverse component of $\mathbf{j}(\mathbf{r})$ follows from the identity

$$\sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{r})\frac{\partial}{\partial\theta}Y^*_{\ell m}(\hat{r}) = \sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{r})\frac{\partial}{\partial\varphi}Y^*_{\ell m}(\hat{r}) = 0, \tag{3.11}$$

where θ and φ are the spherical angles. Equation (3.11), in turn, follows from the property of the spherical harmonics under time reversal and from the addition theorem they satisfy. On the other hand, the radial component of $\mathbf{j}(\mathbf{r})$

$$\hat{r}\cdot\mathbf{j}(\mathbf{r}) = \frac{1}{2im^*}\int_0^\infty dk\sum_\ell\frac{(2\ell+1)}{4\pi}\left(f_{k\ell}(r)\frac{d}{dr}f^*_{k\ell}(r) - f^*_{k\ell}(r)\frac{d}{dr}f_{k\ell}(r)\right) \tag{3.12}$$

also vanishes *provided* the radial functions $f_{k\ell}(r)$ can be taken to be either real or purely imaginary. Assuming this to be true, we can verify that the solutions of the resulting equation are consistent with this assumption. In fact, making use of Eq. (3.10) and averaging over M we obtain a *radial* equation for $f^e_{k\ell}(r)$ (Ref. 12):

$$-\frac{1}{2m^*}\left[\frac{1}{r}\frac{d^2}{dr^2}(rf^e_{k\ell}(r)) - \frac{\ell(\ell+1)}{r^2}f^e_{k\ell}(r)\right] + \omega_k f^e_{k\ell}(r) - \frac{1}{m^*}\frac{1}{R_L(r)}\frac{dR_L(r)}{dr}\frac{d}{dr}f^e_{k\ell}(r) = \mathscr{V}^e_{k\ell}(r), \tag{3.13}$$

whose solutions are either real or purely imaginary for even or odd values of ℓ, respectively, reflecting a similar property of the source term [cf. Eq. (2.11b)].

The following features can be inferred from Eq. (3.13).

(i) Equation (3.13) is *linear* in $f^e_{k\ell}(r)$ and thus it possesses only one solution for all values of the parameters m^* and $\overline{V}^e_k$ (Ref. 13).

(ii) Solutions for increasing $\ell(>0)$ are expected to be progressively suppressed in the region about the core hole and thus they will not contribute appreciably to the relevant portion of the effective potential (3.7) if $R_L(r)$ is sufficiently localized.

(iii) In the limit of large m^* values there is a cancellation between the plasmon relaxations due to the core hole and to the electron.

The properties of the spherical harmonics can also be used to rewrite the effective potential (3.7) in an explicitly invariant form, as shown in the Appendix.

IV. CLOSE-FORM SOLUTION FOR A PARTICULAR CLASS OF SINGLE-PARTICLE ORBITALS

We have shown above that symmetry arguments allow us to reduce the coupled set of equations (3.5) to the simpler radial equations (3.13) and (A4). Solution to these equations has still to be tackled numerically unless the orbital

$R_L(r)$ is restricted, e.g., to a simple hydrogenic form when v_b is a Coulombic potential:

$$R_L(r) = A_L\, r^L e^{-\gamma r}, \tag{4.1}$$

A_L being a normalization constant. In this case a solution to Eq. (3.13) can be obtained in a closed form and it will depend parametrically on γ. To this end, we follow Ref. 6 and express the solution to Eq. (3.13) in terms of the associated Green's function

$$f^e(r) = \int_0^\infty dr'\, \mathscr{G}(r,r')\mathscr{V}^e(r'). \tag{4.2}$$

(The dependence of these functions on k and ℓ is understood throughout.) The Green's function, in turn, can be expressed in terms of the regular and irregular solutions to the homogeneous equation associated with Eq. (3.13)[14]:

$$\mathscr{G}(r,r') = -\frac{1}{W(r')}\begin{cases}\mathscr{R}(r)\mathscr{I}(r') & (r<r'),\\ \mathscr{I}(r)\mathscr{R}(r') & (r>r'),\end{cases} \tag{4.3}$$

where $W(r)$ is the Wronskian

$$W(r) = \mathscr{I}(r)\frac{d\mathscr{R}(r)}{dr} - \mathscr{R}(r)\frac{d\mathscr{I}(r)}{dr}. \tag{4.4}$$

Suitable boundary conditions require the Green's function to remain bounded everywhere.

The solutions to the homogeneous equation associated with Eq. (3.13) whereby $R_L(r)$ is taken of the form (4.1) can be readily obtained by setting

$$F(r) = r^\eta e^{-\epsilon r/2} w(\zeta r), \tag{4.5}$$

where F stands for either $\mathscr{R}$ or $\mathscr{I}$ and (ϵ,η,ζ) are constants to be determined. The transformed equation for w then reads:

$$\begin{aligned}&\frac{d^2}{dr^2}w(\zeta r) + \left[\frac{2(L+\eta+1)}{r} - 2\gamma - \epsilon\right]\frac{d}{dr}w(\zeta r)\\ &\quad + \{[\eta(\eta-1) + 2\eta(L+1) - \ell(\ell+1)](1/r^2)\\ &\quad - [2\gamma\eta + \eta\epsilon + \epsilon(L+1)](1/r)\\ &\quad + \epsilon^2/4 + \epsilon\gamma - 2m^*\omega_k\}w(\zeta r) = 0,\end{aligned} \tag{4.6}$$

which reduces to the standard Kummer's equation[15]

$$\frac{d^2}{dr^2}w(\zeta r) + \left(\frac{b}{r} - \zeta\right)\frac{d}{dr}w(\zeta r) - \frac{a\zeta}{r}w(\zeta r) = 0, \tag{4.7}$$

provided we identify

$$\begin{aligned}&b = 2(L+\eta+1), \quad \zeta = \epsilon + 2\gamma,\\ &\eta^2 + \eta(2L+1) = \ell(\ell+1),\\ &a\zeta = 2\gamma\eta + \eta\epsilon + \epsilon(L+1),\\ &\epsilon^2 + 4\epsilon\gamma - 8m^*\omega_k = 0.\end{aligned} \tag{4.8}$$

The five unknowns here are thus determined uniquely by solving the quadratic equations for ϵ and η:

$$\begin{aligned}&\epsilon = 2((\gamma^2 + 2m^*\omega_k)^{1/2} - \gamma),\\ &\eta = \tfrac{1}{2}\,[(2L+1)^2 + 4\ell(\ell+1))^{1/2} - (2L+1)],\end{aligned} \tag{4.9}$$

where the boundary conditions have been used to fix the sign of the square roots. Notice that every unknown turns out to be positive definite.

The Green's function (4.3) can now be written in terms of the regular (Φ) and irregular (Ψ) Kummer's functions:

$$\begin{aligned}&\mathscr{G}(r,r')\\ &= 2m^*[\Gamma(a)/\Gamma(b)]\,\zeta^{b-1}r^\eta r'^{b-\eta}e^{-2\gamma r'}e^{-(\epsilon/2)(r+r')}\\ &\quad\times\begin{cases}\Phi(a,b,\zeta r)\Psi(a,b,\zeta r') & (r<r'),\\ \Psi(a,b,\zeta r)\Phi(a,b,\zeta r') & (r>r'),\end{cases}\end{aligned} \tag{4.10}$$

where Γ is Euler's gamma function.

The restricted form (4.1) requires us to replace solving the differential equation (A4) for $R_L(r)$ with finding the minimum of the function

$$\begin{aligned}E(\gamma) &= A_L^2\int_0^\infty dr\, e^{-2\gamma r}r^{2L+1}\\ &\quad\times\left[\frac{2(L+1)\gamma - \gamma^2 r}{2m^*} + v_{\text{eff}}(r)r\right]\end{aligned} \tag{4.11}$$

which determines the parameter γ self-consistently together with the screening functions (4.2).

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APPENDIX: EFFECTIVE POTENTIAL FOR THE RADIAL EQUATION

The effective potential (3.7) can be rewritten in terms of the radial functions $f_{k\ell}(r)$ alone. For the last two terms at the right-hand side of Eq. (3.7) this can be simply achieved by using the addition theorem for spherical harmonics. For the second term there, one has to express the gradient operators in spherical coordinates and to make use of the identity

$$\begin{aligned}&\sum_{m=-\ell}^{\ell}\left[\frac{\partial Y_{\ell m}(\hat r)}{\partial\theta}\frac{\partial Y^*_{\ell m}(\hat r)}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial Y_{\ell m}(\hat r)}{\partial\varphi}\frac{\partial Y^*_{\ell m}(\hat r)}{\partial\varphi}\right]\\ &\quad = [(2\ell+1)/4\pi]\ell(\ell+1),\end{aligned} \tag{A1}$$

which follows from Eq. (3.11) after straightforward manipulations. The result is

$$\begin{aligned}&\sum_{\ell m}\nabla f^*_{k\ell m}(\mathbf{r})\cdot\nabla f_{k\ell m}(\mathbf{r})\\ &\quad = \sum_\ell\frac{(2\ell+1)}{4\pi}\left[\left|\frac{df_{k\ell}(r)}{dr}\right|^2 + \frac{\ell(\ell+1)}{r^2}|f_{k\ell}(r)|^2\right],\end{aligned} \tag{A2}$$

so that:

$$\begin{aligned}v_{\text{eff}}(r) &= v_b(r) - \frac{1}{\pi^{1/2}}\int_0^\infty dk\,\mathscr{V}^h_{k0}f_{k0}(r)\\ &\quad + \sum_\ell\frac{(2\ell+1)}{4\pi}\int_0^\infty dk\left\{\frac{1}{2m^*}\left|\frac{df_{k\ell}(r)}{dr}\right|^2\right.\\ &\quad + \left[\frac{\ell(\ell+1)}{2m^*r^2} + \omega_k\right]|f_{k\ell}(r)|^2\\ &\quad \left. - 2\,\mathscr{V}^e_{k\ell}(r)f^*_{k\ell}(r)\right\},\end{aligned} \tag{A3}$$

where the contribution of the hole to $f_{\underset{\sim}{k}\ell}(r)$ is present only for $\ell = 0$ [cf. Eq. (3.9)]. Taking Eqs. (3.8) and (3.10) into account, the effective Schrödinger equation (3.5b) becomes eventually:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_L(r)}{dr}\right) + \left\{2m^*[E - v_{\text{eff}}(r)] - \frac{L(L+1)}{r^2}\right\}R_L(r) = 0. \tag{A4}$$

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[13]This property holds also for the ground state of the free polaron corresponding to zero eigenvalue of the linear momentum (2.7) (cf. Ref. 3).
[14]Compare, e.g., E. A. Kraut, *Fundamentals of Mathematical Physics* (McGraw-Hill, New York, 1967), Sec. 6-22.
[15]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Natl. Bur. Stand., Washington, D. C., 1970), Chap. 13.