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Quantum statistics for a finite number of polarons in a neutralizing background*

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Abstract

The ground-state energy of an N-polaron system, confined to a spherical quantum dot with a neutralizing background charge, is investigated within an all-coupling many-body path-integral variational principle, taking into account both the Fermi statistics of the polarons and the electron–electron interaction. The treatment of the ground-state energy is performed for both closed-shell 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 dependence of the ground-state energy on r_s is very similar to that for a polaron gas in bulk. Hence, 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 potential provided by a neutralizing background charge.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

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 [1] of a *single polaron* provides a superior analytical all-coupling theory. But 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, until now, the stability study [2] was limited to two distinguishable electrons with opposite spin.

Some time ago, two of the present authors [3] contributed to a generalization of the Lee–Low–Pines transformation [4] to the N-polaron problem, that allows one to treat the

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problem (including the statistics) in terms of solely the static structure factor of the electron gas. The method is variational, and limited to the weak electron–phonon coupling regime. More recently, we succeeded [5, 6] 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 strongly relies on the path integral formalism for interacting identical oscillators [7], to which two of the present authors contributed.

In the present paper, we exploit these ideas and techniques to treat the polaron gas, by considering it as a charge-neutral quantum dot which grows in size, while keeping the mean electron density constant.

2. The electron–phonon system

Consider a system of N electrons with mutual Coulomb repulsion, interacting with the lattice vibrations. The system is confined in a sphere of a radius R with a uniform positive background charge density $n_{\rm b}$. The density $n_{\rm b}$ is set equal to the averaged electron density $n_0 = N/(4\pi R^3/3)$, such that the quantum dot is electroneutral. The density can then be expressed in terms of the effective Wigner–Seitz parameter $r_{\rm s}^*$, which is determined by the equation

$$\frac{4\pi}{3}(r_{\rm s}^* a_{\rm B}^*)^3 = \frac{1}{n_0}, \tag{1}$$

with the effective Bohr radius $a_{\rm B}^*$,

$$a_{\rm B}^* = \frac{\hbar^2}{m_{\rm b}(e^2/\varepsilon_\infty)}. \tag{2}$$

$m_{\rm b}$ is the band mass, and ε_∞ is the electronic (high-frequency) dielectric constant. For the study of a polaron gas, this effective Bohr radius is a more appropriate unit of length than the usual unit of length $a_{\rm p}$ of polaron theory

$$a_{\rm p} \equiv \sqrt{\frac{\hbar}{m_{\rm b}\omega_{\rm LO}}}. \tag{3}$$

The total number of electrons is represented as $N = \sum_\sigma N_\sigma$, 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

$$\bar{\mathbf{x}} = \left(\mathbf{x}_{1,-\frac{1}{2}}, \ldots, \mathbf{x}_{N_{-\frac{1}{2}},-\frac{1}{2}}, \quad \mathbf{x}_{1,+\frac{1}{2}}, \ldots, \mathbf{x}_{N_{+\frac{1}{2}},+\frac{1}{2}}\right), \tag{4}$$

the Hamiltonian under consideration is

$$H = \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \frac{\mathbf{p}_{j,\sigma}^2}{2m} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + V_{\rm b}(\bar{\mathbf{x}}) + V_C(\bar{\mathbf{x}}) + \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \sum_{\mathbf{k}} (V_{\mathbf{k}} a_{\mathbf{k}} {\rm e}^{{\rm i}\mathbf{k}\cdot\mathbf{x}_{j,\sigma}} + V_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger {\rm e}^{-{\rm i}\mathbf{k}\cdot\mathbf{x}_{j,\sigma}}), \tag{5}$$

where the electron–phonon interaction is described by the Fröhlich model

$$V_{\mathbf{k}} = \frac{\hbar\omega_{\rm LO}}{{\rm i}k}\left(\frac{4\pi\alpha}{V}\right)^{1/2}\left(\frac{\hbar}{2m\omega_{\rm LO}}\right)^{1/4} \qquad \text{with } \alpha = \frac{e^2}{\hbar c}\sqrt{\frac{m_{\rm b}c^2}{2\hbar\omega_{\rm LO}}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \tag{6}$$

with $\omega_{\rm LO}$ the frequency of the longitudinal optical phonons which 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.

The potential energy from the Coulomb repulsion is

$$V_C(\bar{\mathbf{x}}) = \sum_{\substack{\sigma,\sigma'=\pm\frac{1}{2} \\ (j,\sigma)\neq(l,\sigma')}} \sum_{j=1}^{N_\sigma} \sum_{l=1}^{N_{\sigma'}} \frac{e^2}{2\varepsilon_\infty} \frac{1}{\left|\mathbf{x}_{j,\sigma} - \mathbf{x}_{l,\sigma'}\right|}, \tag{7}$$

and the interaction energy from the background is

$$V_{\mathrm{b}}(\bar{\mathbf{x}}) = \sum_{\sigma} \sum_{j=1}^{N} U_{\mathrm{b}}(|\mathbf{x}|_{j,\sigma}) + V_{bb}, \tag{8}$$

where $U_{\mathrm{b}}(|\mathbf{r}|)$ 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:

$$U_{\mathrm{b}}(r) = -\frac{4\pi e^2 n_{\mathrm{b}}}{3\varepsilon_0} \begin{cases} \dfrac{3R^2 - r^2}{2} & \text{for } r \leqslant R \\ \dfrac{R^3}{r} & \text{for } R \leqslant r, \end{cases} \tag{9}$$

where ε_0 is the static dielectric constant. The ratio η between the high-frequency and low-frequency dielectric constants

$$0 \leqslant \eta = \frac{\varepsilon_\infty}{\varepsilon_0} \leqslant 1 \tag{10}$$

can be used to compare the strength of the electron–electron interaction with the strength of the electron–phonon interaction. The constant term V_{bb} is the potential energy associated with the electrostatic interaction of the background charges with each other:

$$V_{bb} = \frac{3}{5} \frac{e^2 N^2}{\varepsilon_0 R}. \tag{11}$$

If one were able to calculate the partition function $Z(\beta|\{N_\sigma\}) = \mathrm{Tr}(\mathrm{e}^{-\beta H})$ (where $\beta = 1/(k_{\mathrm{B}}T)$ with Boltzmann constant k_{B} and temperature T) for the given number of electrons with spin components σ, one would find the free energy

$$F(\beta|\{N_\sigma\}) = -\frac{1}{\beta} \ln Z(\beta|\{N_\sigma\}), \tag{12}$$

which in the zero-temperature limit $\beta \to \infty$ reduces to the ground-state energy

$$E^0(\{N_\sigma\}) = \lim_{\beta\to\infty} F(\beta|\{N_\sigma\}) \tag{13}$$

of the system.

The trace over the phonon degrees of freedom can be performed in the same way as for the single polaron [1]. The result is the trace of a path integral $K(\bar{\mathbf{x}}, \beta|\bar{\mathbf{x}}')$ (in Euclidean time) over the electron coordinates only:

$$Z(\beta|\{N_\sigma\}) = Z_{\mathrm{ph}}(\beta) Z_{\mathrm{pol}}(\beta|\{N_\sigma\}), \tag{14}$$

$$Z_{\mathrm{pol}}(\beta|\{N_\sigma\}) = \int \mathrm{d}\bar{\mathbf{x}}\, K(\bar{\mathbf{x}}, \beta|\bar{\mathbf{x}}), \tag{15}$$

$$K(\bar{\mathbf{x}}, \beta|\bar{\mathbf{x}}') = \int_{\bar{\mathbf{x}}(0)=\bar{\mathbf{x}}'}^{\bar{\mathbf{x}}(\beta)=\bar{\mathbf{x}}} D\bar{\mathbf{x}}(\tau) \mathrm{e}^{-S[\bar{\mathbf{x}}(\tau)]}, \tag{16}$$

$$S[\bar{\mathbf{x}}(\tau)] = \frac{1}{\hbar} \int_0^{\hbar\beta} \left(\sum_{\sigma} \sum_{j=1}^{N_\sigma} \frac{m_{\mathrm{b}}}{2} \left(\frac{\mathrm{d}\mathbf{x}_{j,\sigma}(\tau)}{\mathrm{d}\tau} \right)^2 + V_{\mathrm{b}}(\bar{\mathbf{x}}(\tau)) + V_C(\bar{\mathbf{x}}(\tau)) \right) \mathrm{d}\tau - \Phi[\bar{\mathbf{x}}(\tau)], \tag{17}$$

where $Z_{\rm ph}(\beta)$ is the partition function of the free phonons, and $Z_{\rm pol}(\beta|\{N_\sigma\})$ is the electronic contribution in which the effect of the electron–phonon interaction is described by an influence functional $\Phi[\bar{\mathbf{x}}(\tau)]$ with a retarded effective electron–electron interaction:

$$\Phi[\bar{\mathbf{x}}(\tau)] = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{2\hbar^2} \int\!\!\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{d}\tau' \frac{\cosh[\omega_{\rm LO}(|\tau-\tau'| - \frac{\hbar\beta}{2})]}{\sinh\left(\frac{1}{2}\beta\hbar\omega_{\rm LO}\right)} \times \sum_{\sigma,\sigma'=\pm\frac{1}{2}} \sum_{j=1}^{N_\sigma} \sum_{j'=1}^{N_{\sigma'}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_{j,\sigma}(\tau) - \mathbf{x}_{j',\sigma'}(\tau'))}. \tag{18}$$

Performing the summation over the phonon wavevectors, this influence functional is expressed as a functional over the retarded Coulomb interaction between the electrons

$$\Phi[\bar{\mathbf{x}}(\tau)] = \frac{\alpha\omega_{\rm LO}}{4}\sqrt{\frac{2\hbar\omega_{\rm LO}}{m_{\rm b}}} \sum_{\sigma,\sigma'=\pm\frac{1}{2}} \sum_{j=1}^{N_\sigma} \sum_{j'=1}^{N_{\sigma'}} \int\!\!\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{d}\tau' \frac{\frac{\cosh\left[\omega_{\rm LO}\left(|\tau-\tau'|-\frac{\hbar\beta}{2}\right)\right]}{\sinh\left(\frac{1}{2}\beta\hbar\omega_{\rm LO}\right)}}{|\mathbf{x}_{j,\sigma}(\tau) - \mathbf{x}_{j',\sigma'}(\tau')|}.$$

However, it should be realized that the propagator $K(\bar{\mathbf{x}}, \beta|\bar{\mathbf{x}}')$ for fermions must satisfy the antisymmetry property

$$K(\bar{\mathbf{x}}, \beta|\bar{\mathbf{x}}') = (-1)^{\xi_{P_\sigma}} K(P_\sigma\bar{\mathbf{x}}, \beta|\bar{\mathbf{x}}'), \tag{19}$$

for any permutation P_σ of the particles with spin component σ, where $\xi_{P_\sigma} = 1$ for even permutations, and $\xi_{P_\sigma} = -1$ for odd permutations.

For the actual calculations it is useful to introduce

$$\rho_{\mathbf{k}} = \sum_{\sigma=\pm1/2} \sum_{j=1}^{N_\sigma} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_{j,\sigma}}, \tag{20}$$

which is proportional to the Fourier transform of the electron density. The potential energy of the electron–electron Coulomb repulsion and the influence functional then take the form

$$V_C(\bar{\mathbf{x}}) = \sum_{\mathbf{k}\neq0} \frac{4\pi e^2}{k^2 V}(\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - N), \tag{21}$$

$$\Phi[\bar{\mathbf{x}}(\tau)] = -\sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{2\hbar^2} \int\!\!\int_0^{\hbar\beta} \mathrm{d}\tau\, \frac{\cosh\left[\omega_{\rm LO}\left(|\tau-\tau'| - \frac{\hbar\beta}{2}\right)\right]}{\sinh\left(\frac{\beta\hbar\omega_{\rm LO}}{2}\right)} \rho_{\mathbf{k}}(\tau)\rho_{-\mathbf{k}}(\tau'). \tag{22}$$

3. The Jensen–Feynman inequality

At present no method is known to calculate the non-Gaussian path integral (15)–(17) analytically. But the Jensen–Feynman variational principle [1] provides a useful approximation technique. It yields a lower bound to the partition function, and hence an upper bound to the free energy:

$$F \leqslant F_{\rm tr} + \frac{1}{\beta}\langle S - S_{\rm tr}\rangle_{S_{\rm tr}}, \tag{23}$$

where $S_{\rm tr}$ is a trial action with corresponding free energy $F_{\rm tr}$, provided that S and $S_{\rm tr}$ are *real* quantities. The angular brackets denote a weighted average over the paths

$$\langle(\bullet)\rangle_{S_{\rm tr}} = \frac{\int \mathrm{d}\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}(0)=\bar{\mathbf{x}}}^{\bar{\mathbf{x}}(\beta)=\bar{\mathbf{x}}} \mathcal{D}\bar{\mathbf{x}}(\tau)(\bullet)\mathrm{e}^{-S_{\rm tr}[\bar{\mathbf{x}}(\tau)]}}{\int \mathrm{d}\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}(0)=\bar{\mathbf{x}}}^{\bar{\mathbf{x}}}(\beta) = \bar{\mathbf{x}}\mathcal{D}\bar{\mathbf{x}}(\tau)\mathrm{e}^{-S_{\rm tr}[\bar{\mathbf{x}}(\tau)]}}. \tag{24}$$

In the present paper, we use a trial action of the form

$$S_{\rm tr}[\bar{\mathbf{x}}(\tau)] = \int_0^{\hbar\beta} \mathrm{d}\tau \left[\sum_{\sigma} \sum_{j=1}^{N_\sigma} \left(\frac{m}{2} \dot{\mathbf{x}}_{j,\sigma}^2(\tau) + \mathsf{A} \mathbf{x}_{j,\sigma}^2(\tau) \right) - \mathsf{B} \sum_{\sigma,\sigma'} \sum_{j=1}^{N_\sigma} \sum_{l=1}^{N_{\sigma'}} \left(\mathbf{x}_{j,\sigma}(\tau) - \mathbf{x}_{l,\sigma'}(\tau) \right)^2 \right] - \mathsf{C} \sum_{j=1}^{N_\sigma} \sum_{l=1}^{N_{\sigma'}} \iint_0^{\hbar\beta} \mathrm{d}\tau \, \mathrm{d}\tau' \frac{\cosh\left(\Omega \left(|\tau - \tau'| - \frac{\hbar\beta}{2} \right) \right)}{\sinh\left(\frac{\beta\hbar\Omega}{2} \right)} \left(\mathbf{x}_{j,\sigma}(\tau) - \mathbf{x}_{l,\sigma'}(\tau') \right)^2 \tag{25}$$

which is similar to the action $S[\bar{\mathbf{x}}(\tau)]$ under study, but with all interactions replaced by quadratic interactions, and with variational parameters A, B, C and Ω. Note that $\langle S - S_{\rm tr} \rangle_{S_{\rm tr}}$ depends on the partition function, the density, the pair correlation function and the dynamic two-point correlation function of the *trial* system. For instance, the expectation value of $\rho_{\mathbf{k}}$ becomes

$$\langle \rho_{\mathbf{k}} \rangle_{S_{\rm tr}} = \sum_{\sigma} \left\langle \sum_{j=1}^{N_\sigma} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_{j,\sigma}} \right\rangle_{S_{\rm tr}} = \sum_{\sigma} N_\sigma \int \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} n_\sigma(\mathbf{r}) \, \mathrm{d}\mathbf{r}, \tag{26}$$

where $n_\sigma(\mathbf{r})$ is the normalized density of electrons with spin component σ in the trial system

$$n_\sigma(\mathbf{r}) = \left\langle \frac{1}{N_\sigma} \sum_{j=1}^{N_\sigma} \delta\left(\mathbf{r} - \mathbf{x}_{j,\sigma} \right) \right\rangle_{S_{\rm tr}}. \tag{27}$$

The trial system now consists of interacting harmonic oscillators in a harmonic confining potential. The required expectation values, including the statistics of the fermions, have been studied before [7]. The bookkeeping to take into account the different spin components is demanding, and the full algebra of this calculation lies beyond the scope of the present report. Most technical details can be found in an earlier paper [6], where a similar treatment was performed for N polarons in a harmonic confinement potential, instead of the uniform spherical background under investigation here. The expectation value of the background potential (8) in the trial system can now be written as

$$\langle V_{\rm b}(\bar{\mathbf{x}}) \rangle_{\rm tr} = \sum_{\sigma} N_\sigma \int U_{\rm b}(|\mathbf{r}|) \, n_\sigma(\mathbf{r}) \, \mathrm{d}\mathbf{r} + V_{bb}, \tag{28}$$

with the density $n_\sigma(\mathbf{r})$ known from previous work, as already mentioned above.

4. Discussion of results

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 executed yet for the large set of parameters which can be of interest (material constants $m_{\rm b}$, $\omega_{\rm LO}$, α, η, doping parameter $r_{\rm s}^*$), but preliminary results indicate that our basic hypothesis holds, i.e., with increasing number of particles for fixed $r_{\rm s}^*$ the ground-state energy converges to the ground-state energy in bulk for a tractable number of particles ($N \sim 50$). We illustrate this with a few representative plots.

In figure 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 with fixed $r_{\rm s}^*$ for two different cases: (i) the

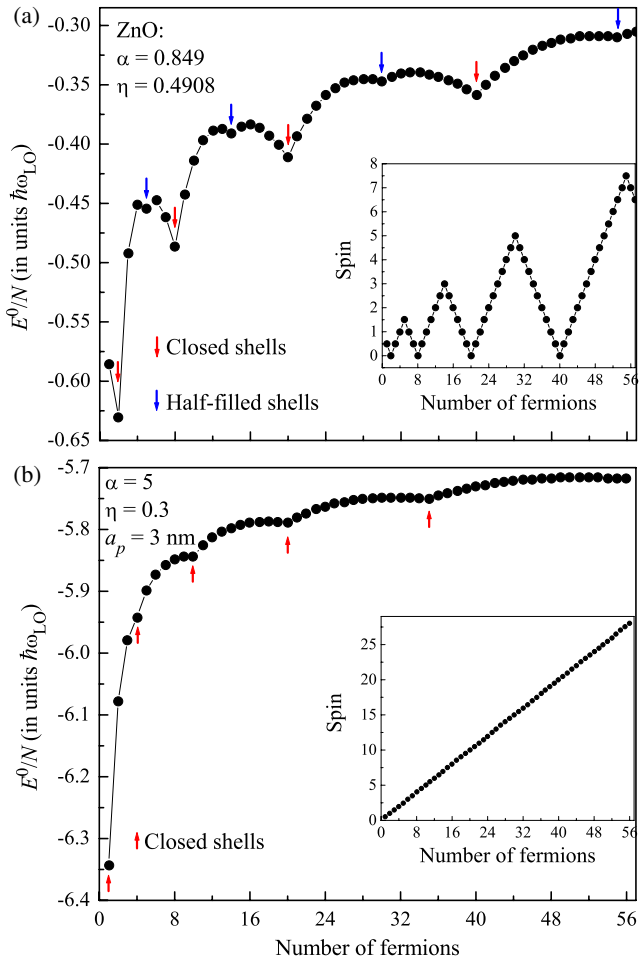

Figure 1. Polaron ground-state energy per particle as a function of the number of fermions. The parameters are taken (a) for ZnO with $\alpha = 0.849$, $\eta = 0.4908$, $r_s^* = 2$, (b) for a polar medium with $\alpha = 5$, $\eta = 0.3$, $r_s^* = 20$. The arrows indicate the number of fermions corresponding to the closed and half-filled shells. *Insets*: the total spin of an N-polaron system as a function of the number of fermions.

case of ZnO with $\alpha = 0.849$, $\eta = 0.4908$, and $\hbar\omega_{LO} = 73.27$ meV, (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 $r_s^* = 2$ (corresponding to a density $n_0 \approx 4.34 \times 10^{19}$ cm^{-3}), the shell filling obeys Hund's rule (see the inset to figure 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 a medium with $\alpha = 5$, $\eta = 0.3$, for $r_s^* = 20$ (corresponding to a density $n_0 \approx 1.14 \times 10^{18}$ cm^{-3}), an N-polaron system in its ground state has the maximal possible spin (see the inset to figure 1(b)). As a result, the ground-state energy as a function of N in figure 1 exhibits kinks for N corresponding to the closed shells of a spin-polarized N-polaron system with parallel spins ($N = 1, 4, 10, 20, 35, \ldots$).

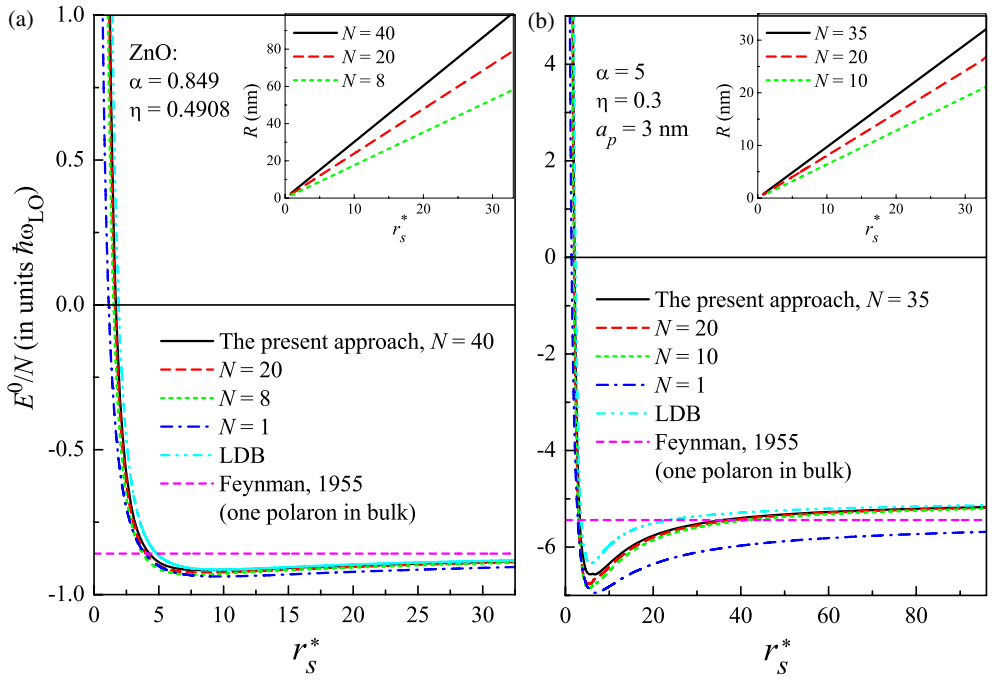

Figure 2. Ground-state energy per particle (and in the insets the radius of the background sphere) as a function of the effective Wigner–Seitz parameter r_s^* for different numbers of fermions. The dash–dotted line represents the results of the generalized Lee–Low–Pines transformation of [3].

In figure 2, the polaron ground-state energy per particle E^0/N is plotted as a function of the effective Wigner–Seitz parameter r_s^* for several numbers of fermions: $N = 1$, 8, 20 and 40 for ZnO (figure 2(a)), and $N = 1$, 10, 20 and 35 for a medium with $\alpha = 5$, $\eta = 0.3$ (figure 2(b)). The insets show the corresponding radius of the background sphere as a function of r_s^*. Notice that, for all considered values of r_s^*, the ground-state energy per particle only slightly varies with N for $N \gtrsim 10$. We can thus assume that, for these numbers of particles, an N-polaron system in a neutral spherical quantum dot reveals properties close to those for a polaron gas in bulk. The dot–dot–dashed lines show the single-polaron ground-state energy for a polaron as calculated with Feynman's path-integral variational method [1]. *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 larger N, the bulk value of the ground-state energy per particle 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 trial system 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 canonical transformation for polarons of [3].

5. Conclusions

We have generalized Feynman's treatment of a single polaron to an N-polaron system, taking into account fermion statistics. For a quantum dot with a spherical neutralizing background, the ground-state energy of the N-polaron system tends to the ground-state energy of a polaron

gas in bulk, if we let the radius of the sphere increase while keeping the density fixed. The results for a relatively low number ($N \lesssim 50$) of polarons converge to the bulk limit. At present we are performing comparisons with other approximations, in particular with those in [8, 9]. Preliminary results confirm the validity of our approach.

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