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Ground state description of bound polarons in parabolic quantum wires

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Abstract. The Feynman-Haken variational path integral theory is, for the first time, generalized to calculate the ground-state energy of an electron coupled simultaneously to a Coulomb potential and to a longitudinal-optical (LO) phonon field in parabolic quantum wires. It is shown that the polaronic correction to the ground-state energy is more sensitive to the electron-phonon coupling constant than the Coulomb binding parameter and monotonically stronger as the effective wire radius decreases. We apply our calculations to several semiconductor quantum wires and find that the polaronic correction can be considerably large.

PACS. 71.38.+i Polarons and electron-phonon interactions – 63.20.Kr Phonon-electron and phonon-phonon interactions

1 Introduction

With the recent progress in microfabrication technology, it becomes possible to fabricate the synthetic polar semiconductor structures with low dimensionality, such as dielectric slabs, heterojunctions, quantum wells, quantum dots, and quantum wires. One subject of interest is the quantum wires [1–3], which now can be fabricated within low-nanometer size. Many investigations have been devoted to the polaronic effects in quasi-one-dimensional systems (an incomplete list is given by Refs. [4–17]).

Polarons in quantum wires are markedly different from those in bulk materials, due to the presence of wire potentials with the form $V(\rho = x, y)$, which confine the carriers motion in the ρ-plane transverse to the wire axis (setting z direction). First, the confining potential may bring about much rich phonon modes [4–7] such as confined phonon modes, interface phonon modes, etc. Second, even for the confining potential itself, there are so many types in the literature. It can be divided into three major types: the rectangular type, cylindrical type, and parabolic type. Further, it can also be characterized as finite or infinite, symmetric or asymmetric. A variety of phonon modes and various types of the wire potential have given rise to rich and varied investigations in this field in the last decade.

Recently, much attention has been attracted to the investigation of the solely effect of the interaction of electron and bulk LO phonons and polaronic properties in quantum wires [7–17]. More recently, the relevant problems of an electron coupled simultaneously to a positive Coulomb impurity and to a longitudinal-optical (LO) phonon field in parabolic quantum wires has been considered in the presence of a electric field [15] and a magnetic field [16], and in rectangular cross section quantum wires has been investigated in the absence of any external field [17]. The bound polaron problem may be more realistic in quantum wires and therefore of much significance.

In the present paper, we will, for the first time, generalize the previous Feynman-Haken [FH] path integral theory [18–21] to study the solely effect of the electron-longitudinal-optical (LO) phonon interactions on the ground-state energy of a bound polaron in polar semiconductor quantum wires with parabolic confinement. Such a choice for the confining potential, besides facilitating the derivations in the theory, is also, more importantly, close to realistic case. Recently, Kash *et al.* [22] have observed some good evidences for the existence of a parabolic potential well in quantum wires produced by strain gradients using a patterned carbon stress.

2 Formula

Following Platzman's work [23] on bound bulk polarons, the Hamiltonian describing bound polarons in quantum wires with parabolic potential can be written as (in Feynman units: $m = \hbar = \omega_{\rm LO} = 1$)

$$H = \frac{\mathbf{p}^2}{2} + V(\rho) - \frac{\beta}{\mathbf{r}} + \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \sum_{\mathbf{k}} (v_{\mathbf{k}} a_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + \mathrm{H.C.}), \quad (1)$$

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where $\mathbf{r} = (\rho, z)$ and $\mathbf{p}$ are the position and the momentum operators of the electron, $V(\rho) = \frac{1}{2}\omega^2\rho^2$ is the confining potential of a quantum wire, with ω being in units of $\omega_{\rm LO}$, measuring the confining strength of the parabolic potential, $a^\dagger_{\mathbf{k}}$ and $a_{\mathbf{k}}$ are respectively the creation and annihilation operators of the LO phonons with the wave vector $\mathbf{k} = (\mathbf{k}_\rho, k_z)$

$$|v_{\mathbf{k}}|^2 = \frac{2\sqrt{2}\pi\alpha}{\nu\mathbf{k^2}}, \quad \beta = \frac{\mathrm{e}^2}{\hbar\omega_{\rm LO}\epsilon_0}\Big/\left(\frac{\hbar}{m\omega_{\rm LO}}\right)^{1/2}. \tag{2}$$

with ν being the crystal volume, α and β being the electron-phonon coupling constant and Coulomb binding parameter. Here we should mention that the impurity-phonon interactions have already been eliminated.

As a first step, following Feynman's [18] first procedure, integrating over the path integral over the phonon coordinates, assuming that they are in their ground-state, we can readily obtain the true action corresponding to Hamiltonian (1)

$$S = \int_{t_a}^{t_b} \mathrm{d}t \left[-\frac{1}{2}\dot{\mathbf{r}}^2 - \frac{1}{2}\omega^2\rho^2 + \frac{\beta}{\mathbf{r}}\right] + \frac{1}{2}\sum_{\mathbf{k}}\int_{t_a}^{t_b}\int_{t_a}^{t_b} |v_{\mathbf{k}}|^2 \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r(t)}-\mathbf{r(s)})}\mathrm{e}^{-|t-s|}\mathrm{d}t\mathrm{d}s. \tag{3}$$

Next task is to choose a path integrable trial action to get a variational expression for the ground-state energy. In this paper, we shall follow the procedure developed by Haken [19] in the treatment of the exciton-phonon problem and later applied to the bound bulk polarons by Matsuura [20] and bound surface polarons by Bhattacharya *et al.* [21]. We choose the trial action S_1 as following

$$S_1 = \int_{t_a}^{t_b} \mathrm{d}t \left[-\frac{1}{2}\dot{\mathbf{r}}^2 - V_{\rm eff}(\mathbf{r(t)})\right] = \int_{t_a}^{t_b} \mathrm{d}t L_{\rm eff}, \tag{4}$$

where $V_{\rm eff}(\mathbf{r(t)})$ is the effective trial potential to be chosen later. The corresponding quantum-mechanical Hamiltonian then satisfies

$$H_{\rm eff}\Phi_n^{\rm eff}(\mathbf{r}) = \left[\frac{1}{2}\mathbf{p^2} + V_{\rm eff}(\mathbf{r})\right]\Phi_n^{\rm eff}(\mathbf{r}) = E_n^{\rm eff}\Phi_n^{\rm eff}(\mathbf{r}), \tag{5}$$

where $\Phi_0^{\rm eff}(\mathbf{r})$ and $E_0^{\rm eff}$ are the ground-state energy and wave function of $H_{\rm eff}$.

After some derivations similar to those in references [19–21], one can obtain the FH energy as

$$E^{\rm FH} = \langle\Phi_0^{\rm eff}(\mathbf{r})|\left[\frac{1}{2}\mathbf{p^2} + \frac{1}{2}\omega^2\rho^2 - \frac{\beta}{\mathbf{r}}\right]|\Phi_0^{\rm eff}(\mathbf{r})\rangle - \sum_j\sum_{\mathbf{k}}\frac{|\langle\Phi_j^{\rm eff}(\mathbf{r})|[v_{\mathbf{k}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}]|\Phi_0^{\rm eff}(\mathbf{r})\rangle|^2}{E_j^{\rm eff} - E_0^{\rm eff} + 1}. \tag{6}$$

It is to note that, if the effective potential $V_{\rm eff}(\mathbf{r})$ is chosen to be such a form that the corresponding Schrödinger equation can be analytically solved, substitution of the relevant energy eigenfunctions and eigenvalues into equations (6) will produce the upper bound to the exact ground state energy of the Hamiltonian (1).

In this paper, according to the symmetry of the system studied, we will choose a variational effective potential as the following Harmonic-Oscillator type which is only isotropic in $\rho-$plane

$$V_{\rm eff}(\mathbf{r}) = \frac{1}{2}\lambda_\rho^2\rho^2 + \frac{1}{2}\lambda_z^2 z^2, \tag{7}$$

where λ_ρ and λ_z is a variational parameter to be determined. Such a form of $V_{\rm eff}(\mathbf{r})$ is different from those in references [19–21] and more suitable for the problem in quantum wires.

The energy eigenfunctions and eigenvalues corresponding to potential (7) are

$$\Phi_j^{\rm eff}(\mathbf{r}) = \left(\frac{\lambda_\rho\lambda_z^{1/2}}{\pi^{3/2}2^{j_x+j_y+j_z}j_x!j_y!j_z!}\right)^{1/2} \times H_{j_x}(\sqrt{\lambda_\rho}x)H_{j_y}(\sqrt{\lambda_\rho}y)H_{j_z}(\sqrt{\lambda_z}z)\mathrm{e}^{-(\lambda_\rho\rho^2/2+\lambda_z z^2/2)}$$

$$E_j^{\rm eff} = (j_x + j_y + 1)\lambda_\rho + \left(j_z + \frac{1}{2}\right)\lambda_z, \tag{8}$$

where $H_n(...)$ is the Hermite polynomial of order n. Then the first line of equation (6) becomes

$$I_1 = \frac{1}{2}\lambda_\rho + \frac{1}{4}\lambda_z + \frac{\omega^2}{2\lambda_\rho} - \frac{\beta}{\pi^{1/2}}\frac{\sqrt{\lambda_z}}{A}\ln\left(\frac{1+A}{1-A}\right) \tag{9}$$

where

$$A = \sqrt{1 - \frac{\lambda_z}{\lambda_\rho}}. \tag{10}$$

Using the transformations

$$\frac{1}{E_j^{\rm eff} - E_0^{\rm eff} + 1} = \int_0^\infty \mathrm{e}^{-(E_j^{\rm eff}-E_0^{\rm eff}+1)t}\mathrm{d}t, \tag{11}$$

and the Slater sum rule for the Hermit polynomials

$$\sum_n \frac{1}{2^n n!}H_n(\lambda x)H_n(\lambda x')\mathrm{e}^{-\frac{1}{2}\lambda^2(x^2+x'^2)-2np} = \frac{\mathrm{e}^p}{\sqrt{2\sinh(2p)}}\mathrm{e}^{-\frac{1}{4}\lambda^2[(x+x')^2\tanh(p)+(x-x')^2\coth(p)]}, \tag{12}$$

one can perform the summation over $j_i, (i = x, y, z)$ in equation (6) easily. Then using

$$\sum_{\mathbf{k}}\frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2} = \frac{\nu}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|}, \tag{13}$$

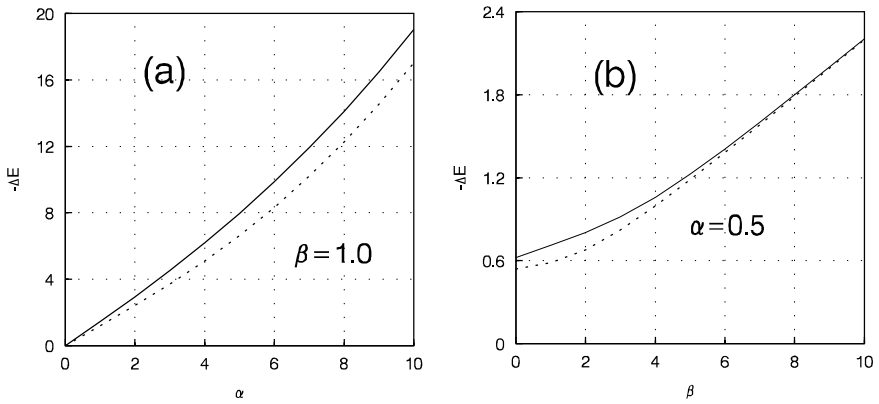

Fig. 1. The polaronic energy correction $-\triangle E^{\rm FH}$ within the FH path integral theory as a function of, (a) α and (b) β, for two the effective wire radius $R = 0.5$ (solid lines) and 1.0 (dotted lines) (in Feynman units).

one can integrate over the electron position vectors $\mathbf{r}$ and $\mathbf{r}'$ by transforming these vectors into the center-of-mass vector $\mathbf{u} = (\mathbf{r} + \mathbf{r}')/2$ and the relative vectors $\mathbf{v} = \mathbf{r} - \mathbf{r}'$, then the second line of equation (6) is simplified to

$$I_2 = -\frac{\alpha}{2\sqrt{\pi}} \int_0^\infty {\rm d}t {\rm e}^{-t} \frac{\sqrt{\lambda_z}}{\sqrt{1-{\rm e}^{-\lambda_z t}}} \frac{1}{\sqrt{1-B}} \times \ln\left(\frac{1+\sqrt{1-B}}{1-\sqrt{1-B}}\right) \tag{14}$$

where

$$B = \frac{\lambda_z(1+\coth(\lambda_z t/2)}{\lambda_\rho(1+\coth(\lambda_\rho t/2)}. \tag{15}$$

Finally the FH energy reads

$$E^{\rm FH} = I_1 + I_2. \tag{16}$$

So far, for given α, β, and ω, one can obtain the ground-state energy of Hamiltonian (1) by minimizing equation (16) respect to λ_ρ and λ_z. It should be pointed out that this Feynman energy expression (16) is suited for the entire range of electron-phonon coupling constant α, strength of the confining potential ω, and Coulomb binding parameters β.

In order to calculate the polaronic correction to the ground-state energy of this system, we also need to have the energy of an impurity in a quantum wire without electron-phonon interaction. Obviously, it can be obtained from equation (9) by finding out the optimal fit to λ_ρ and λ_z. The polaronic energy correction is just the difference between these two energies.

3 Results and discussions

Physically, it is expected that the polaronic energy correction $-\triangle E$ is more pronounced for larger electron-phonon coupling constant α and Coulomb binding parameters β. This is consistent with the our numerical results displayed in Figure 1a and b, where we plot the variation of $-\triangle E$ as the a function of α and β respectively for different effective wire radius $R = 1/\sqrt{\omega}$. It is also found that the value of $-\triangle E$ is more sensitive to the value of α than β and decreases with larger R.

To show the effectiveness of this approach, we will also study this system within well-known Landau-Pekar (LP) variational theory [24]. The main elements of this theory was employed to study bound polarons in quantum wires with rectangular cross section [17]. The adiabatic polaron ground-state can be given through following product ansatz

$$|...\rangle = \phi(\mathbf{r})|A\rangle, \tag{17}$$

where the electron part $\phi(\mathbf{r})$ is chosen as the following product of two Gaussian type wave functions in transverse and longitudinal coordinate

$$\phi(\mathbf{r}) = \varphi(\rho)\chi(z), \quad \varphi(\rho) \sim {\rm e}^{-\lambda_1\rho^2/2}; \quad \chi(z) \sim {\rm e}^{-\lambda_2 z^2/2}, \tag{18}$$

with λ_1 and λ_2 being a variational parameters to be determined, and $|A\rangle$ is the phonon coherent state,

$$|A\rangle = {\rm e}^{\sum_k (f(\mathbf{k})a_\mathbf{k}^\dagger - f^*(\mathbf{k})a_\mathbf{k}}|0\rangle. \tag{19}$$

One can easily derived the LP energy as follows

$$E^{\rm LP} = \frac{1}{2}\lambda_1 + \frac{1}{4}\lambda_2 + \frac{\omega^2}{2\lambda_1} - \frac{\beta}{\pi^{1/2}} \frac{\sqrt{\lambda_2}}{\sqrt{1-\frac{\lambda_2}{\lambda_1}}} \times \ln\left(\frac{1+\sqrt{1-\frac{\lambda_2}{\lambda_1}}}{1-\sqrt{1-\frac{\lambda_2}{\lambda_1}}}\right) - \frac{\alpha}{\sqrt{\pi}} \frac{\sqrt{\lambda_1}}{\sqrt{\frac{\lambda_1}{\lambda_2}-1}} \times \ln\left(\sqrt{\frac{\lambda_1}{\lambda_2}-1} + \sqrt{\frac{\lambda_1}{\lambda_2}}\right). \tag{20}$$

where λ_1 and λ_2 are the variational parameters.

For convenience, we introduce the relative difference, η, between the polaronic energy corrections $-\triangle E$ obtained by these two variational approaches: FH and LP methods

$$\eta = \frac{\triangle E^{\rm FH} - \triangle E^{LP}}{\triangle E^{\rm FH}}. \tag{21}$$

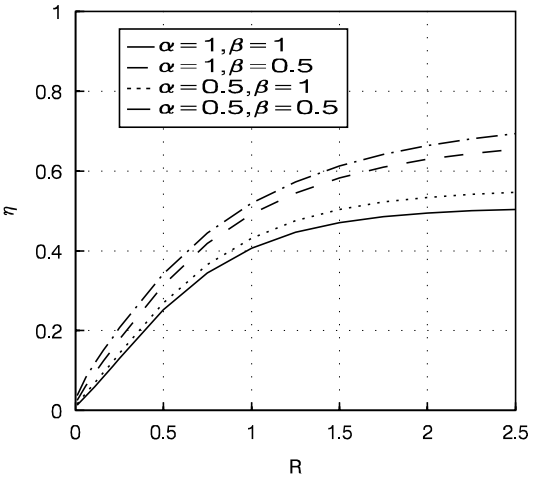

Fig. 2. The relative difference between results for the polaronic energy correction within the FH theory and the LP theory, η, as a function of the wire radius R for different values of α and β (in Feynman units).

In Figure 2, we plot the values of η as a function as a function of the effective wire radius R for coupling constants α and Coulomb binding parameters β which are in the range of parameters of practical materials. It is obviously shown that the polaronic energy correction obtained in the FH method is considerably larger than those obtained within LP theory. From the viewpoint of variational principle, the FH path integral approach is therefore superior to the famous LP theory. Certainly, this superiority will disappear in the limit of $R \to 0$, for the reason that the effective electron-phonon coupling is extremely strengthened in this limit and LP theory is known to be suitable for strong coupling or strong coulomb binding limit.

Here, we should present a few remarks about paper [17] by Osorio *et al.* The author have, in fact, utilized the main idea of LP theory. But the trial wave function for the electron along $x(y)$ direction in equation (6) of reference [17] is just the eigenfunctions corresponding to the system without electron-phonon coupling and the positive Coulomb impurity and thus does not include any variational parameters. Therefore, in principle, their results are even not so good as those obtained by the original LP theory. The latter is further inferior to the present theory. So this can show the importance of the present theory.

Next more important step is to apply our calculations to several semiconductor quantum wires such as CdS, CdSe, CdTe, and GaAs, which are shown in Figure 1. The material parameters used in the calculation are given in Table 1, which are cited from reference [25]. It is clear that the polaronic effects are quite pronounced in these materials when R is below a few nanometers. The polaronic effect decreases monotonically with R and changes very slowly as R approaches asymptotically to the bulk limit. We also find the magnitude of the polaronic correction is predominantly determined by the electron-phonon coupling constant and the optical phonon energy, and only slightly influenced by the coulomb binding parameters β. This is also agree with the observation of Figure 3.

Table 1. Some parameters of CdS, CdSe, CdTe, and GaAs. ($\omega_{\rm LO}$ is in unit of meV and m' in unit of bare electron mass).

Material	m	$\omega_{\rm LO}$	α	β
CdS	0.155	38.26	0.527	1.225
CdSe	0.130	26.58	0.460	1.238
CdTe	0.091	20.84	0.315	1.064
GaAs	0.066	36.7	0.068	0.5447

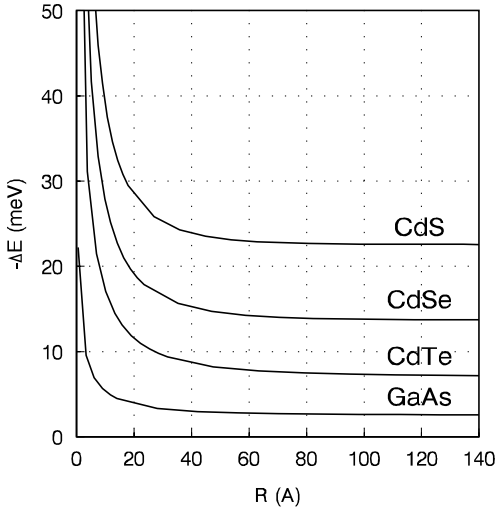

Fig. 3. The polaron energy correction, $-\Delta E$ (in meV) within the FH theory as a function the effective wire radius R (in Å) in CdS, CdSe, CdTe, and GaAs quantum wires with parabolic potential.

In summary, we have studied the polaronic effect of an electron bound to a positive Coulomb impurity in quantum wires within the Feynman-Haken variational path integral theory. By selecting a more general harmonic-type effective potential, we have derived a concise expression for the ground-state energy of this system. Compared to the results obtained by the LP variational theory, the present variational results are more accurate. We observe that the polaronic energy correction is more sensitive to the electron phonon coupling constant than the Coulomb binding parameters. We consider a few selected polar semiconductor quantum wires and show that the polaronic energy correction is substantial when the effective wire radius is made below a few nanometers. Finally we should point out the present derivation can be easily extended to the problems of bound polarons in quantum wells as well as quantum dots.

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References

1. R.G. Wheeler, K.K. Choi, A. Goel, R. Wisnieff, D.E. Prober, Phys. Rev. Lett. **49**, 1674 (1982).
2. T.J. Thornton, M. Pepper, H. Ahmed, D. Andrews, G.J. Davies, Phys. Rev. Lett. **56**, 1198 (1986).
3. R.C. Tonucci, B.L. Justus, A.J. Campillo, C.E. Ford, Science **258**, 783 (1992).
4. M.H. Degani, G.A. Farias, Phys. Rev. B **42**, 11950 (1990).
5. W.S. Li, S.W. Gu, T.C. Au-Yeung, Y.Y. Yeung, Phys. Rev. B **46**, 4630 (1992); Phys. Lett. A **166**, 377 (1992).
6. B. Tanatar, K. Güven, C.R. Bennett, N.S. Constantinou, Phys. Rev. B **53**, 10866 (1996).
7. E.P. Pokatilov, S.N. Klimin, S.N. Balaban, V.M. Fomin, Phys. Stat. Sol. B **191**, 311 (1995).
8. P. Vasilopoulos, P. Warmenbol, F.M. Peeters, J.T. Devreese, Phys. Rev. B **40**, 1810 (1989).
9. V.B. Campos, M.H. Degani, O. Hipólito, Sol. Stat. Commun. **79**, 473 (1991).
10. A. Ercelebi, R.T. Senger, Phys. Rev. B **53**, 11008 (1996).
11. G.Q. Hai, F.M. Peeters, J.T. Devreese, Phys. Rev. B **48**, 12016 (1993).
12. L. Wendler, R. Kügler, J. Phys.-Cond. **6**, 7857 (1994).
13. R. Haupt, L. Wendler, Ann. Phys. (USA) **233**, 214 (1994).
14. L. Wendler, A.V. Chaplik, R. Haupt, O. Hipólito, J. Phys.-Cond. **5**, 8031 (1993).
15. T.C. Au-Yeung, L.H. Hong, S.W. Gu, S.L. Kho, E.M.C. Wong, Phys. Lett. A **192**, 91 (1994).
16. T.C. Au-Yeung, C.C. Jong, S.W. Gu, E.M.C. Wong, Phys. Lett. A **204**, 155 (1995).
17. F.A.P. Osório, M.H. Degani, O. Hipólito, Phys. Rev. B **52**, 4662 (1995).
18. R.P. Feynman, Phys. Rev. **97**, 660 (1955).
19. H. Haken, Z. Phys. **147**, 323 (1957).
20. M. Matsuura, Can. J. Phys. **52**, 1 (1974).
21. M. Bhattachary, A. Chatterjee, T.K. Mitra, Phys. Rev. B **39**, 8351 (1989).
22. K. Kash, B.P. van der Gaag, D.D. Mahooney, A.S. Gozdoz, L.T. Florez, J.P. Harbison, Phys. Rev. Lett. **67**, 1326 (1991).
23. P.M. Platzman, Phys. Rev. **125**, 1961 (1962).
24. L.D. Landau, S.I. Pekar, JETP **18**, 341 (1948); A. Chatterjee, Phys. Rev. B **41**, 1668 (1990).
25. E. Kartheuser, in *Polarons in ionic crystals and polar semiconductors*, edited by J.T. Devreese (North-Holland, Amsterdam, 1972), p. 717.