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Many-electron effects on the two-dimensional D^- centre in a strong magnetic field

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Abstract. The many-electron effects on the two-dimensional D^- centre in a strong magnetic field are investigated in the framework of a static random-phase and low-wavenumber approximation. It is found that the energy levels of the D^- centre oscillate with Landau filling factor. A decrease in the temperature intensifies the oscillation. The screening of the electron gas on the Coulomb potential can be weakened greatly when the Landau filling factor is an integer. It is also found that the state of total angular momentum $L = -2$ can be a bound state only when the Landau filling factor is in a certain region centring at an integer and the temperature is low enough.

1. Introduction

It is well known that a neutral hydrogenic donor can bind a second electron to form a negative ion called the D^- centre. Recently there has been considerable interest in the two-dimensional (2D) or quasi-two-dimensional D^- centre, especially in the limit of a strong magnetic field [1–3]. The experiments reported by Cheng *et al* observing magneto-optical transitions associated with D^- centres in a quasi-2D electron gas and in the presence of a strong magnetic field [1] have motivated the present investigation of screening effects of an electron gas on the 2D D^- centre.

For the 2D neutral centres (D^0) in a zero magnetic field, several linear static screening model calculations have shown that the binding energy of the D^0 centre decreases rapidly as the electron density increases [4]. A non-linear screening calculation for 2D D^0 in a magnetic field [5] has shown that the binding energy of the centre oscillates with the Landau level filling factor. To the best of our knowledge, how the energy spectrum of a 2D D^- centre in a strong magnetic field is influenced by the presence of a 2D electron gas has not been considered theoretically.

In this paper we present an evaluation of the screening effects of a 2D electron gas on the energy spectrum of a 2D D^- centre in a strong magnetic field. In section 2, we outline the theory used in this work. Our numerical results are summarized in section 3.

2. Theory

We consider a 2D system consisting of two electrons and an ionized donor in the presence of a magnetic field (perpendicular to the x–y plane) and in the presence of a 2D electron

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gas. We use $l = (\hbar c/eB)^{1/2}$ as the length unit and employ the complex numbers $z = x + iy$ to describe the 2D position vectors. Using the symmetric gauge with the origin at the donor site, we express the single-particle kinetic energy eigenstates in terms of the Landau level ladder operators [2]

$$a = (1/\sqrt{2})(z/2 - 2\,\partial/\partial z^*) \tag{1}$$

and

$$b = (1/\sqrt{2})(z/2 + 2\,\partial/\partial z^*). \tag{2}$$

They obey the commutation relations $[a, a^\dagger] = [b, b^\dagger] = 1$ and $[a, b] = [a^\dagger, b^\dagger] = 0$. The kinetic energy eigenstates are

$$|N, M\rangle = [(a^\dagger)^N (b^\dagger)^M / \sqrt{N!M!}]|0, 0\rangle. \tag{3}$$

The Hamiltonian of the system is

$$H = H_1 + H_2 + V(|r_1 - r_2|) \tag{4}$$

where

$$H_i = \hbar\omega_c(a_i^\dagger a_i + \tfrac{1}{2}) - V(r_i). \tag{5}$$

Here $\omega_c = eB/mc$ is the cyclotron frequency and m is the band mass of the electron. In equations (4) and (5), $V(r_i)$ is the screened Coulomb potential between the ith electron and the ionized donor, and $V(|r_1 - r_2|)$ is the screened potential between electron 1 and electron 2. Horing and Yildiz [6] have investigated the longitudinal dielectric response properties of a 2D plasma in a magnetic field. They found that, in the framework of the random-phase approximation (RPA), for a low wavenumber, the shielded potential of a point charge in position space is given by

$$V(r) = \int \frac{d^2k}{(2\pi)^2} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \frac{2\pi e^2/\epsilon}{k + (2\pi e^2/\epsilon)\,\partial\rho/\partial\xi}. \tag{6}$$

The quantity $k_0 = (2\pi e^2/\epsilon)\,\partial\rho/\partial\xi$ may be interpreted as an inverse screening length. ρ is the density of the electron gas and ξ the chemical potential. ϵ is the high-frequency dielectric constant of the background. In the degenerate case, for an arbitrary field and an arbitrary temperature, the expression for the electron gas density is given by

$$\rho = \frac{m\omega_c}{\pi\hbar} \sum_{n=0}^{\infty} \eta((n + \tfrac{1}{2})\hbar\omega_c) f_0((n + \tfrac{1}{2})\hbar\omega_c) \tag{7}$$

where $\eta(x)$ is the unit step function and $f_0((n + \frac{1}{2})\hbar\omega_c) = [\![1 + \exp\{\beta[(n + \frac{1}{2})\hbar\omega_c - \xi]\}]\!]^{-1}$ is the Fermi–Dirac distribution function. We take $\xi \simeq E_F = \pi\hbar^2 N_e/m$, where N_e is the average density of the electron gas, and define the filling factor as $\nu = N_e hc/eB$; then we have

$$k_0 = 2\sqrt{2}\beta(R^*\hbar\omega_c)^{1/2} \sum_{n=0}^{\infty} \eta((n + \tfrac{1}{2})\hbar\omega_c)) \frac{\exp[\beta\hbar\omega_c(n + \frac{1}{2} - \nu)]}{[1 + \exp[\beta\hbar\omega_c(n + \frac{1}{2} - \nu)]]^2} \tag{8}$$

where $R^* = me^4/2\epsilon\hbar^2$ is the effective Rydberg. It can be seen from equation (8) that k_0 has delta-function peaks whenever ν equals half an odd integer in the zero-temperature case, reflecting that the Coulomb potential is screened completely in that case.

We now turn our attention to finding the eigenenergies and eigenfunctions of equation (4). According to [2, 3], in the strong-field limit, $|N, M\rangle$ are the eigenfunctions of equation (5), and the eigenfunctions for the D^- centre can be constructed from

$$\Psi^{\pm}(M) = \sum_{M_1=0}^{M} C(M_1, M - M_1)\phi^{\pm}(M_1, M_2) \tag{9}$$

and

$$\phi^{\pm}(M_1, M_2) = |M_1, M_2\rangle_1|M_1, M_2\rangle_2 \pm |M_1, M_2\rangle_2|M_1, M_2\rangle_1. \tag{10}$$

It is easy to show that the above conclusions are correct when the potential is screened. We employ the method presented by MacDonald [2] to solve equation (4). For evaluation of the interaction energy between an electron and the ionized impurity, we have

$$\begin{aligned}\langle N, M|V(r)|N, M\rangle &= \int \frac{d^2k}{(2\pi)^2}\frac{2\pi e^2/\epsilon}{k + k_0}\langle N, M|\exp(-i\boldsymbol{k}\cdot\boldsymbol{r})|N, M\rangle \\ &= \int \frac{d^2k}{(2\pi)^2}\frac{2\pi e^2/\epsilon}{k + k_0}\exp(-\tfrac{1}{2}k^2)G^{NN}(k^*)G^{MM}(k)\end{aligned} \tag{11}$$

where $G^{i'i}(k) = \langle i'|\exp(-ika^\dagger/\sqrt{2})\exp(-ika/\sqrt{2})|i\rangle$. In particular, we have $G^{00}(k) = 1$, $G^{11}(k) = 1 - \frac{1}{2}k^2$ and $G^{22}(k) = 1 - 2(\frac{1}{2}k^2) + \frac{1}{2}(\frac{1}{2}k^2)^2$.

For the elements of the screened Coulomb energy between two electrons, it is convenient to introduce the Landau level ladder operators for the centre-of-mass (R) and relative (r) coordinates. They are related to those for the individual particle operators by [2]

$$a_R^\dagger = (1/\sqrt{2})(a_1^\dagger + a_2^\dagger) \tag{12}$$

and

$$a_r^\dagger = (1/\sqrt{2})(a_1^\dagger - a_2^\dagger). \tag{13}$$

Similarly, we have

$$b_R^\dagger = (1/\sqrt{2})(b_1^\dagger + b_2^\dagger) \tag{14}$$

and

$$b_r^\dagger = (1/\sqrt{2})(b_1^\dagger - b_2^\dagger). \tag{15}$$

For a D^- centre in a strong magnetic field without screening, there are four bound states, namely the total angular momentum $L = 0$ symmetric state, and $L = -1$, -2, and -3 antisymmetric states [2, 3]. The wavefunctions, respectively, are

$$|L = 0\rangle_S = |0, 0\rangle_1|0, 0\rangle_2 = |0, 0\rangle_R|0, 0\rangle_r \tag{16}$$

$$|L = -1\rangle_T = (1/\sqrt{2})(|0, 1\rangle_1|0, 0\rangle_2 - |0, 1\rangle_2|0, 0\rangle_1) = |0, 0\rangle_R|0, 1\rangle_r \tag{17}$$

$$|L = -2\rangle_T = (1/\sqrt{2})(|0, 2\rangle_1|0, 0\rangle_2 - |0, 2\rangle_2|0, 0\rangle_1) = |0, 1\rangle_R|0, 1\rangle_r \tag{18}$$

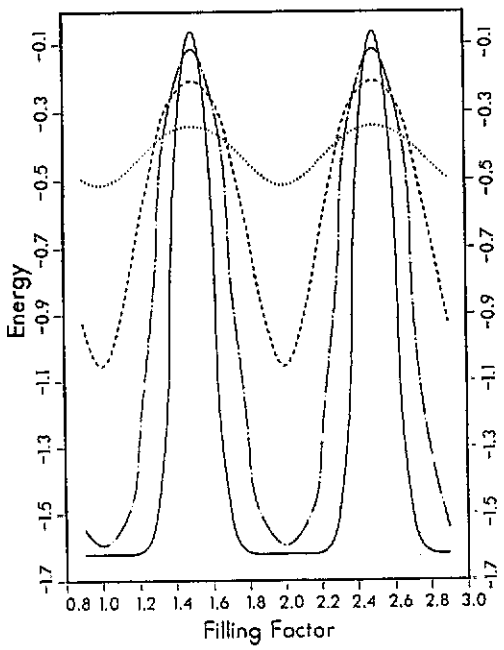

Figure 1. Energy levels of the state $|L = 0\rangle$ with $F = 5$ (· · · · · ·), 10 (– – –), 20 (— · —) and 40 (——).

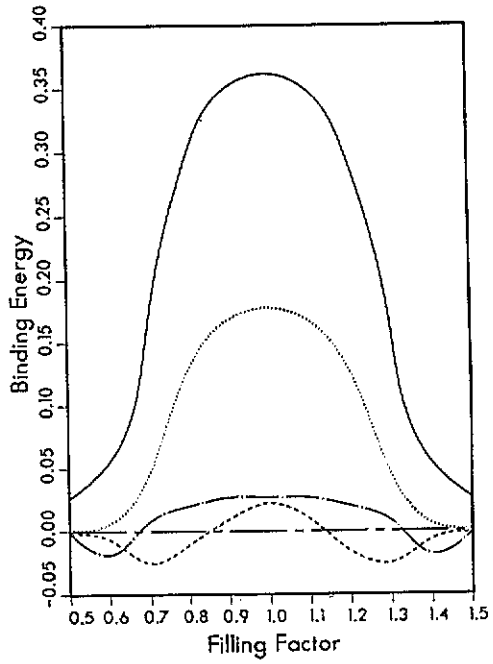

Figure 2. Binding energies of the states $|L = 0\rangle$ (——), $|L = -1\rangle$ (· · · · · ·) and $|L = -2\rangle$ (– – –) with $F = 20$; — · —, binding energy of the state $|L = -2\rangle$ with $F = 40$.

and

$$|L = -3\rangle_T = \tfrac{1}{2}(|0,0\rangle_1|0,3\rangle_2 - |0,0\rangle_2|0,3\rangle_1 + |0,1\rangle_1|0,2\rangle_2 - |0,1\rangle_2|0,2\rangle_1)$$
$$= (1/2\sqrt{2})[(\sqrt{3}-1)|0,2\rangle_R|0,1\rangle_r + (\sqrt{3}+1)|0,0\rangle_R|0,3\rangle_r)]. \tag{19}$$

We believe that the states mentioned above are the bound states of the D^- centre in the presence of the screening, at least in the case when the screening is weakened greatly.

The eigenvalues of equation (4) corresponding to the state $|L = -M\rangle$ are

$$E(L = -M) = \langle L = -M|H|L = -M\rangle. \tag{20}$$

In section 3, we calculate the eigenenergies and the binding energies (defined as the minimum energy required to remove one of the two electrons to infinity) of the D^- centre based on equation (20) numerically.

3. Calculation and conclusion

The energy levels of the 2D D^- centre and the binding energies have been calculated by numerical integration in this work. The parameters that we used are as follows: $\hbar\omega_c = 0.01558$ eV for $B = 9$ T and $m/m_e = 0.067$; the effective Rydberg $R^* = me^4/2\epsilon^2\hbar^2 = 0.0055$ eV. The energies are measured in the unit e^2/l in figures 1 and 2. We take $F = \beta\hbar\omega_c$ as a variable quantity to investigate how the temperature influences the screening effects. The results are given in figures 1–4.

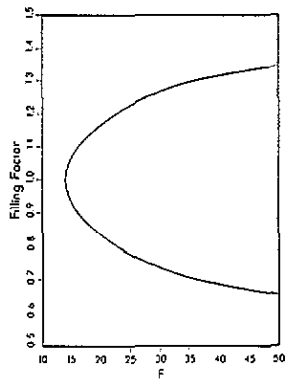

Figure 3. The region when the state $|L = -2\rangle$ is a bound state.

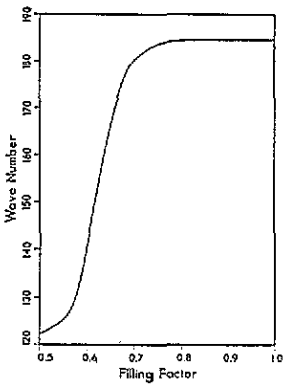

Figure 4. The absorption spectrum for the $L = 0$ symmetric bound state. The wavenumbers are in reciprocal centimetres.

In figure 1, $E(L = 0)$ is presented as a function of the filling factor ν when $F = 5$, 10, 20 and 40. It can be seen that $E(L = 0)$ appears to have an oscillatory behaviour and a decrease in the temperature (or increase in F) intensifies the oscillation. When ν is an integer, $E(L = 0)$ has the maximal absolute values, reflecting the fact that the screening effect is weakened. ν equal to an integer implies that the Fermi energy E_F is between two Landau levels and a few electrons are redistributed to shield the Coulomb potential.

The binding energies of the states $L = 0$ (full curve), $L = -1$ (dotted curve) and $L = -2$ (broken curve) are plotted as functions of ν in figure 2 with $F = 20$. It can be seen from figure 2 that the binding energy of the state $L = -2$ can be a positive quantity only when the filling factor ν is in a certain region. The state $L = -2$ is a bound state within this region and an unbound state outside it. The width of the region depends on F. The chain curve in figure 2 describes the binding energy of the state $L = -2$ with $F = 40$. It is clear that the width of the region increases as F increases. Therefore, there must be a range in the ν–F plane when $|L = -2\rangle$ is a bound state. This range is plotted in figure 3. We have evaluated the binding energy of state $L = -3$ up to $F = 50$ and did not find that the state $L = -3$ is a bound state.

We also calculated the infrared absorption spectrum of the D^- centre. The absorption spectrum for the $L = 0$ symmetric state consists of a single line at the energy [2]

$$\Delta_S(L = 0) = \hbar\omega_c - E_1(0) + E_0(1). \tag{21}$$

The numerical results are presented in figure 4. It can be seen that the transition frequency increases as the filling factor increases from 0.5. On the other hand, it is reasonable to expect that the transition frequency will decrease when the filling factor increases from 1 to 1.5.

In summary, we have investigated the many-electron effects on the energy spectrum of a 2D D^- centre in a strong magnetic field. It was found that the energy levels of the 2D D^- centre oscillate with the filling factor ν. A decrease in the temperature intensifies the oscillation. For ν equal to an integer, the screening effects can be weakened greatly. We also found that the state $|L = -2\rangle$ can exist as a bound state in a certain region centring on ν equal to an integer only when F is large enough.

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