Path-integral approach to the ground-state energy of a homogeneous polaron gas

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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 treatment of the ground-state energy is performed for both closed- and open-shell systems. The average fermion density in the neutral spherical dot is characterized by the Wigner-Seitz parameter r_s. For a sufficiently large but finite number of polarons, the dependency of the ground-state energy on r_s is very similar to that for a polaron gas in bulk. From this, we can conclude that the ground-state energy of a polaron gas in bulk can be qualitatively described using a model of a finite number of polarons in a confinement potential provided by a neutralizing background charge.

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I. INTRODUCTION

Many-polaron systems are gaining increasing interest because polaron effects influence the thermodynamic and optical properties in high-T_c superconductors (see, e.g., Refs. 1 and 2). Experiments on the infrared optical absorption of high-T_c materials (see Refs. 3–5 and references therein) reveal features which are convincingly attributed to polarons.

In the present paper we address the problem of the ground-state energy of a polaron gas, starting from considerations on a system of a finite number of polarons in a quantum dot.

It is well known that Feynman's variational path-integral treatment[6] of a single polaron provides a superior analytical all-coupling theory. However, the generalization of this approach to many polarons is far from trivial, not only because of the Coulomb repulsion. A major problem is also the treatment of the Fermi-Dirac statistics of the electrons. Even for the bipolaron, up till now, stability study[7] was limited to two distinguishable electrons with opposite spin.

Some time ago, two of the present authors[8] contributed to a generalization of the Lee-Low-Pines transformation[9] to the N-polaron problem, which allows the problem (including the statistics) to be treated in terms of the static structure factor of the electron gas; the method was used in the Hartree-Fock approximation. The method is variational, but the upper bound to the ground-state energy is accurate only for sufficiently weak electron-phonon coupling. Based on this approach, a weak-coupling theory was developed,[10] taking into account the static screening of the electron-phonon interaction and using various approximations for the static dielectric function. A different treatment of the ground-state properties of a polaron gas at intermediate coupling was developed in Refs. 11, using an effective self-consistent electron-electron potential due to LO phonon exchange, with the parameters determined within a variational approach.

For arbitrary electron-phonon coupling, we succeeded[12,13] in generalizing Feynman's variational approach to a finite number of polarons in a quantum dot, to study the possible occurrence of bipolarons, tripolarons, and multipolarons. This method relies on the path-integral formalism for interacting identical oscillators.[14]

Another extension of the Feynman path-integral variational method for a many-polaron system has been developed in Refs. 15–17, starting from the low-density regime, where the particles localize due to the Coulomb repulsion and form a Wigner crystal. When the coupling to the LO phonons is turned on, the electron Wigner crystal is progressively transformed into a polaronic Wigner crystal. In Refs. 15–17, the electrons are considered as distinguishable particles. This approximation is justified inside the solid phase, where the overlap between the wave functions of different localized electrons is negligible. In Ref. 17, the method[15,16] was generalized, taking into account the Wigner crystal normal modes rather than a single mean frequency in the minimization procedure of the variational free energy.

On the one hand, taking account of the Fermi-Dirac statistics of polarons is of particular importance at high density of polarons where exchange effects bring a significant contribution to their ground-state energy. On the other hand, the formalism of Refs. 12 and 13 is not aimed at treating the low-density limit or, in particular, at describing the Wigner crystallization. The density range in which the approach of Refs. 12 and 13 and that of Refs. 15–17 are adequate are complementary to each other.

In the present work, we exploit the ideas and techniques of Refs. 12 and 13, and treat the ground-state energy of a system of N interacting polarons confined to a quantum dot by a uniform spherical positive background charge which exactly compensates the charge of the electrons. Indeed, if we let the quantum dot with a neutralizing background have a radius that tends to infinity, we have in practice a uniform electron gas dressed with polaron effects. In this connection, a quantum dot, in which confinement is provided by a neutralizing background, can be a relevant model for a polaron gas in bulk.

The paper is subdivided as follows. In Sec. II, the N-polaron system under consideration is described. In Sec. III, we determine the variational functional for the ground-state energy of that system. In Sec. IV, we discuss the numerical results and compare the ground-state energy and various contributions 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. V, the conclusions are presented.

II. ELECTRON-PHONON SYSTEM

Consider a system of N electrons with mutual Coulomb repulsion and interacting with the lattice vibrations. The system is confined by a sphere of a radius R with a uniform positive background charge density n_b. The density n_b is set equal to the averaged electron density $n_0=N/(4\pi R^3/3)$, such that the quantum dot is electrically neutral. The density can then be expressed in terms of the effective Wigner-Seitz parameter r_s^*, which is determined by the equations

$$\frac{4\pi}{3}(r_s^* a_B^*)^3 = \frac{1}{n_0}, \quad a_B^* = \frac{\hbar^2}{m_b(e^2/\varepsilon_\infty)} \tag{1}$$

with the effective Bohr radius a_B^*, the band mass m_b, and the electronic (high-frequency) dielectric constant ε_∞.

The total number of electrons is represented by $N=\Sigma_\sigma N_\sigma$, where N_σ is the number of electrons with spin projection $\sigma=\pm 1/2$. The electron coordinates are denoted by $\mathbf{x}_{j,\sigma}$ with $j=1,\ldots,N_\sigma$. Introducing the generalized electron coordinate

$$\bar{\mathbf{x}} = (\mathbf{x}_{1,-1/2},\ldots,\mathbf{x}_{-N_{-1/2},-1/2},\mathbf{x}_{1,+1/2},\ldots,\mathbf{x}_{N_{+1/2},+1/2}), \tag{2}$$

the Hamiltonian under consideration is

$$H = \sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma}\frac{\mathbf{p}_{j,\sigma}^2}{2m} + \sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + V_b(\bar{\mathbf{x}}) + V_C(\bar{\mathbf{x}}) + \sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma}\sum_{\mathbf{k}}(V_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}_{j,\sigma}} + V_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{x}_{j,\sigma}}), \tag{3}$$

The potential energy from the Coulomb repulsion is

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

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 interaction energy from the background is

$$V_b(\bar{\mathbf{x}}) = \sum_\sigma\sum_{j=1}^{N} U_b(|\mathbf{x}|_{j,\sigma}) + V_{bb}, \tag{6}$$

where $U_b(|\mathbf{r}|)$ is the electrostatic background potential of an electron with position $\mathbf{r}$. In the case of the uniform neutralizing background sphere described above, this potential energy is readily calculated, and is harmonic inside the sphere:

$$U_b(r) = -\frac{4\pi e^2 n_b}{3\varepsilon_0}\times\begin{cases}\dfrac{3R^2-r^2}{2} & \text{for } r\leqslant R,\\ \dfrac{R^3}{r} & \text{for } R\leqslant r,\end{cases} \tag{7}$$

where ε_0 is the static dielectric constant. The constant term V_{bb} is the potential energy associated with 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 electron-phonon interaction is described by the Fröhlich model,

$$V_{\mathbf{k}} = \frac{\hbar\omega_{\mathrm{LO}}}{ik}\left(\frac{4\pi\alpha}{V}\right)^{1/2}\left(\frac{\hbar}{2m\omega_{\mathrm{LO}}}\right)^{1/4}, \quad \text{with} \quad \alpha = \frac{e^2}{\hbar c}\sqrt{\frac{m_b c^2}{2\hbar\omega_{\mathrm{LO}}}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right), \tag{9}$$

with ω_{LO} the frequency of the longitudinal optical phonons that are created and annihilated by $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$, and with the electronic and static dielectric constants ε_∞ and ε_0, respectively.

Observe that the usual unit of length a_p of polaron theory is given by

$$a_p \equiv \sqrt{\frac{\hbar}{m_b\omega_{\mathrm{LO}}}}. \tag{10}$$

Its relation to the effective Bohr radius is

$$\frac{a_B^*}{a_p} = \frac{1-\eta}{\sqrt{2}\alpha}, \tag{11}$$

where η is the ratio between the high- and low-frequency dielectric constants,

$$0\leqslant\eta=\frac{\varepsilon_\infty}{\varepsilon_0}\leqslant 1. \tag{12}$$

Therefore, in terms of the number of polarons and the radius of the background sphere, the parameter r_s^* can be rewritten as

$$r_s^* = \frac{\sqrt{2}\alpha}{1-\eta}\frac{R}{N^{1/3}}. \tag{13}$$

As shown in Ref. 13, the partition function of a system of interacting polarons can be represented as the path integral over the electron coordinates only,

$$Z_p(\{N_\sigma\},\beta) = \sum_P\frac{(-1)^{\xi_P}}{N_{1/2}!N_{-1/2}!}\int d\bar{\mathbf{x}}\int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}(\tau)e^{-S_p[\bar{\mathbf{x}}(\tau)]}, \tag{14}$$

with the action functional

$$S_p[\bar{\mathbf{x}}(\tau)] = -\frac{1}{\hbar}\int_0^{\hbar\beta}\left[-\sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma}\frac{m_b}{2}\left(\frac{d\mathbf{x}_{j,\sigma}}{d\tau}\right)^2 - V_C(\bar{\mathbf{x}}(\tau)) - V_b(\bar{\mathbf{x}}(\tau))\right]d\tau + \Phi[\bar{\mathbf{x}}(\tau)], \tag{15}$$

and where Σ_P denotes the sum over all permutations $P\bar{\mathbf{x}}$ over the electron coordinates with the same spin component. Throughout the present treatment, the Euclidean time variable $\tau = it$ is used, where t is the real time variable.

The "influence phase" of the phonons,

$$\Phi[\bar{\mathbf{x}}(\tau)] = -\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' \times\frac{\cosh[\omega_{\mathrm{LO}}(|\tau-\tau'|-\hbar\beta/2)]}{\sinh(\beta\hbar\omega_{\mathrm{LO}}/2)}\rho_{\mathbf{k}}(\tau)\rho_{-\mathbf{k}}(\tau'), \tag{16}$$

describes the phonon-induced retarded interaction between the electrons, including the retarded self-interaction of each electron.

The free energy of a system of interacting polarons $F_p(\{N_\sigma\},\beta)$ is related to their partition function (14) by the equation

$$F_p(\{N_\sigma\},\beta) = -\frac{1}{\beta}\ln Z_p(\{N_\sigma\},\beta). \tag{17}$$

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

$$E^0(\{N_\sigma\}) = \lim_{\beta\to\infty} F_p(\{N_\sigma\},\beta). \tag{18}$$

III. VARIATIONAL PRINCIPLE

At present no method is known to calculate the non-Gaussian path integral (14) analytically. For distinguishable particles, the Jensen-Feynman variational principle[6] 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. 18 and 19 that keeping the appropriate symmetry for a trial system (see the discussion in Ref. 19), the variational inequality for identical particles takes the same form as the Jensen-Feynman variational principle:

$$F_p \leqslant F_0 + \frac{1}{\beta}\langle S_p - S_0\rangle_{S_0}, \tag{19}$$

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

$$\langle(\cdots)\rangle_{S_0} = \frac{\sum_P \frac{(-1)^{\xi_P}}{N_{1/2}!N_{-1/2}!}\int d\bar{\mathbf{x}}\int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}(\tau)(\cdots)e^{-S_0[\bar{\mathbf{x}}(\tau)]}}{\sum_P \frac{(-1)^{\xi_P}}{N_{1/2}!N_{-1/2}!}\int d\bar{\mathbf{x}}\int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}(\tau)e^{-S_0[\bar{\mathbf{x}}(\tau)]}}. \tag{20}$$

In the present paper, we use a trial action in which the background potential and the Coulomb interaction are simulated by harmonic terms,

$$S_0[\bar{\mathbf{x}}(\tau)] = \frac{1}{\hbar}\int_0^{\hbar\beta}\sum_\sigma\sum_{j=1}^{N_\sigma}\frac{m_b}{2}[\dot{\mathbf{x}}_{j,\sigma}^2(\tau)+\Omega^2\mathbf{x}_{j,\sigma}^2(\tau)]d\tau - \frac{1}{\hbar}\int_0^{\hbar\beta}\sum_{\sigma,\sigma'}\sum_{j=1}^{N_\sigma}\sum_{l=1}^{N_{\sigma'}}\frac{m_b\omega^2}{4}[\mathbf{x}_{j,\sigma}(\tau)-\mathbf{x}_{l,\sigma'}(\tau)]^2d\tau + \Phi_0[\bar{\mathbf{x}}(\tau)], \tag{21}$$

with an influence phase of the form

$$\Phi_0[\bar{\mathbf{x}}(\tau)] = -C\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' \times\frac{\cosh[\Omega_f(|\tau-\tau'|-\hbar\beta/2)]}{\sinh(\beta\hbar\Omega_f/2)}\mathbf{X}(\tau)\cdot\mathbf{X}(\tau'), \tag{22}$$

where $\mathbf{X}$ is the center-of-mass coordinate of the electrons,

$$\mathbf{X} = \frac{1}{N}\sum_\sigma\sum_{j=1}^{N_\sigma}\mathbf{x}_{j,\sigma}. \tag{23}$$

The trial action $S_0[\bar{\mathbf{x}}(\tau)]$ thus contains three variational frequencies Ω, ω, and Ω_f, and the factor C which accounts for the strength of the electron-phonon interaction. The diagonalization of this system results in four eigenfrequencies, say Ω_1 (the frequency of the relative motion of the centers of mass of the electrons and the harmonic interaction field), Ω_2 (the frequency of the motion of the center of mass of the model system as a whole), w_0 (the frequency characterizing the coupling of harmonic interaction field to the electrons, analogous to the frequency W in the Feynman polaron model), and w (the frequency of the motion of the electrons in the relative coordinate system), which are known functions of Ω, ω, Ω_f, and C.

The oscillator setup of the trial action does not describe some physical features which exist for a many-electron system in a background-charge potential, such as Friedel oscillations of the electron density. The Friedel oscillations do not arise for a three-dimensional (3D) fermion gas in a parabolic trap, although they exist, e.g., for a one-dimensional fermion gas in a parabolic potential.[20] The treatment of the spatial correlations of the polaron density is beyond the scope of the present work, because our particular interest is to investigate the bulk limit of a homogeneous polaron gas (where the Friedel oscillations do not appear) using a model with a finite number of polarons.

As a result, we obtain the following upper bound to the ground-state energy of an N-polaron system in a spherical compensating background:

$$E_{\mathrm{var}}(\{N_\sigma\}) = \mathbb{E}_F(\{N_\sigma\},w) - \frac{m_b}{2}(\Omega^2 - N\omega^2)\left\langle \sum_{j=1}^{N} \mathbf{x}_j^2 \right\rangle_{S_0} - \frac{m_b\omega^2 N^2}{2}\langle \mathbf{X}^2\rangle_{S_0} + \lim_{\beta\to\infty}\frac{1}{\beta}\langle\Phi_0\rangle_{S_0} + \langle U_b(\bar{\mathbf{x}})\rangle_{S_0} + E_C + E_{e\text{-ph}}. \quad (24)$$

The terms E_C and $E_{e\text{-ph}}$ arise from the Coulomb repulsion between the electrons and the Fröhlich electron-phonon interaction, and are discussed below. The first term $\mathbb{E}_F(N,w)$ is the energy of N noninteracting fermionic oscillators with frequency w:

$$w = \sqrt{\Omega^2 - N\omega^2}, \quad (25)$$

$$\mathbb{E}_F(\{N_\sigma\},w) = \hbar w \sum_{\sigma=\pm 1/2}\left[(N_\sigma - N_{L_\sigma})\left(L_\sigma + \frac{3}{2}\right) + \sum_{n=0}^{L_\sigma - 1}\left(n+\frac{3}{2}\right)g(n)\right], \quad (26)$$

where L_σ is the lowest not fully occupied level for the N_σ electrons with spin projection σ. The energy levels of a 3D oscillator are degenerate, and

$$g(n) = \frac{1}{2}(n+1)(n+2) \quad (27)$$

is the degeneracy of the nth energy level. The parameter

$$N_{L_\sigma} = \frac{1}{6}L_\sigma(L_\sigma+1)(L_\sigma+2) \quad (28)$$

is the number of electrons at all fully filled levels. After some algebra, in the Feynman units ($\hbar=1$, $m_b=1$, $\omega_{\mathrm{LO}}=1$) the variational functional (24) takes the form

$$E_{\mathrm{var}}(\{N_\sigma\}) = \frac{\Omega_0^2 + w^2}{2w}\left(\sum_\sigma \mathcal{F}(N_\sigma) - \frac{3}{2}\right) + \frac{3}{4\Omega_1\Omega_2(\Omega_1+\Omega_2)}(\Omega_1\Omega_2^3 + \Omega_1^3\Omega_2 + 3\Omega_1^2\Omega_2^2 + \Omega_0^2\Omega_1\Omega_2 - 2\Omega_1\Omega_2^2 w_0 + \Omega_1\Omega_2 w_0^2 - 2\Omega_1^2\Omega_2 w_0 + \Omega_0^2 w_0^2) + \langle U_b(\bar{\mathbf{x}})\rangle_{S_0} + E_C + E_{e\text{-ph}}, \quad (29)$$

where the function $\mathcal{F}(N_\sigma)$ is given by

$$\mathcal{F}(N_\sigma) = \frac{1}{8}L_\sigma(L_\sigma+1)^2(L_\sigma+2) + (N_\sigma - N_{L_\sigma})\left(L_\sigma + \frac{3}{2}\right).$$

The term E_C is the Coulomb contribution,

$$E_C = \frac{1}{4\pi^2}\frac{\sqrt{2}\alpha}{1-\eta}\int d\mathbf{q}\frac{1}{q^2}[\,\mathcal{G}(\mathbf{q},0|N_+,N_-)|_{\beta\to\infty} - N] \quad \text{with} \quad \eta = \frac{\varepsilon_\infty}{\varepsilon_0},$$

and $E_{e\text{-ph}}$ is the polaron contribution,

$$E_{e\text{-ph}} = -\frac{\sqrt{2}\alpha}{4\pi^2}\int d\mathbf{q}\frac{1}{q^2}\int_0^\infty d\tau\, e^{-\tau}\,\mathcal{G}(\mathbf{q},\tau|N_+,N_-)|_{\beta\to\infty},$$

where $\mathcal{G}(\mathbf{q},\tau|N_+,N_-)$ is the dynamic two-point correlation function for the electron density operators:

$$\mathcal{G}(\mathbf{q},\tau|N_+,N_-) = \langle \rho_{\mathbf{q}}(\tau)\rho_{-\mathbf{q}}(0)\rangle_{S_0}.$$

This correlation function, for which the path integral calculation was developed in Ref. 21, was described in Ref. 13, and factorizes as follows:

$$\mathcal{G}(\mathbf{q},\tau|N_+,N_-) = \exp\left(-\frac{q^2 D(\tau)}{2N}\right)\tilde{\mathcal{G}}(\mathbf{q},\tau|\{N_\sigma\},\beta). \quad (30)$$

Here, the function $D(\tau)$ is provided by the centers-of-mass motion,

$$D(\tau) = 2\frac{\Omega_1^2 - w_0^2}{\Omega_1^2 - \Omega_2^2}\frac{\sinh(\Omega_1\tau/2)\sinh[\Omega_1(\hbar\beta-\tau)/2]}{\Omega_1\sinh(\beta\hbar\Omega_1/2)} + 2\frac{w_0^2 - \Omega_2^2}{\Omega_1^2 - \Omega_2^2}\frac{\sinh(\Omega_2\tau/2)\sinh[\Omega_2(\hbar\beta-\tau)/2]}{\Omega_2\sinh(\beta\hbar\Omega_2/2)} - \frac{\sinh(w\tau/2)\sinh[w(\hbar\beta-\tau)/2]}{w\sinh(\beta\hbar w/2)}, \quad (31)$$

and $\tilde{\mathcal{G}}(\mathbf{q},\tau|\{N_\sigma\},\beta)$ is the two-point correlation function for the degrees of freedom of an N-polaron system describing the motion of fermions relative to their center of mass,

$$\tilde{\mathcal{G}}(\mathbf{q},\tau|\{N_\sigma\},\beta) = \sum_{\mathbf{n},\mathbf{n}',\sigma}|\langle\mathbf{n}|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}'\rangle|^2 e^{w\tau(n-n')}[f_1(n,\sigma|N_\sigma,\beta) - f_2(n,\sigma;n',\sigma|\{N_\sigma\},\beta)] + \sum_{\mathbf{n},\sigma,\mathbf{n}',\sigma'}\langle\mathbf{n}|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}\rangle \times\langle\mathbf{n}'|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}'\rangle f_2(n,\sigma;n',\sigma'|\{N_\sigma\},\beta), \quad (32)$$

where $\langle\mathbf{n}|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}'\rangle$ is the one-electron matrix element,

$$\langle\mathbf{n}|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}'\rangle = \int e^{i\mathbf{q}\cdot\mathbf{x}}\psi_{\mathbf{n}}^*(\mathbf{x})\psi_{\mathbf{n}'}(\mathbf{x})d\mathbf{x}. \quad (33)$$

$\psi_{\mathbf{n}}(\mathbf{x})$ is the eigenfunction of a 3D oscillator with the frequency ω. The index $\mathbf{n}$ denotes the set $\mathbf{n}=\{n,l,m\}$, where n is the number of the energy level, l is the quantum number of the orbital angular momentum, and m is the quantum number of the z projection of the orbital angular momentum, and $f_1(n,\sigma|N_\sigma,\beta)$ and $f_2(n,\sigma;n',\sigma'|\{N_\sigma\},\beta)$ are one-electron and two-electron distribution functions for a *canonical* ensemble of fermions described in detail in the Appendix of Ref. 13.

Finally, the potential energy of electrons in a uniformly charged background sphere with the radius R is found to be

$$\langle U_b(\bar{\mathbf{x}})\rangle_{S_0} = -\frac{\sqrt{2}\alpha\eta N}{\pi(1-\eta)}\sum_{\sigma}\sum_{n=0}^{\infty} f_1(n,\sigma|N_\sigma,\beta) \times\sum_{k=0}^{n}\frac{(-1)^k}{k!}\binom{n+2}{n-k}\Gamma\left(k+\frac{1}{2}\right) \times\frac{1}{A^{k+1/2}}\left(\frac{1}{2w}\right)^k {}_1F_1\left(k+\frac{1}{2};\frac{5}{2};-\frac{R^2}{4A}\right)+V_{bb}, \tag{34}$$

with the parameter

$$A \equiv \frac{1}{4N}\left(\frac{\Omega_1\Omega_2+w_0^2}{\Omega_1\Omega_2(\Omega_1+\Omega_2)}+\frac{N-1}{w}\right). \tag{35}$$

IV. DISCUSSION OF RESULTS

The minimization of the variational ground-state energy with respect to the variational parameters has to be done numerically. We discuss some of the most relevant results. We have restricted the range of r_s^* in the figures to low and intermediate values, where the contribution to the ground-state energy owing to Wigner crystallization is presumably small.

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 $\eta=0.4908$, and (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 $r_s^*=2$ (which corresponds to the density $n_0\approx 4.34\times 10^{19}$ 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 $r_s^*=20$ (which corresponds to the density $n_0\approx 1.14\times 10^{18}$ 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, 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 ($N=1,4,10,20,35,\ldots$).

The polaron contribution to the ground-state energy can be subdivided into two parts, which behave differently when the number of fermions is increased. Indeed, the correlation function given by Eq. (32) consists of two terms:

$$\tilde{\mathcal{G}}(\mathbf{q},\tau|\{N_\sigma\},\beta)=\tilde{\mathcal{G}}_1(\mathbf{q},\tau|\{N_\sigma\},\beta)+\tilde{\mathcal{G}}_2(\mathbf{q},\tau|\{N_\sigma\},\beta), \tag{36}$$

with

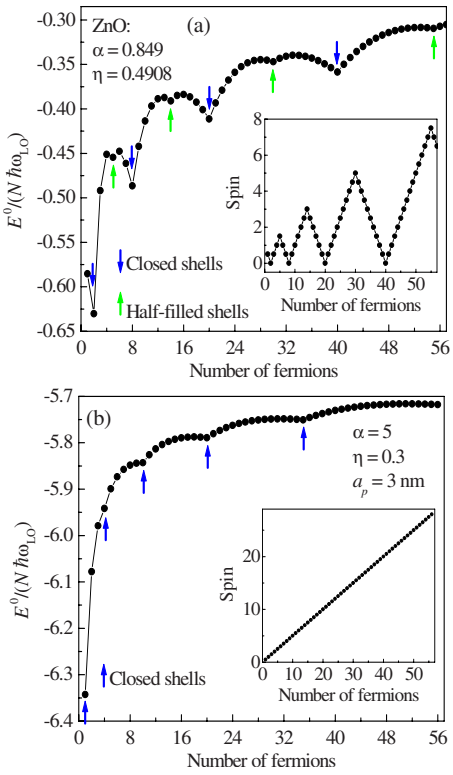

FIG. 1. (Color online) Polaron ground-state energy per particle in an N-polaron quantum dot as a function of the number of fermions. The parameters are taken (a) for ZnO with $\alpha=0.849$, $\varepsilon_0=8.15$, $\varepsilon_\infty=4.0$, and $\hbar\omega_{\mathrm{LO}}=73.27$ meV, and (b) for a polar medium with $\alpha=5$, $\eta=0.3$, and $a_p=3$ nm. The value of the parameter r_s^* is (a) 2, which corresponds to the fermion density $n_0=4.34\times 10^{19}$ cm^{-3}, and (b) 20, corresponding to $n_0=1.14\times 10^{18}$ 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.

$$\tilde{\mathcal{G}}_1(\mathbf{q},\tau|\{N_\sigma\},\beta)\equiv\sum_{\mathbf{n},\mathbf{n}',\sigma}|\langle\mathbf{n}|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}'\rangle|^2 e^{w\tau(n-n')}[f_1(n,\sigma|N_\sigma,\beta) - f_2(n,\sigma;n',\sigma|\{N_\sigma\},\beta)], \tag{37}$$

$$\tilde{\mathcal{G}}_2(\mathbf{q},\tau|\{N_\sigma\},\beta)\equiv\sum_{\mathbf{n},\sigma,\mathbf{n}',\sigma'}\langle\mathbf{n}|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}\rangle \times\langle\mathbf{n}'|e^{i\mathbf{q}\cdot\mathbf{x}}|\mathbf{n}'\rangle f_2(n,\sigma;n',\sigma'|\{N_\sigma\},\beta). \tag{38}$$

In accordance with Eq. (36), we subdivide the Coulomb and polaron contributions:

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

$$E_{e\text{-ph}}=E_{e\text{-ph}}^{(1)}+E_{e\text{-ph}}^{(2)}.$$

For sufficiently large N (in practice, already for $N\geqslant 5$), we can with a high accuracy replace the two-electron distribution function by the product of one-electron distribution functions,

$$f_2(n,\sigma;n',\sigma'|\{N_\sigma\},\beta) \approx f_1(n,\sigma|N_\sigma,\beta) f_1(n',\sigma'|N_{\sigma'},\beta), \tag{39}$$

which allows us to express $\tilde{\mathcal{G}}_2(\mathbf{q},\tau|\{N_\sigma\},\beta)$ as

$$\tilde{\mathcal{G}}_2(\mathbf{q},\tau|\{N_\sigma\},\beta) = \langle\rho_{\mathbf{q}}(\tau)\rangle\langle\rho_{-\mathbf{q}}(0)\rangle = |\langle\rho_{\mathbf{q}}\rangle|^2 \tag{40}$$

and consequently

$$E_C^{(2)} = \frac{e^2}{4\pi^2\varepsilon_\infty}\int d\mathbf{q}\frac{1}{q^2}|\langle\rho_{\mathbf{q}}\rangle|^2.$$

This means that Eq. (38) represents the potential energy of the direct Coulomb electron-electron interaction in the Coulomb contribution. An analogous term occurs for the polaron contribution:

$$E_{e\text{-ph}}^{(2)} = -\frac{\sqrt{2}\alpha}{4\pi^2}\int d\mathbf{q}\frac{1}{q^2}|\langle\rho_{\mathbf{q}}\rangle|^2.$$

With increasing N at a fixed average electron density, the magnitude of $\langle\rho_{\mathbf{q}}\rangle$ increases proportionally to N for sufficiently large N. Therefore, the contributions $E_C^{(2)}$ and $E_{e\text{-ph}}^{(2)}$ under the same conditions increase proportionally to N^2. In the limit of large N, the leading terms of $E_C^{(2)}$ and of $E_{e\text{-ph}}^{(2)}$ can be determined if the electron density

$$n(\mathbf{r}) = \frac{1}{(2\pi)^3}\int \langle\rho_{\mathbf{q}}\rangle e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{q}$$

is uniform inside the background-charge sphere: $n(\mathbf{r}) = n_0\Theta(R-r)$. As a result, we obtain for these leading terms

$$E_C^{(2)}|_{N\gg1} \approx \frac{3}{5}\frac{e^2N^2}{\varepsilon_\infty R}, \quad E_{e\text{-ph}}^{(2)}|_{N\gg1} \approx -\frac{3}{5}\frac{e^2N^2}{\varepsilon^* R},$$

where $1/\varepsilon^* \equiv 1/\varepsilon_\infty - 1/\varepsilon_0$. These terms are precisely compensated by the leading term in the potential energy from the background sphere, confirming the correct treatment of the charge neutrality.

Within the approximation (39), the term (37) is

$$\tilde{\mathcal{G}}_1(\mathbf{q},\tau|\{N_\sigma\},\beta)|_{N\gg1} \approx \sum_{\mathbf{n},\mathbf{n}',\sigma} |(e^{i\mathbf{q}\cdot\mathbf{x}})_{\mathbf{n}\mathbf{n}'}|^2 \exp\left(\frac{\tau}{\hbar}(\varepsilon_n - \varepsilon_{n'})\right) f_1(n,\sigma|N_\sigma,\beta) \times[1 - f_1(n',\sigma'|N_{\sigma'},\beta)], \tag{41}$$

so that (41) is a direct analog of the two-point correlation function in bulk within the Hartree-Fock approximation:

$$\langle\rho_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(0)\rangle|_{\text{bulk,HF}} = \sum_{\mathbf{k},\mathbf{k}'} \exp\left[\tau\left(\frac{k^2}{2} - \frac{(k')^2}{2}\right)\right] \times f_{\mathbf{k}}(1 - f_{\mathbf{k}'})\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}. \tag{42}$$

Therefore, in the "bulk limit" $E_C^{(1)}$ becomes the Coulomb exchange energy, and $E_{e\text{-ph}}^{(1)}$ becomes the polaron contribution for a polaron gas in bulk.

In Fig. 2, we have plotted the polaron contributions $E_{e\text{-ph}}^{(1)}/N$ as a function of N for a quantum dot in ZnO and in a polar medium with $\alpha=5$, $\eta=0.3$. In the insets, the spin of the N-polaron system is represented as a function of the number of fermions. As seen from Fig. 2(a), the polaron contribution $E_{e\text{-ph}}^{(1)}/N$ in ZnO as a function of N oscillates, taking maxima for N corresponding to the closed shells $N=2,8,20,40,\ldots$ and for half-filled shells $N=5,14,30,55\ldots$. In the case of the medium with $\alpha=5$, $\eta=0.3$, for $r_s^*=20$ (corresponding to the density $n_0 \approx 1.14\times10^{18}$ cm^{-3}), the polaron contribution $E_{e\text{-ph}}^{(1)}/N$ oscillates, taking maximal values at the fermion numbers which correspond to closed shells for a spin-polarized system with parallel spins $N=1,4,10,20,35,\ldots$.

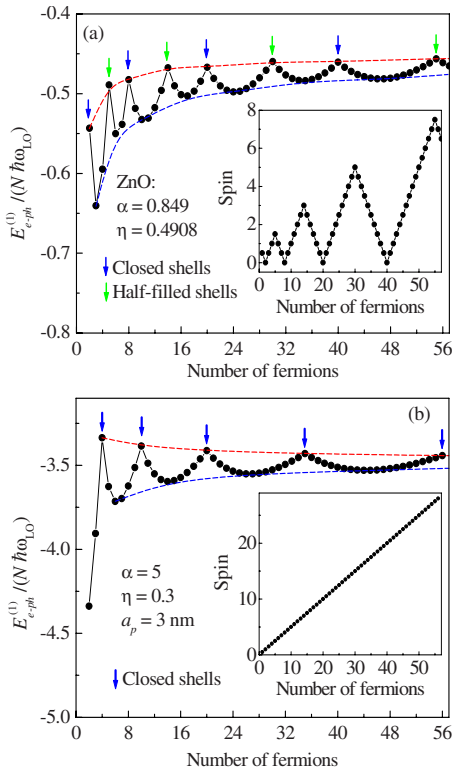

FIG. 2. (Color online) Polaron contribution to the ground-state energy per particle $E_{e\text{-ph}}^{(1)}/N$ in an N-polaron quantum dot as a function of the number of fermions. The values of the parameters are the same as those in Fig. 1.

The dashed curves in Fig. 2 are the envelopes for the local maxima (closed shells) and the local minima of $E_{e\text{-ph}}^{(1)}/N$, respectively. When these envelopes are extrapolated to a larger number of fermions, the distance between the envelopes decreases. Therefore, the magnitude of the variations of $E_{e\text{-ph}}^{(1)}/N$ related to the shell filling diminishes with increasing N, and it is safe to suppose that, in the limit of large N, the envelopes tend to each other at a value that corresponds to the "bulk" limit $\lim_{N\to\infty}(E_{e\text{-ph}}^{(1)}/N)$.

In Fig. 3, the polaron ground-state energy E^0/N per particle is plotted as a function of the effective Wigner-Seitz parameter r_s^* determined by Eq. (13) for different regimes: for the weak-coupling regime with $\alpha=0.01$ [Fig. 3(a)], for the case of ZnO [Fig. 3(b)], and for a medium with $\alpha=5$, $\eta=0.3$ [Fig. 3(c)]. In the insets, the radius of the background sphere R is represented as a function of the number of fer-

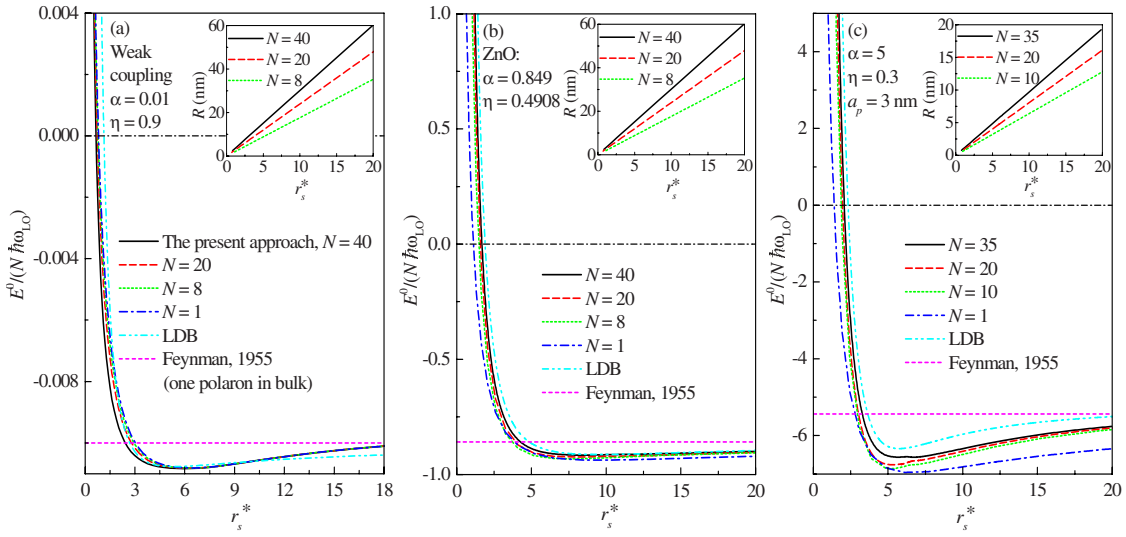

FIG. 3. (Color online) Ground-state energy per particle of an N-polaron system in a quantum dot as a function of the parameter r_s^* for different numbers of fermions. Insets: The radius of a background-charge sphere as a function of r_s^*.

mions. For all considered values of r_s^*, the ground-state energy per particle varies only slightly with N for $N \gtrsim 10$. For a sufficiently large number of particles, an N-polaron system in a quantum dot thus reveals properties close to those for a polaron gas in bulk. The short-dashed lines in Fig. 3 show the one-polaron ground-state energy for a polaron in bulk calculated within the Feynman path-integral variational method.[6] 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 $N=1$, this value analytically coincides with that obtained within the Feynman method. For $N>1$, the limit of an N-polaron energy per particle at $r_s^* \to \infty$ is slightly higher than the Feynman one-polaron ground state energy [except in the weak-coupling regime, Fig. 3(a)]. This difference is due to the fact that the model of Ref. 13 for $N \neq 1$ in the limit $r_s^* \to \infty$ differs from the Feynman model (N times repeated) for a single polaron. In fact, the model applied in the present approach and in Ref. 13 is equivalent to N electrons interacting through an elastic bond with a single fictitious particle, while the Feynman approach assumes an individual fictitious particle for each electron. However, even for relatively high values of r_s^*, the present approach provides lower ground-state energies than those given by the single-polaron Feynman theory. In the weak-coupling regime, the limit of an N-polaron energy per particle at $r_s^* \to \infty$ coincides with the one-polaron ground-state energy in bulk.

In Fig. 4, the polaron contribution $E^{(1)}_{e\text{-ph}}/N$ to the ground state energy per particle is represented as a function of r_s^*. The polaron contribution $E^{(1)}_{e\text{-ph}}/N$ for $\alpha=5$, $\eta=0.3$ [Fig. 4(b)] versus r_s^* has a discontinuity at $r_s^* \approx 6.4$. The total spin as a function of r_s^* for a quantum dot with $\alpha=5$, $\eta=0.3$ is shown in the inset, which reveals that this discontinuity of the polaron contribution is related to a transition from the ground state obeying Hund's rule to the spin-polarized ground state with parallel spins. In the regime governed by Hund's rule, the numbers of electrons $N=10$, 20, and 35 correspond to *different* values of the total spin $S=1$, 0, and 3.5, respectively. We see that those values of the total spin do not monotonically increase with N. As a result, $E^{(1)}_{e\text{-ph}}/N$ in the regime governed by Hund's rule is not a monotonically increasing function of N. It is worth noting that the total ground-state energy changes continuously with varying r_s^*, although partial contributions can be discontinuous at the aforesaid transition.

In Fig. 5, the total ground-state energy and the polaron contribution for a single polaron in a quantum dot are plotted as a function of r_s^* determined by Eq. (13). With increasing r_s^*, the polaron ground-state energy in a quantum dot tends to the ground-state energy of the Feynman polaron[6] in bulk. It should be noted that the dependence of the polaron ground-state energy in a quantum dot on r_s^* is qualitatively similar to that for a polaron gas in bulk[8] even for a single polaron.

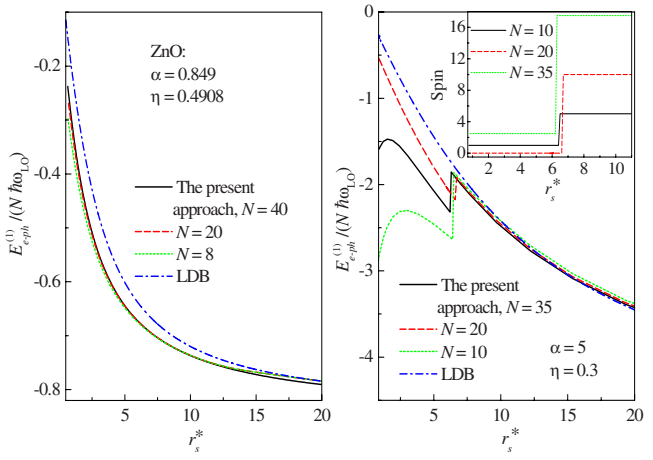

FIG. 4. (Color online) Polaron contribution to the ground-state energy per particle $E^{(1)}_{e\text{-ph}}/N$ of an N-polaron system in a quantum dot as a function of the parameter r_s^* for different numbers of fermions. Inset: The total spin of an N-polaron system as a function of r_s^*.

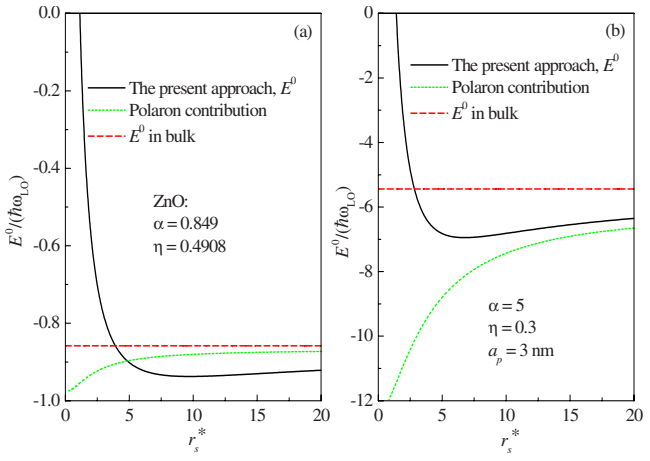

FIG. 5. (Color online) Ground-state energy and the polaron contribution to the ground-state energy $E_{e\text{-ph}}$ for a single polaron in a quantum dot as a function of the parameter r_s^*.

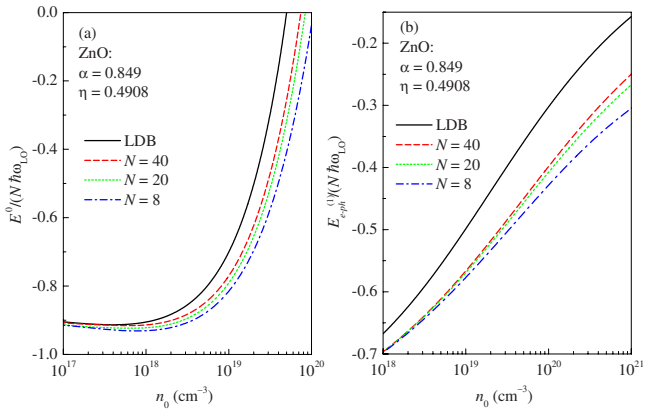

FIG. 6. (Color online) (a) Ground-state energy per particle. (b) Polaron contribution to the ground-state energy per particle $E_{e\text{-ph}}^{(1)}/N$ of an N-polaron system in a quantum dot as a function of the fermion density.

In Figs. 6(a) and 6(b), we plot the polaron ground-state energy per particle and the polaron contribution $E_{e\text{-ph}}^{(1)}/N$ calculated within our variational path-integral method for different numbers of fermions, compared, respectively, with the ground-state energy per particle and with the polaron contribution for a polaron gas in bulk from Ref. 8. As seen from Fig. 6, our all-coupling variational method provides lower values for the ground-state energy and for the polaron contribution than those obtained in Ref. 8. The difference between the polaron contribution calculated within our method and that of Ref. 8 is smaller at low densities and increases in magnitude with increasing density. Note that the ground-state energy per polaron derived within our variational approach for N polarons behaves as a function of density similarly to that for the polaron gas in bulk as described in Ref. 8.

V. CONCLUSIONS

We have generalized Feynman's treatment of a single polaron to an N-polaron system, taking into account fermion statistics. The formalism was applied to a quantum dot with a spherical neutralizing background, which we let grow in size, keeping the electron density fixed. We thus obtain 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- and open-shell systems. For a relatively low number ($N \lesssim 40$) of polarons, the results for the ground-state energy already converge to the bulk limit.

ACKNOWLEDGMENTS

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