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Energy spectrum of a two-dimensional screened donor in a constant magnetic field of arbitrary strength

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Abstract

We compute the energy levels of a two-dimensional screened hydrogenic donor when a constant magnetic field is applied. In order to describe the screening of the Coulomb field we introduce a Yukawa potential. With the help of a mixed-basis variational method, as well as the shifted $1/N$ method, we calculate the binding energies of the $1S$, $2P^-$ and $3D^-$ ground states and we show how they depend on the screening strength. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

There has been a considerable amount of work in recent years devoted to the study of semiconductor confined structures because of their applicability in electronics and optoelectronics devices. Recent developments in nanostructure technology has permitted one to study the behavior of electrons and impurities in quasi two-dimensional configurations (quantum wells) [1–6].

A very interesting problem in quantum low-dimensional structures is to understand how an atom, i.e. an impurity, modifies the energy spectrum of the system. Quantum wells present confinement in one space dimension, the growth direction, and the inclusion of strong magnetic fields can form quantum dots. The most representative example of this configuration are the regions of GaAs which act as well of the conduction electrons, separated by regions of $Ga_{1-x}Al_xAs$ which act as barriers. The application of a magnetic field perpendicular to confinement plane is expected to provide further band-structure data and binding energy information.

The potential interaction due to hydrogenic impurities can be modified by the presence of induced charges surrounding the donor. One can

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consider the impurity as a hydrogenic atom in a plasma. The Coulomb potential Z/r is screened by the electrons and this effect should be considered when one considers the effective electrostatic potential. Taking into account that, for a stationary donor, the effective potential can be computed with the help of the expression [7,8]

$$V(\vec{r}) = \frac{Z}{(2\pi)^3} \int d^3q \frac{4\pi}{q^2 \varepsilon(\vec{q})} e^{i\vec{q}\cdot\vec{r}} \quad (1)$$

and that in the Thomas–Fermi approximation, the dielectric constant is

$$\varepsilon = 1 + \frac{k_s^2}{q^2}, \quad k_s^2 = \frac{3k_F}{\pi a_0}, \quad (2)$$

where $a_0 = \hbar^2 \varepsilon / m^* e^2$ is the Bohr radius. The screened potential takes the form

$$V(\vec{r}) = \frac{Z}{(2\pi)^3} \int d^3q \frac{4\pi}{q^2 + k_s^2} e^{i\vec{q}\cdot\vec{r}} = \frac{Z}{r} e^{-k_s r} \quad (3)$$

with

$$k_s = \left(\frac{16}{3\pi^2} \right)^{1/3} \left(\frac{r_s}{a_0} \right)^{1/2} k_F = \frac{2.95}{(r_s/a_0)^{1/2}} \text{Å}^{-1} \quad (4)$$

corresponding to a screening length $l_s = 1/k_s$. Taking into account that for most of cases the ratio r_s/a_0 is between 2 and 6, we have that $1.2 \leq k_s \leq 2.1$. In this article we adopt the atomic units $\hbar = M = e = 1$, in the CGS system.

The size of the screening length can also depend on the absolute temperature T . In fact, in plasma theory, the screening length is called the Debye screening length and is given by [9,10].

$$l_s = \left(\frac{4\pi}{\kappa T} \sum_j \rho_j e^2 Z_j^2 \right)^{-1/2}, \quad (5)$$

where T is the temperature of the plasma, ρ_j is the density of particles of type j , and eZ_j is the charge. According to Eq. (5), the screening length will decrease as the density of free electrons increases or the absolute temperature T of the system decreases, therefore screening effects become important for many electron configurations.

The ground bound state of Coulomb impurity screened by free carriers in a quantum well, in the absence of magnetic fields, was calculated in Refs.

[11,12]. Here the authors also discussed the influence of the temperature on the binding energy.

The influence of the magnetic field strength B on the density-of-states (DOS) and, consequently, on the screening k_s is a complicate many-body problem. At zero temperature the screening constant is proportional to the DOS evaluated at the Fermi level [7]. For two-dimensional systems the DOS behaves as a series of steps

$$\frac{dN}{dE} \propto \frac{d}{dE} \sum_{\varepsilon_i < E} (E - \varepsilon_i), \quad (6)$$

where ε_i are the energy levels of the system. For weak magnetic fields we can simply add to ε_i the first term in the perturbation series which will be proportional to the cyclotronic frequency ω_c , shifting slightly the positions of the steps in the DOS, but the shape remains the same. The case of strong magnetic field was discussed in Ref. [13], where a self-consistent solution is given to this non-trivial problem, showing that for strong magnetic fields there are qualitative changes in the shape of the DOS. In the present article we assume that k_s is the same for all values of B , but given the value of k_s , all the eigenvalues can be readily obtained using the described techniques.

In order to discuss the influence of the screening potential on the energy spectrum of a two-dimensional hydrogenic donor we solve the two-dimensional Schrödinger equation in the presence of a Yukawa potential $e^{-k_s r}/r$. For this purpose, we have at our disposal different analytic and numerical techniques that have been successfully applied for computing the energy levels of hydrogenic donors in magnetic fields [14–16].

It is the purpose of the present article is to compute the energy levels of a two-dimensional hydrogenic donor in an electrostatic Yukawa potential and a magnetic field of arbitrary strength. In order to calculate the binding energies we apply the shifted $1/N$ method [17–19], and mixed variational method [14–16]. The results are compared with those obtained using the numeric Schwartz [20] interpolation technique.

2. Method

The non-relativistic Hamiltonian for a hydrogenic impurity or a hydrogenic atom with a Yukawa binding potential when a constant magnetic field B is applied perpendicular to the x - y plane can be written as

$$H = \frac{1}{2m^*} \left(-i\hbar\nabla - \frac{e\mathbf{A}}{c} \right)^2 - \frac{e^2}{\varepsilon\rho} \exp(-k_s\rho), \quad (7)$$

where ε is the dielectric constant of the medium, m^* is the electron effective mass. We select the vector potential \mathbf{A} in the symmetric gauge

$$\mathbf{A} = \frac{B}{2}(-y, x, 0) = \frac{Br}{2}\hat{\phi} \quad (8)$$

with a uniform magnetic field $\mathbf{B} = B\hat{k}$. If the effective Rydberg constant $\mathcal{R}_0^* = m^*e^4/2\hbar^2\varepsilon^2$ is the energy unit and effective Bohr radius $a_0 = \varepsilon\hbar^2/m^*e^2$ is the length unit, expression (7) becomes

$$H = -\nabla^2 + \gamma L_z - \frac{2e^{-k_s\rho}}{\rho} + \frac{\gamma^2\rho^2}{4}. \quad (9)$$

The coupling constant γ , which measures the ratio between the magnetic energy and Coulomb energy, is defined as $\gamma = \varepsilon^2\hbar^3 B/(ce^3 m^{*2})$ where m^* is the effective mass, ε the dielectric constant of the host material, ∇^2 is the two-dimensional Laplacian, and L_z is the angular momentum operator $-i\hbar\partial/\partial\phi$ with eigenvalue $\hbar m$. The units of energy are given in terms of the effective Rydberg constant.

The substitution

$$\Psi(\mathbf{r}) = e^{im\phi}\Psi(\rho) \quad (10)$$

reduces the Schrödinger equation $H\Psi = E\Psi$ to the following second-order ordinary differential equation

$$\left[-\frac{d^2}{d\rho^2} - \frac{1}{\rho} \frac{d}{d\rho} + \frac{m^2}{\rho^2} + \frac{\gamma^2\rho^2}{4} - \frac{2e^{-k_s\rho}}{\rho} + m\gamma - E \right] \times \Psi(\rho) = 0. \quad (11)$$

Exact solutions of Eq. (11) cannot be expressed in closed form in terms of special functions. In the present article, we tackle the problem of computing the energy spectrum using a two-terms mixed-basis variational approach. We compare our results with those obtained using the numeric

Schwartz [20] interpolation technique, as well as the shifted $1/N$ method, showing that the variational results fit very well to those computed numerically for any range of values of the magnetic strength B .

In order to apply the variational method to our problem [21], we look for a trial wave function. Since Eq. (11) reduces to the hydrogen atom equation when $\gamma = 0$, and $k_s = 0$, we can consider as a basis for $\gamma \ll 1$ the hydrogen wave functions Ψ_H . Since $\langle \Psi_H | H | \Psi_H \rangle > E$, we obtain an upper bound of the energy for small values of the parameter γ . The solution of Eq. (11) when $\gamma = 0$ is

$$\Psi_H(\rho) = D_{m,n} e^{-\rho/(1/2+n_\rho+|m|)} \rho^{|m|} L\left(n_\rho, 2|m|, \frac{2\rho}{(1/2+n_\rho+|m|)}\right), \quad (12)$$

where $D_{m,n}$ is a normalization constant, and $L(a, b, x)$ are the Laguerre polynomials [22]. Consequently the energy spectrum in the zero-field limit takes the form,

$$E_H = -\frac{1}{(1/2+n_\rho+|m|)^2}. \quad (13)$$

Conversely, for large values of γ and distances $\rho > l_s$, a good trial basis is that of the spherical oscillator. In this case the solution of Eq. (11) has the form

$$\Psi_{\text{Osc}}(r) = C_{m,n} e^{-\gamma\rho^2/4} \rho^{|m|} L\left(n_\rho, |m|, \frac{\gamma}{2}\rho^2\right) \quad (14)$$

and in the high-field limit, the energy levels are

$$E_{\text{Osc}} = \gamma(2n_\rho + |m| + m + 1). \quad (15)$$

If we attempt to apply the variational method using the hydrogen atom basis, we will obtain good agreement with the accurate results for small values of γ , but this approach fails for large γ even if we consider a many term basis. An analogous situation occurs when we use the oscillator basis, in which case we obtain a good agreement for large γ but the convergence is very slow for small values of γ [14]. In order to solve this problem, we propose a mixed-basis approach. The idea is to use as trial function, for any quantum level n , a linear

combination of the form

$$\Psi_n = \sum_i^N c_{iH} \Psi_{iH} + c_{N+iO} \Psi_{iOsc}, \quad (16)$$

where $N \geq i \geq n$; Ψ_{iH} and Ψ_{iOsc} are the corresponding hydrogen and oscillator wave functions associated with the quantum level i ; c_{iO} and c_{iH} are constants to be calculated. It is worth noticing that our mixed basis is not orthogonal under the inner product $\int_0^\infty \Psi_i \Psi_j \rho \, d\rho$. We proceed to minimize the expectation value $\langle \Psi | H | \Psi \rangle$ with the normalization condition, $\langle \Psi | \Psi \rangle = 1$.

Applying the variational approach to the basis coefficients c_i , we reduce our problem to that of solving the matrix equation

$$[\langle \Psi_i | H | \Psi_j \rangle - \lambda \langle \Psi_i | \Psi_j \rangle] c_j = 0, \quad (17)$$

where the lowest value of λ will be the energy of the level. When $j \leq 3$ we can analytically compute the eigenvalues λ and eigenvectors c_j . The advantage of this approach is twofold. First, the eigenvalues satisfy the inequality $\lambda > E$ and therefore we have a lower bound for our energy levels. Second, we obtain a relatively simple expression for the normalized eigenfunctions. This approach can be extended to many term bases but, in this case, the resulting eigenvalue equation has to be solved numerically.

In this paper, we choose to work with a two term trial variational function of the form $\Psi = c_H \Psi_H + c_O \Psi_O$, and with a three term mixed-variational basis, in this case we can solve the resulting third-order algebraic equation (17) with the help of the Cardano method.

The shifted $1/N$ expansion has become a very useful tool for computing the energy spectrum of radial potentials. Using the general prescription presented by Imbo [17,18] and particularized to the 2D hydrogen atom by Mustafa [19] we also compute the energy levels with the help of the shifted $1/N$ method. The underlying idea of this method is that if N is the dimensionality of the theory, then the theory can may have large N generalization which can be solved explicitly in the limit $N \rightarrow \infty$. The method allows one the compute physical observables such as the energy eigenvalues by expanding them in powers of $1/\bar{k} = 1/(k - a)$ where $k = N + 2l$ and a is a suitable shift. The

shift parameter is chosen in such a way that the first order correction to the large \bar{k} energy vanishes.

The numerical computations of the energy spectra associated with Eq. (11) are carried out with the help of the Schwartz method [20] which is a generalization of the mesh point technique for numerical approximation of functions. This method gives highly accurate results given a thoughtful choice of the reference function. For Eq. (11) we chose as the interpolation function

$$f(\rho) = \sum_m f_m \frac{u(\rho)}{(\rho - \rho_m) a_m}, \quad (18)$$

where

$$u(\rho) = \sin[\pi(\rho/h)^{1/2}]. \quad (19)$$

Here r_m is a zero of $u(\rho)$, a_m is a zero of its derivative, and h is the step of the quadratic mesh. The use of this scheme on Eq. (11) leads to an algebraic eigenvalue problem, giving as result a non-symmetric matrix to be diagonalized in order to obtain the energy values.

3. Analysis of the results

As illustration of the mixed-basis and $1/N$ methods, we present two different expansions of the $1S$, $2P^-$ and $3D^-$ quantum states of the 2D Hydrogenic Hamiltonian (9). We plot the energy against $\gamma' = \gamma/(\gamma + 1)$ as the horizontal scale.

Figs. 1, 3 and 5 compare, for different screening parameters k_s , the energy eigenvalues obtained via the mixed variational method and with the help of the $1/N$ method with those obtained numerically. It is easy to see that even for a two term mixed basis a good fitting is obtained in the weak and strong field regimes. One of the bases gives a reasonable good fitting in the intermediate region. We also have that for the $2P^-$ and $3D^-$ states the mixed-basis variational approach gives very good results.

The accuracy of the mixed variational and the shifted $1/N$ methods makes difficult, from Figs. 1, 3 and 5, to decide how technique is better suited for computing the hydrogen energy levels. Figs. 2, 4 and 6 show that the shifted $1/N$ method always

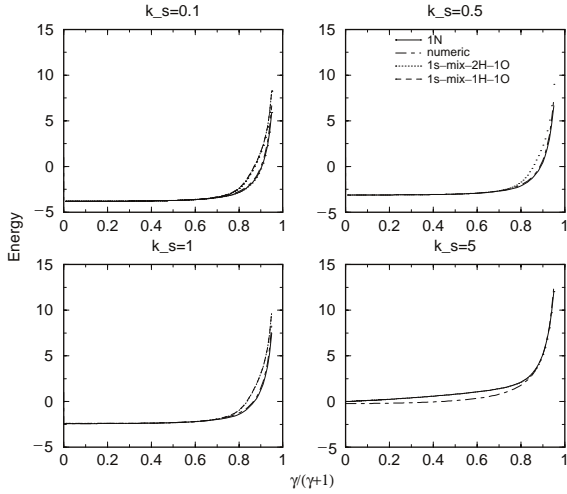


Fig. 1. Energy of the 1S state as a function of γ' . The thin solid line is obtained with the help of the shifted $1/N$ method; the dotted line is obtained using a three term mixed 1S, 2S hydrogen and 1S oscillator bases variational method. The dashed line is obtained via a two term variational method with the 1S hydrogen and oscillator bases. The dot-dashed line is obtained by numerical methods.

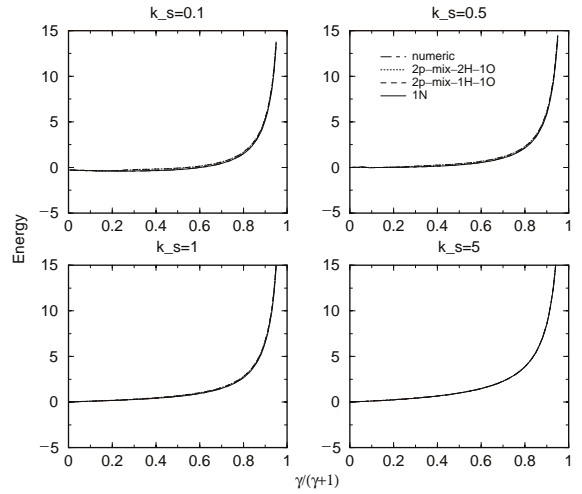


Fig. 3. Energy of the $2P^-$ state as a function of γ' . The thin solid line is obtained with the help of the shifted $1/N$ method; the dotted line is obtained using a three term mixed $2P^-$, $3P^-$ hydrogen and $2P^-$ oscillator bases variational method. The dashed line is obtained via a two term variational method with the $2P^-$ hydrogen and oscillator bases. The dot-dashed line is obtained by numerical methods.

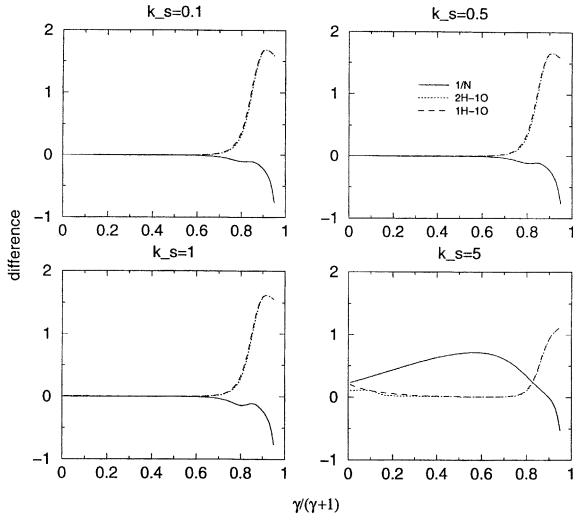


Fig. 2. The figure shows the difference between the numerical result for the 1S energy spectrum and the energy values computed with the help of the two term mixed variational (dashed line), three term variational (dotted line), and the shifted $1/N$ method (thin solid line).

gives results below the numeric energy levels. Among the analytic methods, Figs. 2, 4 and 6 show that the mixed variational method gives the

best results even for large values of γ' . We also have the three term mixed basis gives better results than the two terms basis. Nevertheless, this improvement in the approximation is accompanied by further complications in the computation of the coefficients c_H and c_O .

It can be seen that in the weak magnetic field regime the $1/N$ and variational methods work quite good but the shifted $1/N$ approach systematically underestimates the numerical result. On the other hand, the accuracy of the shifted $1/N$ methods decreases as the magnetic field strength increases.

Tables 1–3 show the energy eigenvalues obtained for different magnetic field strengths and for different values of the screening parameter k_s . It can be seen that, the Yukawa potential shifts up the energy levels as long as the screening parameter increases. The presence of the magnetic field B avoids that the energy levels for the $2P^-$ and $3D^-$ levels shift away towards the continuum. As long as the screening parameter k_s increases, the contribution of the magnetic field becomes more important and the energy eigenvalues are closer to those given by the oscillator energy expression.

From Tables 2 and 3 we can see that for strong magnetic fields and $k_s = 5$ expression (15) is a good approximation for the energy levels.

It is worth mentioning that, in opposition to the three-dimensional case, the attractive 2D Yukawa

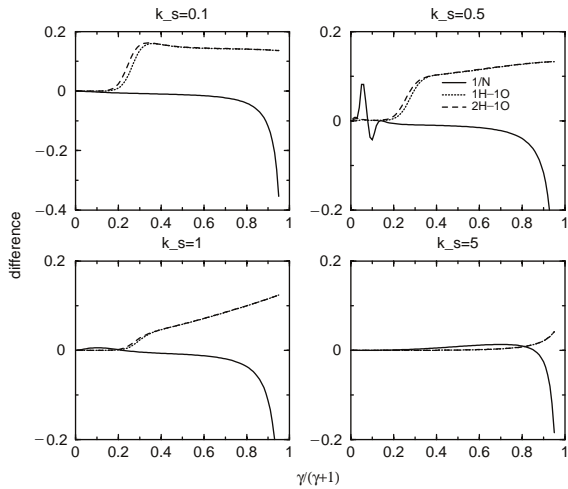


Fig. 4. The figure shows the difference between the numerical result for the $2P^-$ energy spectrum and the energy values computed with the help of the two term mixed variational (dashed line), three term variational (dotted line), and the shifted $1/N$ method (thin solid line).

potential does not possess critical k_s value for which it stops binding the electron in the S state. The behavior for P and higher states resembles

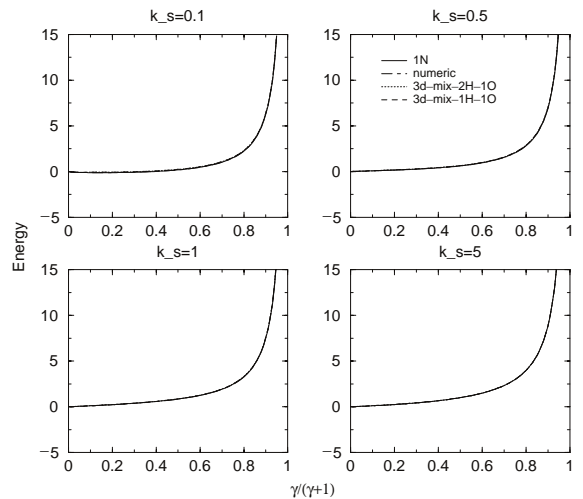


Fig. 5. Energy of the $3D^-$ state as a function of γ' . The thin solid line is obtained with the help of the shifted $1/N$ method; the dotted line is obtained using a three term mixed $3D^-, 4D^-$ hydrogen and $3D^-$ oscillator bases variational method. The dashed line is obtained via a two term variational method with the $3D^-$ hydrogen and oscillator bases. The dot-dashed line is obtained by numerical methods.

Table 1

Energy eigenvalues of the 1S state for different values of the screening parameter k_s

γ'	$k_s = 0$	$k_s = 0.1$	$k_s = 0.5$	$k_s = 1$	$k_s = 5$
0.05	-3.9997404	-3.80461995	-3.11172254	-2.40907312	-0.21942279
0.10	-3.9988434	-3.80372109	-3.11078632	-2.40803509	-0.21271210
0.15	-3.9970851	-3.80195929	-3.10895170	-2.40600232	-0.20098787
0.20	-3.9941592	-3.79902756	-3.10589999	-2.40262488	-0.18381506
0.25	-3.9896419	-3.79450105	-3.10119102	-2.39742229	-0.16052271
0.30	-3.9829381	-3.78778425	-3.09420934	-2.38972736	-0.13010736
0.35	-3.9732025	-3.77803021	-3.08408217	-2.37860122	-0.09112799
0.40	-3.9592116	-3.76401385	-3.06955100	-2.36270128	-0.04154484
0.45	-3.9391601	-3.74392757	-3.04876523	-2.34006997	0.02154095
0.50	-3.9103193	-3.71504033	-3.01893847	-2.30778452	0.10231754
0.55	-3.8684466	-3.67310570	-2.97575297	-2.26135193	0.20699611
0.60	-3.8067060	-3.61128306	-2.91227534	-2.19361038	0.34511992
0.65	-3.7135808	-3.51805027	-2.81686105	-2.09261069	0.53203989
0.70	-3.5685234	-3.37285171	-2.66878860	-1.93721108	0.79395892
0.75	-3.3319623	-3.13610462	-2.42824082	-1.68698589	1.17925336
0.80	-2.9191742	-2.72307009	-2.01012558	-1.25589955	1.78741126
0.85	-2.1180589	-1.92162136	-1.20172946	-0.42962247	2.85080963
0.90	-0.2422031	-0.04529561	0.68454941	1.48268453	5.13856651
0.95	6.4634700	6.66111196	7.40688023	8.24788125	12.56877898

Table 2

Energy eigenvalues of the $2P^-$ state for different values of the screening parameter k_s

γ'	$k_s = 0$	$k_s = 0.1$	$k_s = 0.5$	$k_s = 1$	$k_s = 5$
0.05	-0.4894827	-0.3159597	0.0021555	0.0463278	0.0525854
0.10	-0.5239504	-0.3491058	0.0014463	0.0889856	0.1109077
0.15	-0.5482152	-0.3718141	0.0065433	0.1317992	0.1759646
0.20	-0.5629132	-0.3849681	0.0178916	0.1771905	0.2490002
0.25	-0.5681960	-0.3887934	0.0361708	0.2271036	0.3315865
0.30	-0.5635941	-0.3828323	0.0624779	0.2834710	0.4257396
0.35	-0.5479613	-0.3659302	0.0984332	0.3485122	0.5340888
0.40	-0.5193465	-0.3361225	0.1463561	0.4250151	0.6601297
0.45	-0.4747349	-0.2903797	0.2095603	0.5166941	0.8086149
0.50	-0.4095808	-0.2241423	0.2928481	0.6287261	0.9861770
0.55	-0.3169840	-0.1304972	0.4033550	0.7686295	1.2023646
0.60	-0.1862031	0.0013101	0.5520556	0.9478051	1.4714512
0.65	0.0001686	0.1886992	0.7566079	1.1844251	1.8157860
0.70	0.2719562	0.4615100	1.0471344	1.5092807	2.2724809
0.75	0.6842918	0.8748928	1.4791538	1.9788312	2.9080906
0.80	1.3504374	1.5421344	2.1664872	2.7083376	3.8552547
0.85	2.5422466	2.7351274	3.3819020	3.9730244	5.4225250
0.90	5.1012487	5.2954749	5.9686985	6.6211075	8.5339259
0.95	13.4006100	13.5965322	14.3046639	15.0435465	17.8187438

Table 3

Energy eigenvalues of the $3D^-$ state for different values of the screening parameter k_s

γ'	$k_s = 0$	$k_s = 0.1$	$k_s = 0.5$	$k_s = 1$	$k_s = 5$
0.05	-0.2288102	-0.0806745	0.0462468	0.0521290	0.0526313
0.10	-0.2605089	-0.1041185	0.0865113	0.1081107	0.1111086
0.15	-0.2734835	-0.1115386	0.1265188	0.1683547	0.1764609
0.20	-0.2731927	-0.1071244	0.1695468	0.2338573	0.2499737
0.25	-0.2612880	-0.0919454	0.2178662	0.3059796	0.3332737
0.30	-0.2377636	-0.0656970	0.2735897	0.3864755	0.4284507
0.35	-0.2015205	-0.0271088	0.3390943	0.4776187	0.5382344
0.40	-0.1504340	0.0260516	0.4173552	0.5824195	0.6662604
0.45	-0.0811497	0.0972105	0.5123381	0.7049706	0.8174794
0.50	0.0113883	0.1914753	0.6295732	0.8510058	0.9988114
0.55	0.1348103	0.3165155	0.7770885	1.0288376	1.2202342
0.60	0.3009099	0.4841559	0.9670410	1.2510080	1.4966834
0.65	0.5286556	0.7133926	1.2187654	1.5373780	1.8515727
0.70	0.8503051	1.0365097	1.5649294	1.9213558	2.3238164
0.75	1.3250359	1.5127133	2.0652227	2.4637233	2.9832332
0.80	2.0734797	2.2626706	2.8409976	3.2875551	3.9689355
0.85	3.3828235	3.5736206	4.1806001	4.6841869	5.6041136
0.90	6.1341553	6.3267471	6.9673454	7.5429775	8.8536548
0.95	14.8572149	15.0520267	15.7367568	16.4157527	18.5196924

that observed in the three-dimensional problem. The critical binding values for a pure 2D Yukawa potential are $k_s = 0.4244$ and $k_s = 0.13594$ for $2P^-$ and $3D^-$ states, respectively. The

shifted $1/N$ method fails to give an accurate value for the energy eigenstates for screening values close to the critical binding value, as can be seen from Fig. 4.

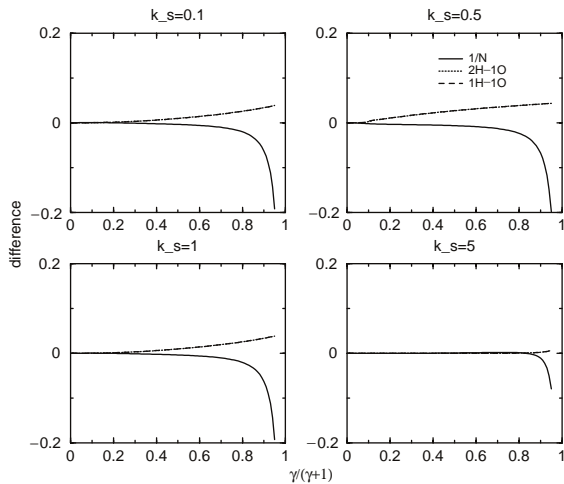


Fig. 6. The figure shows the difference between the numerical result for the $3D^-$ energy spectrum and the energy values computed with the help of the two term mixed variational (dashed line), three term variational (dotted line), and the shifted $1/N$ method (thin solid line).

The results reported in this article show that the presence of bounded states in a 2D Yukawa hydrogenic atom strongly depends on the strength of the screening parameter. The inclusion of magnetic field B permits one to recover the Landau energy levels. Figs. 1–6 show that the mixed variational approach gives the most close to numerical results even for large values of γ' .

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