# *N*-POLARON SYSTEM IN CHARGE BACKGROUND

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## Abstract

The ground state energy of an *N*-polaron system confined to a quantum dot with a neutralizing background charge is investigated within an all-coupling many-body path-integral variational principle taking into account both Fermi statistics of polarons and the electron-electron interaction. The obtained polaron parameters are compared with those for a polaron gas in bulk.

## 1. Introduction

During recent years, thermodynamic and optical properties of interacting many-polaron systems attract an increasing interest because of a possible role of polarons in those properties of high-$T_c$ superconductors (see, e.g., Refs. [1, 2]). Experiments on the infrared optical absorption of high-$T_c$ substances (see Refs. [3-5] and references therein) demonstrate features that are convincingly attributed to large and small polarons.

The ground-state properties of a weak-coupling interacting large-polaron gas have been treated in Refs. [6-8]. For small polarons, the formation of a finite density multi-polaron state in the Holstein model is analyzed in Refs. [9, 10]. To the best of our knowledge, at present there is no results on the ground-state energy and on the optical conductivity of an arbitrary-coupling large-polaron gas in bulk consistently accounting for the many-body effects.

In the present work, we treat the ground-state energy of a system of $N$ interacting polarons confined to a quantum dot taking into account a background-charge potential. In the case when the total background charge exactly compensates the charge of the electrons (i.e., when a quantum dot is electroneutral), at $N \to \infty$ the physical quantities of this system, e.g., the ground-state energy, should tend to those in bulk. Indeed, if we let the quantum dot with a neutralizing background have a radius, which tends to infinity, we have in practice a uniform electron gas dressed with polaron effects. In this connection, a quantum dot, in which a confinement is provided by a neutralizing background, can be a relevant model for a polaron gas in bulk. A problem of a particular interest is to perform the comparison of the ground-state energy of an *N*-polaron system with the ground-state energy of a polaron gas in bulk.

In Sec. 2, the $N$ -polaron system under consideration is described. In Sec. 3, we determine the variational functional for the ground-state energy of that system. In Sec. 4, we discuss the numerical results and compare the ground-state energy and various contri-

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butions to the ground-state energy of an $N$ -polaron system confined to a quantum dot with the corresponding quantities of a polaron gas in bulk. In Sec. 5, the conclusions are represented.

## 2. Electron-phonon system

We consider a system of $N$ electrons with mutual Coulomb repulsion and interacting with the lattice vibrations. The system is assumed to be confined to a parabolic potential characterized by the frequency parameter $\Omega_0$ and to a static background-charge potential uniformly distributed with the charge density $en_b$ in a sphere of a radius $R$. In the particular case, when the density $n_b$ is equal to the averaged electron density $n_0 = 3N/(4\pi R^3)$, the quantum dot is electroneutral, because the charge of electrons is compensated by the background charge.

The total number of electrons is represented as $N = \sum_\sigma N_\sigma$, where $N_\sigma$ is the number of electrons with the spin projection $s = \pm 1/2$. The electron coordinates are denoted by $\mathbf{x}_{j,\sigma}$ with $j = 1,\ldots, N_\sigma$. As was shown in Refs. [11, 12], the partition function of a system of interacting polarons can be represented as the path integral over the electron coordinates only,

$$Z_p\left(\{N_\sigma,\beta\}\right) = \sum_P \frac{(-1)^{\xi_P}}{N_{1/2}!N_{-1/2}!}\int d\bar{\mathbf{x}}\int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}(\tau)e^{-S_p[\bar{\mathbf{x}}(\tau)]} \tag{1}$$

with the action functional

$$S_p[\bar{\mathbf{x}}(\tau)] = -\frac{1}{\hbar}\int_0^{\hbar\beta}\left[L_e\left(\dot{\bar{\mathbf{x}}}(\tau),\bar{\mathbf{x}}(\tau)\right) - V_C\left(\bar{\mathbf{x}}(\tau)\right) - V_b\left(\bar{\mathbf{x}}(\tau)\right)\right]d\tau + \Phi[\bar{\mathbf{x}}(\tau)]. \tag{2}$$

Throughout the present treatment, the Euclidean time variable $\tau = it$ is used, where $t$ is the real time variable. In the action (2), $L_e\left(\dot{\bar{\mathbf{x}}},\bar{\mathbf{x}}\right)$ is the Lagrangian of $N$ electrons with band mass $m_b$ in a parabolic confinement potential,

$$L_e\left(\dot{\bar{\mathbf{x}}},\bar{\mathbf{x}}\right) = -\sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma}\frac{m_b}{2}\left(\dot{\mathbf{x}}_{j,\sigma}^2 + \Omega_0^2\mathbf{x}_{j,\sigma}^2\right), \qquad \dot{\mathbf{x}} \equiv \frac{d\mathbf{x}}{d\tau}, \tag{3}$$

$\Omega_0$ is the confinement frequency, $V_C\left(\bar{\mathbf{x}}\right)$ is the potential energy of the electron-electron Coulomb repulsion in the medium with the high-frequency dielectric constant $\varepsilon_\infty$:

$$V_C\left(\bar{\mathbf{x}}\right) = \sum_{\substack{\sigma,\sigma'=\pm 1/2\\(j,\sigma)\neq(l,\sigma')}}\sum_{j=1}^{N_\sigma}\sum_{l=1}^{N_{\sigma'}}\frac{e^2}{2\varepsilon_\infty}\frac{1}{\left|\mathbf{x}_{j,\sigma}-\mathbf{x}_{l,\sigma'}\right|} = \sum_{\mathbf{q}\neq 0}\frac{4\pi e^2}{q^2 V}\left(\rho_{\mathbf{q}}\rho_{-\mathbf{q}} - N\right), \tag{4}$$

where $\rho_{\mathbf{q}}$ is the Fourier transform of the electron density operator:

$$\rho_{\mathbf{q}} = \sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma} e^{i\mathbf{q}\cdot\mathbf{x}_{j,\sigma}}, \tag{5}$$

and $V$ is the volume of the crystal.

The term $V_b\left(\bar{\mathbf{x}}\right)$ in action (2) is the potential energy of $N$ electrons in the potential of the background charge,

$$V_b\left(\bar{\mathbf{x}}\right) = \sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma} U_b\left(r_{j,\sigma}\right) + V_{bb}, \quad r = |\mathbf{x}|, \tag{6}$$

$$U_b(r) = -\frac{4\pi e^2 n_b}{3\varepsilon_0}\left[\Theta(r<R)\frac{3R^2-r^2}{2} + \Theta(R>r)\frac{R^3}{r}\right], \tag{7}$$

where $\varepsilon_0$ is the static dielectric constant of a crystal. The constant term $V_{bb}$ is the potential energy of the electrostatic interaction of the background charges with each other:

$$V_{bb} = \frac{3}{5}\frac{e^2N^2}{\varepsilon_0 R}. \tag{8}$$

The static dielectric constant $\varepsilon_0$ appears instead of the high-frequency dielectric constant $\varepsilon_\infty$ in Eqs. (7) and (8) due to screening of a background-charge potential by the LO phonons.
The "influence phase" of phonons

$$\Phi[\bar{\mathbf{x}}(\tau)] = -\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\frac{\cosh\left[\omega_{\mathbf{k}}\left(|\tau-\tau'|-\frac{\hbar\beta}{2}\right)\right]}{\sinh\left(\frac{\hbar\beta\omega_{\mathbf{k}}}{2}\right)}\rho_{\mathbf{k}}(\tau)\rho_{-\mathbf{k}}(\tau') \tag{9}$$

describes the phonon-induced retarded interaction between the electrons, including the retarded self-interaction of each electron, $V_{\mathbf{k}}$ is the amplitude of the electron-phonon interaction. In the present work, we consider electrons interacting with the long-wavelength longitudinal optical (LO) phonons with a dispersionless frequency $\omega_{\mathbf{k}}=\omega_{\mathrm{LO}}$, for which the amplitude $V_{\mathbf{k}}$ is [13]

$$V_{\mathbf{k}} = \frac{\hbar\omega_{\mathrm{LO}}}{iq}\left(\frac{2\sqrt{2}\pi\alpha}{V}\right)^{1/2}\left(\frac{\hbar}{m_b\omega_{\mathrm{LO}}}\right)^{1/4}, \tag{10}$$

where $\alpha$ is the electron-phonon coupling constant.

The free energy of a system of interacting polarons $F_p(\{N_\sigma\},\beta)$ is related to their partition function (1) by the equation:

$$F_p(\{N_\sigma\},\beta) = -\frac{1}{\beta}\ln Z_p(\{N_\sigma\},\beta). \tag{11}$$

In the zero-temperature limit, the free energy turns into the $N$-polaron ground-state energy,

$$E^0(\{N_\sigma\}) = \lim_{\beta\to\infty} F_p(\{N_\sigma\},\beta). \tag{12}$$

## 3. Variational principle

At present no method is known to calculate the non-gaussian path integral (1) analytically. For distinguishable particles, the Jensen-Feynman variational principle [14] provides a powerful approximation technique. It yields a lower bound to the partition function and, hence, an upper bound to the free energy. It was demonstrated in Refs. [15, 16] that keeping the appropriate symmetry for a trial system (see the discussion in Ref. [16]), the variational inequality for identical particles takes the same form as the Jensen-Feynman variational principle

$$F_p \le F_0 + \frac{1}{\beta}\left\langle S_p - S_0\right\rangle_{S_0}, \tag{13}$$

where $S_0$ is a model action with corresponding free energy $F_0$. The angular brackets mean a weighted average over the paths

$$\left\langle\left(\bullet\right)\right\rangle_{S_0}=\frac{\sum\limits_P\frac{(-1)^{\xi_P}}{N_{1/2}!N_{-1/2}!}\int d\bar{\mathbf{x}}\int\limits_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}}D\bar{\mathbf{x}}(\tau)(\bullet)e^{-S_0[\bar{\mathbf{x}}(\tau)]}}{\sum\limits_P\frac{(-1)^{\xi_P}}{N_{1/2}!N_{-1/2}!}\int d\bar{\mathbf{x}}\int\limits_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}}D\bar{\mathbf{x}}(\tau)e^{-S_0[\bar{\mathbf{x}}(\tau)]}} \tag{14}$$

In the present paper, we use the trial action

$$\begin{aligned}S_0[\bar{\mathbf{x}}(\tau)]=&\frac{1}{\hbar}\int\limits_0^{\hbar\beta}\sum_{\sigma=\pm1/2}\sum_{j=1}^{N_\sigma}\frac{m_b}{2}\left[\dot{\mathbf{x}}_{j,\sigma}^2(\tau)+\Omega^2\mathbf{x}_{j,\sigma}^2(\tau)\right]d\tau\\&-\frac{1}{\hbar}\int\limits_0^{\hbar\beta}\sum_{\sigma,\sigma'=\pm1/2}\sum_{j=1}^{N_\sigma}\sum_{l=1}^{N_{\sigma'}}\frac{m_b\omega^2}{4}\left[\mathbf{x}_{j,\sigma}(\tau)-\mathbf{x}_{l,\sigma'}(\tau)\right]^2d\tau\;+\;\Phi_0[\bar{\mathbf{x}}(\tau)],\end{aligned} \tag{15}$$

with the influence phase of $N_f$ fictitious particles of the mass $m_f$ interacting with the electrons through elastic bonds with the elastic constant $k=m_f\Omega_f^2$

$$\Phi[\bar{\mathbf{x}}(\tau)]=-\frac{k^2N^2N_f}{4m_f\hbar\Omega_f}\int\limits_0^{\hbar\beta}d\tau\int\limits_0^{\hbar\beta}d\tau'\frac{\cosh\left[\Omega_f\left(|\tau-\tau'|-\frac{\hbar\beta}{2}\right)\right]}{\sinh\left(\frac{\hbar\beta\Omega_f}{2}\right)}\mathbf{X}(\tau)\cdot\mathbf{X}(\tau'),$$

where **X** is the center-of-mass coordinate of the electrons. As a result, we arrive at a variational functional for the ground-state energy of an *N*-polaron system in a parabolic confinement potential taking into account a charge background. The expectation values entering that functional, including the fermion statistics, have been studied earlier [12, 17, 18].

## 4. Discussion of results

The further numerical treatment of the ground-state energy of an N-polaron system confined to a quantum dot is performed under the following suppositions.

(1) We set the confinement frequency $\Omega_0 = 0$, so that the confinement is realized only by the background charge.

(2) We set the charge of the background sphere equal to (*eN*), so that the system is electro-neutral. In this model, the average electron density can be defined as

$$n_0\equiv\frac{N}{V}=\frac{3N}{4\pi R^3}. \tag{16}$$

The density is expressed in terms of the parameter $r_s^*$, which is determines by the equation

$$\frac{4\pi}{3}\left(r_sa_B^*\right)^3=\frac{1}{n_0}, \tag{17}$$

where $a_B^*$ is the effective Bohr radius related to the Bohr radius in the vacuum $a_B$ by the equality

$$a_B^*=\frac{m_e\varepsilon_\infty}{m_b}a_B. \tag{18}$$

In the Feynman units, the effective Bohr radius is expressed through the electron-phonon coupling constant α and the ratio of the dielectric constants η

$$a_B^*=\frac{1-\eta}{\sqrt{2\alpha}}. \tag{19}$$

Therefore, the parameter $r_s^*$ is determined through the number of polarons and the radius of a background-charge sphere

$$r_s^* = \frac{\sqrt{2}\alpha}{1-\eta}\frac{R}{N^{1/3}}. \tag{20}$$

Although most required quantities (partition function, density, two point correlation function) could be expressed in closed form (finite series), the time integral in the influence functional and the minimization of the ground state energy with respect to the variational parameters have to be performed numerically. No detailed calculations have been done for the very large set of parameters which can be of interest (material constants $m_b$, $\omega_{LO}$, $\alpha$, $\eta$, the parameter $r_s^*$, but preliminary results seem to reveal that our basic hypothesis holds, i.e., with increasing number of particles for fixed $r_s^*$ the ground state energy seems to converge to the one in bulk for a tractable number of particles (order of magnitude say $N$). We illustrate this with a few representative plots.

In Fig. 1, the ground-state energy per particle for an $N$-polaron system in a quantum dot is plotted as a function of the number of polarons keeping constant values of the parameter $r_s^*$ for two different cases: (i) the case of ZnO with $\alpha = 0.849$ and $\eta = 0.4908$, (ii) the case of a polar medium with $\alpha = 5$, $\eta = 0.3$. In the insets, the total spin of an $N$-polaron system in its ground state is represented as a function of $N$.

In an $N$-polaron quantum dot in ZnO for $r_s^* = 2$ (what corresponds to the density $n_0 = 4.34\times10^{19}$ cm$^{-3}$), the shell filling obeys Hund's rule [see the inset to Fig. 1 (a)]. This shell filling is manifested in the ground-state energy, where the pronounced minima correspond to the closed shells ($N = 2, 8, 20, 40,\ldots$) and weakly expressed minima correspond to the half-filled shells ($N = 5, 14, 30, 56, \ldots$). In the case of the medium with $\alpha = 5$, $\eta = 0.3$, for $r_s^* = 20$ (what corresponds to the density $n_0 = 1.14\times10^{18}$ cm$^{-3}$), an $N$-polaron system in its ground state has a maximal possible spin [see the inset to Fig. 1(b)]. As a result,

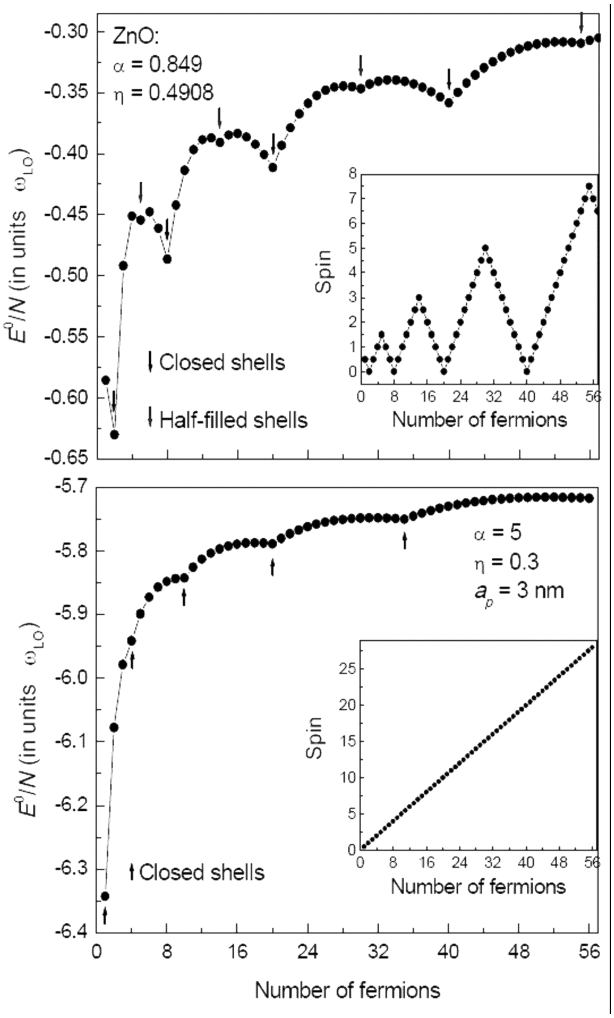


Fig. 1. Polaron ground-state energy per particle in an $N$-polaron quantum dot as a function of the number of fermions. The parameters are taken (a) for ZnO with $\alpha = 0.849$, $\varepsilon_0 = 8.15$, $\varepsilon_\infty = 4.0$ and $\hbar\omega_{LO} = 73.27$ meV, (b) for a polar medium with $\alpha = 5$, $\eta = 0.3$ and $a_p = 3$ nm. The value of the parameter $r_s^*$ is (a) $r_s^* = 2$, what corresponds to the fermion density $n_0 = 4.34\times10^{19}$ cm$^{-3}$, (b) $r_s^* = 20$, what corresponds to $n_0 = 1.14\times10^{18}$ cm$^{-3}$. The arrows indicate the number of fermions corresponding to the closed and half-filled shells. *Insets*: the total spin of an $N$-polaron system as a function of the number of fermions. (After Ref. [18].)

the ground-state energy as a function of $N$ in Fig. 1 has kinks for $N$ corresponding to the closed shells for a spin-polarized $N$-polaron system with parallel spins ($N = 1, 4, 10, 20, 35, \ldots$).

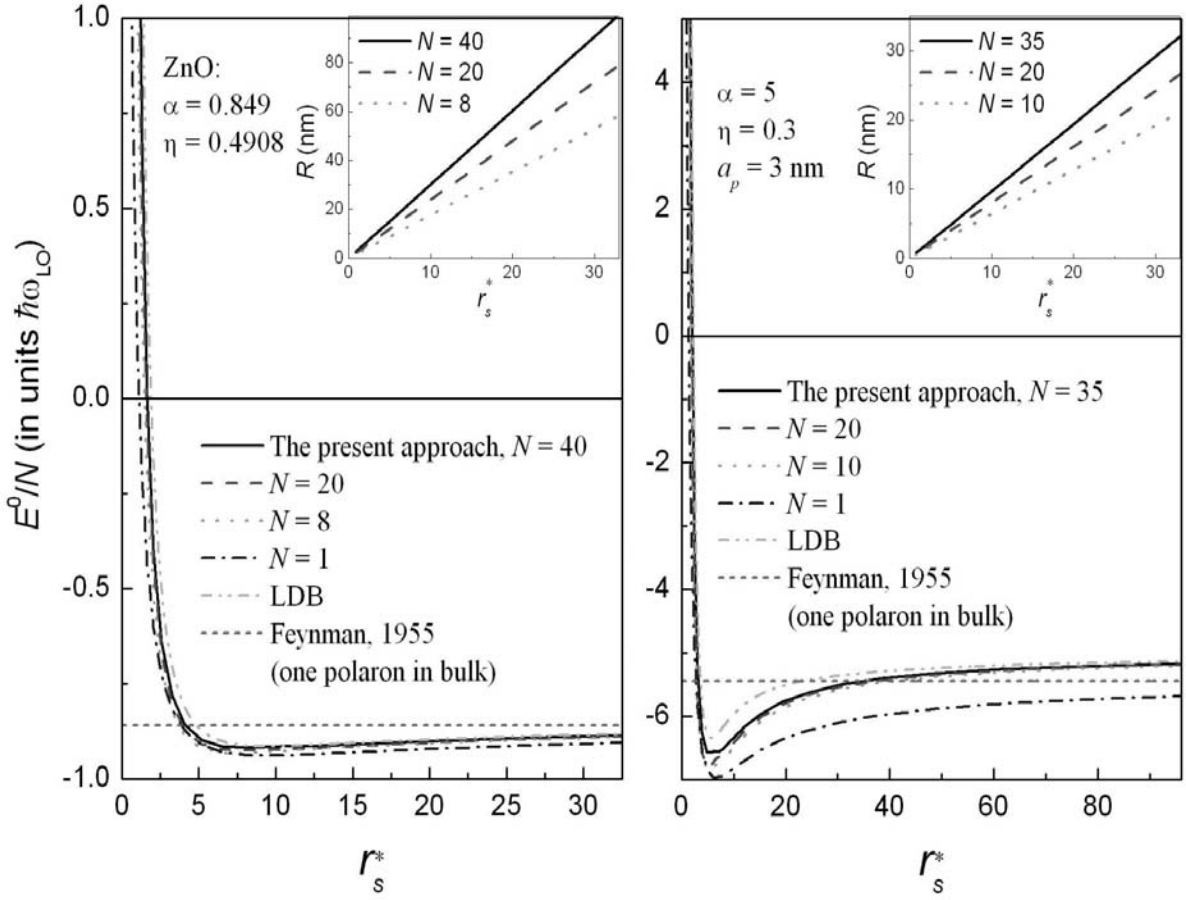


Fig. 2. Ground-state energy per particle of an $N$-polaron system in a quantum dot as a function of the parameter $r_s^*$ for different numbers of fermions. The dash-dotted line represents the results of the generalized Lee-Low-Pines transformation of Ref. [6]. (After Ref. [18].)]

In Fig. 2, the polaron ground-state energy per particle $E^0/N$ is plotted as a function of the effective parameter $r_s^*$ determined by Eq. (20) for several numbers of fermions: $N = 1$, 8, 20 and 40 for ZnO [Fig. 2(a)], and $N = 1$, 10, 20 and 35 for a medium with $\alpha = 5$, $\eta = 0.3$ [Fig. 2(b)]. We see that for all considered values of $r_s^*$, the ground-state energy per particle only slightly varies with $N$ for $N \geq 10$. Hereof, we can suppose that for these numbers of particles, an $N$-polaron system in a quantum dot reveals properties close to those for a polaron gas in bulk.

It appears that $E^0/N$ as a function of $r_s^*$ tends to a finite (bulk) value of the ground-state energy at large $r_s^*$. For $N = 1$, that value analytically coincides with that obtained within the Feynman method. For other $N$, the bulk value of the ground-state energy is higher than the Feynman one-polaron ground-state energy, as seen from the graph for $\alpha = 5$. This difference is due to the fact that the model of Refs. [11, 12] for $N \neq 1$ in the limit $r_s^* \to \infty$ differs from the Feynman model ($N$ times repeated) for a single polaron. The dash-dotted line represents the results of the generalized Lee-Low-Pines transformation of Ref. [6].

## 5. Conclusions

We have derived the ground-state energy of an $N$-polaron system at arbitrary coupling strength in a confinement potential, which is a combination of a parabolic potential and of a potential induced by a background charge. The many-body path-integral variational principle provides a rigorous upper bound for the ground-state energy of $N$ polarons taking into account both the Fermi statistics and the Coulomb interaction between fermions. The treatment of the ground-state energy is performed for both closed-shell and open-shell systems. In the case when a confinement is provided by a background charge and a quantum dot is electroneutral, the ground-state energy and the electron-phonon contribution to the ground-state energy as a function of the number of fermions demonstrate a trend to their values in bulk with increasing $N$. For a finite $N$, the dependences of the ground-state energy and of the polaron contribution on the parameter $r_s^*$, which determines the average fermion density in a quantum dot, are very similar to those for a polaron gas in bulk. Hereof, we can conclude that the ground-state properties of a polaron gas in bulk can be qualitatively described using a model of a finite number of polarons in a confinement provided by a background charge.

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