

# On the ground state energy of a gas of interacting polarons in a magnetic field

K. Putteneers\*, F. Brosens, S.N. Klimin, J.T. Devreese

*Department Fysica, Universiteit Antwerpen, Universiteitsplein 1, B-2610 Antwerpen, Belgium*

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## Abstract

The ground-state energy of a three-dimensional polaron gas in a magnetic field is investigated. An upper bound for the ground-state energy is derived within a variational approach which is based on a many-body generalization of Lee-Low-Pines transformation. The basic contributing ingredients found are the ground-state energy and the static structure factor of the homogeneous electron gas in a magnetic field. Both these quantities are derived in the Hartree–Fock approximation. The resulting ground-state energy of the polaron gas is analyzed as a function of the electron density and of the magnetic field strength.

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## 1. Introduction

Increasing interest in the polaron gas problem is stimulated by intense experimental investigations of polar materials (see, for review, Refs. [1–4]). The electron–phonon interaction is manifested, in particular, in experiments on the cyclotron resonance in bulk [5] and quasi-2D [6–8] systems, giving evidence for a resonant magneto-polaron effect [9]. Cyclotron-resonance measurements on semiconductor quantum wells with high electron density [10–12] reveal that the CR lines are shifted and split as compared to those in low-density quantum wells. In Ref. [13], these effects are interpreted within the framework of the polaron concept, which thus remains valid for high-electron density systems. In this connection, the investigation of the ground-state properties of an interacting polaron gas is an important ingredient.

In the present work, we analyze an interacting polaron

gas at  $T=0$ . However, the obtained results can also be applied to a polaron gas at nonzero temperature if the thermal energy is small as compared to both the LO-phonon energy and the Fermi energy ( $k_B T \ll \hbar \omega_{LO}$ ,  $k_B T \ll E_F$ ). An upper bound for the ground-state energy of a polaron gas in an applied homogenous magnetic field is derived using a many-body generalization [14] of the familiar Lee-Low-Pines transformation [15] for the polaron. The Hamiltonian of the polaron gas is given by

$$\begin{aligned}
 H = & \frac{1}{2m} \sum_{\sigma} \int d^3 r \Psi_{\sigma}^{\dagger}(\mathbf{r}) \left( \frac{\hbar}{i} \nabla + \frac{e}{c} \mathbf{A}(\mathbf{r}) \right)^2 \Psi_{\sigma}(\mathbf{r}) \\
 & + \frac{1}{2} \sum_{\sigma\sigma'} \int d^3 r \int d^3 r' \Psi_{\sigma}^{\dagger}(\mathbf{r}) \Psi_{\sigma'}^{\dagger}(\mathbf{r}') v(\mathbf{r} - \mathbf{r}') \Psi_{\sigma'}(\mathbf{r}') \Psi_{\sigma}(\mathbf{r}) \\
 & + \sum_{\mathbf{k}} \hbar \omega_{LO} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \sum_{\mathbf{k}\sigma} (V_{\mathbf{k}}^* a_{-\mathbf{k}}^{\dagger} + V_{\mathbf{k}} a_{\mathbf{k}}) \\
 & \times \int d^3 r \Psi_{\sigma}^{\dagger}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \Psi_{\sigma}(\mathbf{r}) \\
 & + \sum_{\sigma} \int d^3 r \Psi_{\sigma}^{\dagger}(\mathbf{r}) g \mu_B B \sigma \Psi_{\sigma}(\mathbf{r})
 \end{aligned} \tag{1}$$

where  $a_{\mathbf{k}}^{\dagger}$  and  $a_{\mathbf{k}}$  are the creation and annihilation operators

\* Corresponding author.

E-mail addresses: [katrijn.putteneers@ua.ac.be](mailto:katrijn.putteneers@ua.ac.be) (K. Putteneers), [fons.brosens@ua.ac.be](mailto:fons.brosens@ua.ac.be) (F. Brosens), [sergei.klimin@ua.ac.be](mailto:sergei.klimin@ua.ac.be) (S.N. Klimin), [jozef.devreese@ua.ac.be](mailto:jozef.devreese@ua.ac.be) (J.T. Devreese).

for the longitudinal optical (LO) phonons with frequency  $\omega_{\text{LO}}$ ,  $g$  is the effective Landé factor,  $\mu_{\text{B}}$  is the Bohr magneton,  $m$  is the band mass, and  $\Psi_{\sigma}^{\dagger}(\mathbf{r})$  and  $\Psi_{\sigma}(\mathbf{r})$  are the fermion creation and annihilation field operators for the charge carriers in position  $\mathbf{r}$  with spin projection  $\sigma = \pm 1/2$  along the  $z$  axis which is chosen in the direction of the magnetic field  $\mathbf{B}$ . The electron–phonon interaction strength is described by the amplitude

$$V_k = -i\hbar\omega_{\text{LO}} \left( \frac{4\pi\alpha}{Vk^2} \right)^{1/2} \left( \frac{\hbar}{2m\omega_{\text{LO}}} \right)^{1/4}, \quad (2)$$

$$\alpha = \frac{1}{2} \frac{e^2}{\hbar\omega_{\text{LO}}} \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_0} \right) \left( \frac{2m\omega_{\text{LO}}}{\hbar} \right)^{1/2}$$

where  $\alpha$  is the dimensionless electron–phonon coupling constant with the high-frequency and static dielectric constants  $\varepsilon_{\infty}$  and  $\varepsilon_0$ , and  $v(\mathbf{r})$  is the Coulomb interaction between the electrons, with the Fourier transform

$$v(k) = \frac{1}{V} \frac{4\pi e^2}{\varepsilon_{\infty} k^2} \quad (3)$$

where  $V$  is the crystal volume.

In Ref. [14], the ground-state energy was studied for a polaron gas in the absence of a magnetic field by introducing the following unitary phonon translation operator, which is the many-particle generalization of the Lee-Low-Pines transformation [15]:

$$U = \exp \left[ \sum_{\sigma} \int d^3r \Psi_{\sigma}^{\dagger}(\mathbf{r}) \left( \sum_{\mathbf{k}} (f_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} - f_{\mathbf{k}}^* a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k} \cdot \mathbf{r}}) \right) \Psi_{\sigma}(\mathbf{r}) \right] \quad (4)$$

By applying exactly the same unitary transformation for the polaron gas in the presence of a magnetic field and calculating the expectation value  $\langle \Psi_{\text{GT}} | U^{-1} H U | \Psi_{\text{GT}} \rangle$  in a trial ground state  $|\Psi_{\text{GT}}\rangle = |vac\rangle \cdot |\Psi_{\text{el}}\rangle$  which is the product of the phonon vacuum and an electron state, we found an upper bound to the ground-state energy

$$E = NE_B - \frac{1}{2} N \sum_{\mathbf{k}} v(k) (1 - S(\mathbf{k}))$$

$$+ N \sum_{\mathbf{k}} \left( \hbar\omega_{\text{LO}} S(\mathbf{k}) + \frac{\hbar^2 k^2}{2m} \right) f_{\mathbf{k}} f_{\mathbf{k}}^* \quad (5)$$

$$- N \sum_{\mathbf{k}} (V_k f_{\mathbf{k}}^* + V_k^* f_{\mathbf{k}}) S(\mathbf{k})$$

where  $E_B$  is the energy of a gas of non-interacting electrons in an applied magnetic field  $B$ , and  $S(\mathbf{k})$  is the static structure factor of a homogeneous electron gas in a magnetic field.

Minimizing (5) with respect to  $f_{\mathbf{k}}^*$  we obtained the same formal expression for the optimal values of  $f_{\mathbf{k}}$  as in [14]:

$$f_{\mathbf{k}} = \frac{V_{\mathbf{k}}}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k^2}{2mS(\mathbf{k})}} \quad (6)$$

This results in the following expression for the variational ground-state energy per particle:

$$E_0 = E_B - \frac{1}{2} \sum_{\mathbf{k}} v(k) [1 - S(\mathbf{k})] - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2 S(\mathbf{k})}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k^2}{2mS(\mathbf{k})}} \quad (7)$$

The ground-state energy (7) is structurally similar to that obtained in [14] in the absence of a magnetic field. The basic ingredients  $E_B$  and  $S(\mathbf{k})$  are different though, because of the magnetic field. The static and dynamic structure factors can be calculated using various approximations (see, e.g. Ref. [16] for a confined 3D electron gas and Refs. [17–19] for a 2D electron gas).

In the present paper, we calculate  $E_B$  and  $S(\mathbf{k})$  in the Hartree–Fock approximation, which is variational in nature. The contribution  $E_B$  is treated in Section 2.1. The static structure factor  $S(\mathbf{k})$  will be discussed in Section 2.2. The upper bound to the ground-state energy per particle, taking both contributions into account, is discussed in Section 3. For the numerical calculations and illustrations the degenerate polar semiconductor GaAs is used (Table 1).

## 2. Ingredients contributing to the ground-state energy

### 2.1. Energy of non-interacting electrons in a magnetic field

The energy of non-interacting electrons in a magnetic field is calculated starting from the energy for a single particle in a magnetic field and applying the Pauli principle. Expressing that the number of particles  $N$  equals the number of occupied states we arrive at the equation

$$\nu \sum_{\sigma=\pm\frac{1}{2}} \sum_{n=0}^{\infty} \sum_{k_z} \Theta \left( E_F - \hbar\omega_c \left( n + \frac{1}{2} \right) - g\mu_{\text{B}} B \sigma - \frac{\hbar^2 k_z^2}{2m} \right) = N \quad (8)$$

where  $\nu$  is the degeneration factor of each Landau level,  $k_z$  represents the wave vector component along the magnetic field,  $\omega_c$  is the cyclotron frequency and  $E_F$  stands for the Fermi energy. The function  $\Theta(x)$  is defined as

$$\Theta(x) = \begin{cases} 1 & \text{if } x \text{ is true} \\ 0 & \text{if } x \text{ is false} \end{cases} \quad (9)$$

Table 1

Parameters and material constants of GaAs which are used for the calculations

$m/m_{\text{e}}$	$\hbar\omega_{\text{LO}}$ (meV)	$\varepsilon_{\infty}$	$\varepsilon_0$	$\alpha$	$g$
0.0653 [20]	36.3 [21]	10.89 [21]	13.18 [21]	0.068 [22]	−0.44 [23]

By summing all one-electron energies obeying the Pauli principle one obtains

$$E_B = \frac{m\omega_c}{2\pi^2\hbar n_0} \sum_{\sigma=\pm\frac{1}{2}} \sum_{n=0}^{n_{\max}(\sigma)} \times \left[ \left( \hbar\omega_c \left( n + \frac{1}{2} \right) + g\mu_B B\sigma \right) \kappa_{n,\sigma} + \frac{\hbar^2 \kappa_{n,\sigma}^3}{6m} \right] \quad (10)$$

$$\kappa_{n,\sigma} = \sqrt{\frac{2m}{\hbar^2} \left( E_F - \hbar\omega_c \left( n + \frac{1}{2} \right) - g\mu_B B\sigma \right)} \quad (11)$$

where  $n_0 = N/V$  is the electron density and  $\kappa_{n,\sigma}$  is the maximal wave vector in  $z$ -direction of an electron with the spin projection  $\sigma$  in the  $n$ -th Landau level. The integer

$$n_{\max}(\sigma) = \left\lfloor \frac{E_F - g\mu_B B\sigma}{\hbar\omega_c} - \frac{1}{2} \right\rfloor \quad (12)$$

denotes the number of fully occupied Landau levels with the spin projection  $\sigma$ . The energy contributions clearly depend on the electron density and on the magnitude of the applied magnetic field via the Fermi energy and the number of occupied Landau levels.

## 2.2. Structure factor

Within the Hartree–Fock approximation, the expression for the static structure factor is calculated based on the second quantization form

$$S(\mathbf{k}) = 1 + \frac{1}{N} \sum_{\sigma\sigma'} \int d^3r \int d^3r' e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \times \langle \Psi_{\text{el}} | \Psi_{\sigma'}^{\dagger}(\mathbf{r}) \Psi_{\sigma'}^{\dagger}(\mathbf{r}') \Psi_{\sigma'}(\mathbf{r}') \Psi_{\sigma}(\mathbf{r}) | \Psi_{\text{el}} \rangle \quad (13)$$

The calculations were performed with periodic boundary conditions on a cube with volume  $V$ , and the limit  $V \rightarrow \infty$  is taken keeping the density  $n_0$  constant. Writing out the field operators in the energy representation and applying Wick's theorem, the structure factor is expressed in terms of integrals over wave vectors and summations over eigenstates of electrons in a magnetic field. Using the orthogonality relations for the eigenstates one is left with an exchange term which involves integrals of the form [24]

$$\int_{-\infty}^{\infty} dx e^{-x^2} H_m(x + \alpha) H_n(x + \beta) = 2^n \sqrt{\pi} m! \beta^{n-m} L_m^{n-m}(-2\alpha\beta) \quad \text{for } m < n \quad (14)$$

where  $H_n(x)$  is the Hermite polynomial of the  $n$ -th order and where  $L_j^k(x)$  is an Laguerre polynomial.

The resulting expression for the static structure factor of

an electron gas in a magnetic field is

$$S(\mathbf{k}) = 1 - \frac{1}{(2\pi l_B)^2 n_0} e^{-\frac{l_B^2 k_{\perp}^2}{2}} \times \sum_{\sigma} \sum_n^{n_{\max}(\sigma)} \sum_{n'}^{n_{\max}(\sigma)} \frac{n_{<}!}{n_{>}!} \left( \frac{l_B^2 k_{\perp}^2}{2} \right)^{n_{>} - n_{<}} \times \left[ L_{n_{<}}^{n_{>} - n_{<}} \left( \frac{l_B^2 k_{\perp}^2}{2} \right) \right]^2 \zeta(n, n', \sigma, k_z) \quad (15)$$

$$\zeta(n, n', \sigma, k_z) = 2\kappa_{n_{>},\sigma} \Theta(|k_z| \leq \kappa_{n_{<},\sigma} - \kappa_{n_{>},\sigma}) + (\kappa_{n_{>},\sigma} + \kappa_{n_{<},\sigma} - |k_z|) \times \Theta(\kappa_{n_{<},\sigma} - \kappa_{n_{>},\sigma} \leq |k_z| \leq \kappa_{n_{>},\sigma} + \kappa_{n_{<},\sigma}) \quad (16)$$

where  $l_B = \sqrt{\frac{\hbar c}{eB}}$  is the magnetic length,  $k_{\perp}$  denotes the component of the wave vector perpendicular to the applied magnetic field,  $n_{>} \equiv \max(n, n')$  and  $n_{<} \equiv \min(n, n')$ . In order to avoid numerical underflow or overflow in the recurrence relations, it is important to consider renormalized associated Laguerre polynomials

$$\mathcal{L}_{n-p}^p(x) = \sqrt{\frac{p!(n-p)!}{n!}} L_{n-p}^p(x)$$

It is clear from (15) that the dependence of  $S(\mathbf{k})$  on the wave vector component perpendicular to the magnetic field and on the wave vector component along the magnetic field can be treated separately, and that the introduction of a magnetic field results in an anisotropy of the structure factor.

In the present calculations, the electron density is described through the parameter  $r_s = r_0/\alpha_B^*$ , where  $r_0 = (4\pi n_0/3)^{-1/3}$  is the Wigner-Seitz radius, and  $\alpha_B^* = \hbar^2 \epsilon_{\infty}/(e^2 m)$  is the effective Bohr radius.

In Fig. 1, the static structure factor  $S(k_{\perp}, k_z)$  is plotted for the value  $r_s = 1$ , corresponding to the electron density  $n_0 \approx 3.75 \times 10^{17} \text{ cm}^{-3}$  in GaAs. The dependence of the structure factor on  $k_{\perp}$  is shown in Fig. 1(a), which reveals that the structure factor  $S(k_{\perp}, k_z)|_{k_z=0}$  is a smooth function with limiting values  $S(0,0)=0$  and  $S(\infty,0)=1$ . The curvature however, increases with increasing magnetic field, with a smaller slope for small  $k$ , and an increasing value of the wave vector before the high wave vector limit is reached.

Fig. 1(b) reveals that the structure factor as a function of the wave vector component along the magnetic field is far less smooth. Relatively pronounced kinks appear in  $S(0, k_z)$  where the slope suddenly changes, and the number of kinks for  $S(\mathbf{k}) < 1$  exactly equals the number of fully occupied Landau levels. The static structure factor  $S(k)$  thus allows to count the number of occupied Landau levels of a polaron gas with given density and magnetic field strength. Furthermore,  $S(k_{\perp}, k_z)$  more rapidly tends to unity in the  $z$ -directions, parallel to  $B$ , than the  $xy$ -plane. Furthermore,

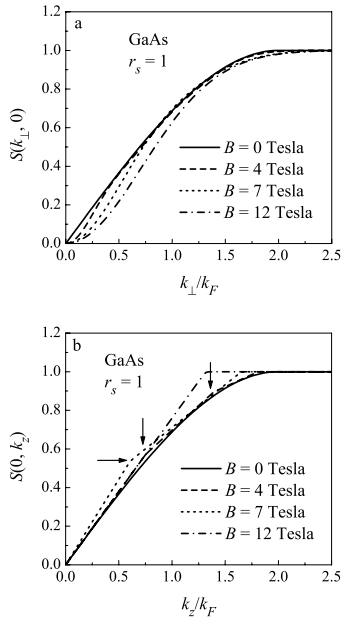


Fig. 1. Hartree-Fock static structure factor  $S(k_{\perp}, k_z)$  of an electron gas as a function of the wavevector component  $k_{\perp}$  perpendicular to the applied magnetic field (a) and as a function of the wavevector component  $k_z$  along the applied magnetic field (b). In both cases the other wavevector component is equal to zero. In the panel 'b', the downward pointing arrows indicate the two kinks corresponding to the magnetic field of 4 T ( $n_{\max}=2$ ), and the horizontal pointing arrow indicates the kink corresponding to 7 T ( $n_{\max}=1$ ).

this anisotropy enhances with increasing  $B$ . As a result,  $S(k_{\perp}, 0)$  is, as a general trend, a decreasing function of  $B$ , whereas  $S(0, k_z)$  increases with increasing  $B$ . The physical reason for this anisotropy is the following. A magnetic field applied along the  $z$ -axis hinders the translation of the electrons in the  $xy$ -plane analogously to a parabolic confinement potential with the frequency  $\omega_c$  and with confinement length  $l_B = \sqrt{\frac{\hbar c}{eB}}$ . The magnetic length decreases with increasing magnetic field strength, and hence the region of  $k_{\perp}$ , in which  $S(k_{\perp}, k_z)$  substantially varies, increases because it is of the order of  $l_B^{-1}$ , as seen from the factor  $\exp(-l_B^2 k_{\perp}^2 / 2)$  in Eq. (15). However, the anisotropy is non-monotonous: it is accompanied by oscillations due to the de Haas-van Alphen effect [25].

### 3. Ground state energy: results and discussion

Converting the sums in (7) to integrals over cylinder coordinates, introducing dimensionless variables, reducing the singularity in the origin and using two-dimensional open Romberg integration, we calculated the variational ground-state energy per particle numerically.

In Fig. 2(a) the ground-state energy per particle is plotted as a function of the magnetic field. Both the many-polaron

ground-state energy and the Fermi energy are oscillating functions of the magnetic field. At well-defined magnetic fields inflection points occur in  $E_0(B)$ . This phenomenon can be understood if we look at the Fermi energy: the inflection points of the ground-state energy coincide with the local maxima of the Fermi energy, and therefore those inflection points are a direct consequence of the de Haas-van Alphen effect. For comparison, we also have plotted in Fig. 2(a) the ground-state energy calculated for  $\alpha=0$  (the dashed curve), i.e. without the polaron contribution. As seen from the figure, the electron-phonon interaction substantially shifts the ground-state energy to lower values with respect to that calculated for  $\alpha=0$ . This shift is practically independent on the magnetic field strength.

The described dependence of the energy on the magnetic field is also seen in Fig. 3(a), which shows the energy as a function of the parameter  $r_s$ . From this figure, it is clear that by applying a magnetic field, the minimum of the ground-state energy occurs at a finite value of  $r_s$ .

Similarly as in Fig. 2(a), kinks appear due to the change of the number of fully occupied Landau levels, as is more clearly illustrated in Fig. 3(b) where the Fermi energy is shown as a function of  $r_s$ . For all values of the magnetic field, the magnitude of the difference between  $E^0$  and  $E^0|_{B=0}$  falls down with increasing density, so that the influence of the magnetic field on the ground-state energy of a polaron gas is larger for lower densities. This behavior of  $E^0$  as a

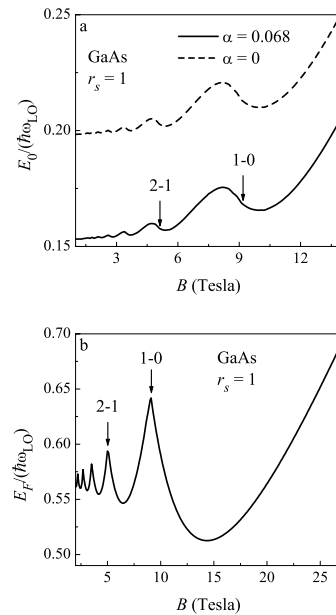


Fig. 2. The ground-state energy per particle (a) and the Fermi energy (b) as a function of the magnetic field for a polaron gas in GaAs with  $r_s=1$ . The arrows and numbers indicate the changes of the number of filled Landau levels  $n_{\max}$ . The dashed curve shows the ground-state energy calculated without the polaron contribution. Notice the different scale in the abscises of both panels.

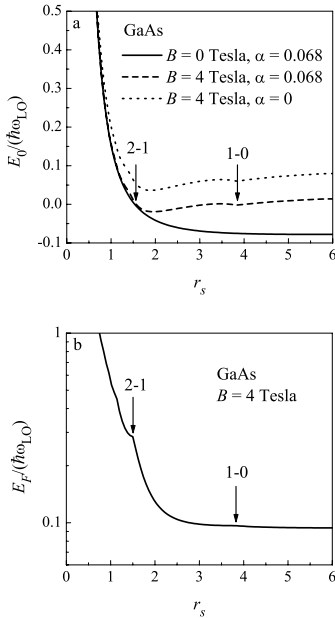


Fig. 3. The ground-state energy per particle with and without applied magnetic field (a) and the Fermi energy for  $B=4$  T (b) for a polaron gas in GaAs as a function of the parameter  $r_s$ . The arrows and numbers indicate the changes of  $n_{\max}$ . The dotted curve shows the ground-state energy calculated without the polaron contribution.

function of the density is explained by the fact that, when the density is high enough, a large number of Landau levels are filled. In this case, the magnetic field should be considered as relatively weak with respect to the characteristic frequency of the electron gas  $E_F/\hbar$  ( $\omega_c \ll E_F/\hbar$ ).

When comparing in Fig. 3 the density dependence of the ground-state energy for a polaron gas with that calculated without the electron–phonon interaction, we see that the magnitude of the polaron contribution decreases with decreasing  $r_s$  due to screening. The same trend was indicated also for a polaron gas in the absence of a magnetic field in Ref. [14].

#### 4. Conclusion

We have extended the variational approach to the many-polaron problem [14] to a system of interacting polarons in an external homogeneous magnetic field. The rigorous upper bound for the ground-state energy of an interacting polaron gas in a magnetic field has been obtained in terms of the static structure factor. Due to the presence of a magnetic field, the static structure factor as a function of the electron density reveals features related to the filling of the Landau levels, when the Fermi energy crosses a Landau level. The other result of an applied magnetic field is the field-induced anisotropy of the structure factor  $S(\mathbf{k})$ , which should be observable experimentally.

The application of a magnetic field has pronounced effects on the behavior of the ground-state energy as a function of the electron density. The most prominent feature, which is also observed in the ground-state energy as a function of the magnetic field, is the occurrence of kinks in the ground-state energy, which occur as a consequence of the de Haas–van Alphen effect as soon as a Landau level becomes fully occupied. Although the ground-state energy is not directly observable, these phenomena should influence experimental data, e.g. the optical absorption of the polaron gas in a magnetic field, which are currently being studied.

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