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## Solution of the Schrödinger equation for two-dimensional $D^-$ centres with correlation functions

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### Abstract

The Schrödinger equation for two-dimensional  $D^-$  centres is directly solved by expanding the wavefunction in terms of hyperspherical harmonics and generalized Laguerre polynomials. An exponential correlation function is introduced to accelerate the speed of convergence. The inclusion of 144 hyperspherical harmonics and 21 generalized Laguerre polynomials yields the ground-state energy  $-2.240\,2399$  au, which is converged to an error in the sixth significant figure.

A two-dimensional  $D^-$  centre consists of a fixed positive ion and two electrons, all confined to the  $x$ - $y$  plane. Since its first experimental identification in selectively doped GaAs–GaAlAs multiple-quantum-well structures in 1990 [1], there have been many calculations of the ground-state energy [2–6]. In the presence of a strong perpendicular magnetic field or in a quantum dot, a two-dimensional  $D^-$  centre is confined by a parabolic potential in the  $x$ - $y$  plane, and the wavefunctions decay as  $\exp(-\rho^2)$ , where  $\rho$  is a size parameter. Exact eigenenergies can be obtained by diagonalizing the Hamiltonian with oscillator harmonics as basis functions [2, 6]. Without the magnetic field or the static electric field which defines a quantum dot, the system is governed by the long-range Coulomb interaction. The wavefunctions decay as  $\exp(-\rho)$ . More sophisticated methods are then required to obtain accurate eigenenergies. Already, there have been a number of variational or diffusion quantum Monte Carlo calculations of the ground-state energies based on trial wavefunctions with several variational parameters [3]. In this paper, we directly solve the problem by expanding the trial eigenfunctions in terms of the hyperspherical harmonics and generalized Laguerre polynomials. Obviously, when the wavefunction is expanded in a complete set of basis functions, it is guaranteed that the eigenfunctions and the eigenenergies converge to the correct ones. Calculations based on an incomplete set do not offer this advantage. Hence, the present work represents the first well founded solution of the problem.

The solution of the Coulomb few-body problems with hyperspherical harmonics has a long tradition [7–12]. However, it is also very well known that the direct expansion of the wavefunction in a series of hyperspherical harmonics converges very slowly [10]. This results from the fact that the particles tends to form subclusters in the system. The imitation of this feature requires many hyperspherical harmonics. In this paper, we accelerate the convergence by introducing a Jastrow-type correlation factor, and exact ground-state energies have been obtained.

For two electrons moving in the Coulomb field of a donor ion in an ideal two-dimensional quantum well, the Schrödinger equation in effective atomic units (au) is

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2) = E\Psi(\mathbf{r}_1, \mathbf{r}_2) \quad (1)$$

with

$$H = -\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 - \frac{1}{r_1} - \frac{1}{r_1} + \frac{1}{r_{12}} \quad (2)$$

where  $\mathbf{r}_i$  is the position vector of the  $i$ th particle from the donor ion in the  $x$ - $y$  plane.

To deal with the singularity of the attractive Coulomb interactions in equation (1), which is responsible for the formation of subcluster structures in the system, we write the wavefunction as a product of two parts:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi'(\mathbf{r}_1, \mathbf{r}_2)\chi \quad (3)$$

with

$$\chi = \exp[-a(r_1 + r_2)] \quad (4)$$

where  $a$  is a free parameter. The eigenequation for determining  $\Psi'$  is given by

$$H'\Psi'(\mathbf{r}_1, \mathbf{r}_2) = E\Psi'(\mathbf{r}_1, \mathbf{r}_2) \quad (5)$$

where

$$H' = -\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 + a\left(\frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_2}\right) + \frac{a}{2}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - a^2. \quad (6)$$

The introduction of hyperspherical coordinates takes advantage of the homogeneity of the Coulomb interactions. Let  $(x_i, y_i)$  be the cartesian coordinates of the  $i$ th electron; the two equivalent sets of hyperspherical coordinates that can be assigned to the system are defined as

$$\begin{aligned} (x_1, y_1) &= (R \cos \phi^\alpha \cos \varphi_1^\alpha, R \cos \phi^\alpha \sin \varphi_1^\alpha) \\ (x_2, y_2) &= (R \sin \phi^\alpha \cos \varphi_2^\alpha, R \sin \phi^\alpha \sin \varphi_2^\alpha) \end{aligned} \quad (7)$$

and

$$\begin{aligned} (x_{rel}, y_{rel}) &= (x_2 - x_1, y_2 - y_1) = (\sqrt{2}R \cos \phi^\beta \cos \varphi_1^\beta, \sqrt{2}R \cos \phi^\beta \sin \varphi_1^\beta) \\ (x_{cm}, y_{cm}) &= \left(\frac{x_2 + x_1}{2}, \frac{y_2 - y_1}{2}\right) = (\sqrt{1/2}R \sin \phi^\beta \cos \varphi_2^\beta, \sqrt{1/2}R \sin \phi^\beta \sin \varphi_2^\beta) \end{aligned} \quad (8)$$

where

$$0 \leq R < \infty \quad 0 \leq \phi^j \leq \frac{\pi}{2} \quad 0 \leq \varphi_1^j, \varphi_2^j \leq 2\pi \quad j = \alpha, \beta$$

and where  $(x_{rel}, y_{rel})$  denote the relative coordinates and  $(x_{cm}, y_{cm})$  denote the centre-of-mass coordinates of the two electrons.

With hyperspherical coordinates, the Hamiltonian  $H'$  can be rewritten as

$$H' = -\frac{1}{2}\left[\frac{\partial^2}{\partial R^2} + \frac{3}{R}\frac{\partial}{\partial R} - \frac{\Lambda^2(\Omega)}{R^2}\right] + a\left[U^{(1)}(\Omega)\frac{\partial}{\partial R} + U^{(2)}(\Omega)\frac{1}{R}\right] + U^{(3)}(\Omega)\frac{1}{R} - a^2 \quad (9)$$

where

$$U^{(1)}(\Omega) = \cos \phi^\alpha + \sin \phi^\alpha \tag{10}$$

$$U^{(2)}(\Omega) = (\cos \phi^\alpha - \sin \phi^\alpha) \frac{\partial}{\partial \phi^\alpha} + \frac{1}{2} \left( \frac{1}{\cos \phi^\alpha} + \frac{1}{\sin \phi^\alpha} \right) \tag{11}$$

$$U^{(3)}(\Omega) = -\frac{1}{\cos \phi^\alpha} - \frac{1}{\sin \phi^\alpha} + \frac{1}{\sqrt{2} \cos \phi^\beta}. \tag{12}$$

Here  $\Omega$  stands for a set of collective hyperspherical angles  $\{\phi^j, \phi_1^j, \phi_2^j\}$ .  $\Lambda^2(\Omega)$  is the grand orbital operator, the eigenfunctions of which are called a set of four-dimensional hyperspherical harmonics  $Y_{\{v l_1 l_2\}}(\Omega)$ , given by

$$Y_{\{v l_1 l_2\}}(\Omega) = \Theta_v^{l_1 l_2} P_v^{l_1 l_2}(\phi^j) e^{i l_1 \phi_1^j} e^{i l_2 \phi_2^j} \tag{13}$$

where  $\Theta_v^{l_1 l_2}$  is a normalization constant, and  $P_v^{l_1 l_2}$  is a Jacobi polynomial.

We expand the trial wavefunction  $\Psi'$  in terms of hyperspherical harmonics in the following manner:

$$\Psi'(R, \Omega) = \sum_{\{v l_1 l_2\}} F_{\{v l_1 l_2\}}(R) Y_{\{v l_1 l_2\}}(\Omega). \tag{14}$$

Then equation (5) is transformed into a set of coupled differential equations:

$$\begin{aligned} & \left\{ -\frac{1}{2} \left[ \frac{d^2}{dR^2} + \frac{3}{R} \frac{d}{dR} - \frac{\lambda(\lambda+2)}{R^2} \right] - a^2 - E \right\} F_{\{v l_1 l_2\}}(R) \\ & + \sum_{\{v' l_1' l_2'\}} \left\{ a \left[ U_{\{v l_1 l_2, \{v' l_1' l_2'\}}^{(1)} \frac{d}{dR} + U_{\{v l_1 l_2, \{v' l_1' l_2'\}}^{(2)} \frac{1}{R} \right] + U_{\{v l_1 l_2, \{v' l_1' l_2'\}}^{(3)} \frac{1}{R} \right\} F_{\{v' l_1' l_2'\}}(R) \\ & = 0 \end{aligned} \tag{15}$$

where  $\lambda = 2v + |l_1| + |l_2|$ , and

$$U_{\{v l_1 l_2, \{v' l_1' l_2'\}}^{(i)} = \int Y_{\{v l_1 l_2\}}^*(\Omega) U^{(i)}(\Omega) Y_{\{v' l_1' l_2'\}}(\Omega) d\Omega \tag{16}$$

which can be evaluated analytically [13].

In matrix notation, equation (15) can be more succinctly written as

$$\left\{ -\frac{1}{2} \left[ \frac{d^2}{dR^2} + \frac{3}{R} \frac{d}{dR} - \frac{\bar{\Gamma}}{R^2} \right] + a \left[ \bar{\mathbf{U}}^{(1)} \frac{d}{dR} + \bar{\mathbf{U}}^{(2)} \frac{1}{R} \right] + \bar{\mathbf{U}}^{(3)} \frac{1}{R} - a^2 - E \right\} \bar{\mathbf{F}}(R) = 0 \tag{17}$$

where  $\bar{\Gamma}$  is a diagonal matrix with elements  $\lambda(\lambda+2)\delta_{\{v l_1 l_2, \{v' l_1' l_2'\}}$ ,  $\bar{\mathbf{U}}^{(i)}$  is a square matrix with elements  $U_{\{v l_1 l_2, \{v' l_1' l_2'\}}^{(i)}$ ,  $\bar{\mathbf{F}}(R)$  is a one-column matrix with elements  $[F_{\{v' l_1' l_2'\}}(R)]$ .

We expand the hyperradial wavefunction  $\bar{\mathbf{F}}(R)$  according to

$$\bar{\mathbf{F}}(R) = \sum_n \bar{\mathbf{C}}_n L_n^{(2)}(\rho) \tag{18}$$

where  $\bar{\mathbf{C}}_n$  are one-column matrices of the expansion coefficients and  $\rho = 2aR$ .  $L_n^{(\gamma)}(\rho)$  are the generalized Laguerre polynomials, which form a complete set and obey the following relations:

$$\frac{d^2}{d\rho^2} L_n^{(\gamma)}(\rho) + \left( \frac{\gamma+1}{\rho} - 1 \right) \frac{d}{d\rho} L_n^{(\gamma)}(\rho) + \frac{n}{\rho} L_n^{(\gamma)}(\rho) = 0 \tag{19}$$

$$(\gamma+n)L_{n-1}^{(\gamma)}(\rho) - (\gamma+2n+1-\rho)L_n^{(\gamma)}(\rho) + (n+1)L_{n+1}^{(\gamma)}(\rho) = 0 \tag{20}$$

$$\rho \frac{d}{d\rho} L_n^{(\gamma)}(\rho) = nL_n^{(\gamma)}(\rho) - (\gamma+n)L_{n-1}^{(\gamma)}(\rho). \tag{21}$$

Substituting equation (18) into equation (17), and considering equation (19), we arrive at

$$\sum_n \left\{ (\bar{\mathbf{U}}^{(1)} - 1) \frac{d}{d\rho} + \frac{\bar{\Gamma}}{\rho^2} + \left[ n + \bar{\mathbf{U}}^{(2)} + \frac{1}{a} \bar{\mathbf{U}}^{(3)} \right] \frac{1}{\rho} - \epsilon \right\} \bar{C}_n L_n^{(2)}(\rho) = 0 \quad (22)$$

where  $\epsilon = (a^2 + E)/(2a^2)$ . With the help of equation (21), we have

$$\sum_n \left\{ \left[ n \bar{\mathbf{U}}^{(1)} + \bar{\mathbf{U}}^{(2)} + \frac{1}{a} \bar{\mathbf{U}}^{(3)} \right] \rho L_n^{(2)}(\rho) + (n+2)(1 - \bar{\mathbf{U}}^{(1)}) \rho L_{n-1}^{(2)}(\rho) + (\bar{\Gamma} - \epsilon \rho^2) L_n^{(2)}(\rho) \right\} \bar{C}_n = 0. \quad (23)$$

By repeatedly using equation (20) in equation (23), the power of  $\rho$  can be reduced to zero. Then, setting the coefficients of each  $L_n^{(2)}(\rho)$  to zero, we obtain a set of linear and homogeneous equations for determining the column-matrix coefficients  $\bar{C}_n$ :

$$\begin{aligned} & -\epsilon(n-1)n\bar{C}_{n-2} + \left\{ -n \left[ (n-1)\bar{\mathbf{U}}^{(1)} + \bar{\mathbf{U}}^{(2)} + \frac{1}{a} \bar{\mathbf{U}}^{(3)} \right] + 4\epsilon n(n+1) \right\} \bar{C}_{n-1} \\ & + \left\{ (2n+3) \left[ n\bar{\mathbf{U}}^{(1)} + \bar{\mathbf{U}}^{(2)} + \frac{1}{a} \bar{\mathbf{U}}^{(3)} \right] \right. \\ & \left. - n(n+2)(1 - \bar{\mathbf{U}}^{(1)}) + \bar{\Gamma} - 6\epsilon(n+1)(n+2) \right\} \bar{C}_n \\ & + (n+3) \left\{ - \left[ (n+1)\bar{\mathbf{U}}^{(1)} + \bar{\mathbf{U}}^{(2)} + \frac{1}{a} \bar{\mathbf{U}}^{(3)} \right] \right. \\ & \left. + (2n+3)(1 - \bar{\mathbf{U}}^{(1)}) + 4\epsilon(n+2) \right\} \bar{C}_{n+1} \\ & - \epsilon(n+3)(n+4)\bar{C}_{n+2} = 0 \end{aligned} \quad (24)$$

the secular equation of which determines the eigenenergies.

In our numerical calculations, in view of some physical considerations, two values of  $a$ -parameter in equation (4) have been tried:

- (i) With  $a = \sqrt{|E|}$  in equation (4), the correlation factor  $\chi$  correctly represents the asymptotic behaviour of the full function  $\Psi$  as  $r_1, r_2 \rightarrow \infty$ , or the interaction term  $1/r_{12}$  tends to vanish. The calculated ground-state energies with some selected numbers of bases are presented in table 1. The numbers of generalized Laguerre polynomials used are 3, 4, 5, 6, 7, 8, while the numbers of hyperspherical harmonics used are 4, 16, 36, 64, 100, corresponding to the maximum  $\lambda$ -values 4, 12, 20, 28, 36 respectively. For comparison, also included in table 1 are the ground-state energies calculated with the same numbers of bases but with a different  $\chi$ -factor [14]:

$$\chi = \exp\{-\gamma(r_1^2 + r_2^2)^{1/2}\} \quad \gamma^2 = 2|E| \quad (25)$$

which is invariant under the transformation of coordinates (note that  $(r_1^2 + r_2^2)^{1/2} = R$  is the hyperradius in hyperspherical coordinates).

It is clear in table 1 that with  $\chi = \exp[-\sqrt{|E|}(r_1 + r_2)]$ , the ground-state energies converge faster in the expansion of hyperspherical harmonics but slightly slower in the expansion of Laguerre polynomials than with equation (25).

- (ii) With  $a = 2$  in equation (4),  $\chi$  represents the ground state of a system without the electron-electron interaction. The Coulomb terms  $(1/r_1 + 1/r_2)$  in equation (6) are completely cancelled. The calculated ground-state energies are presented in table 2, where the numbers of the generalized Laguerre polynomials used are significantly bigger than in table 1. It can be seen that the convergence in the expansion of hyperspherical harmonics

**Table 1.** Ground-state (<sup>1</sup>S<sub>1</sub>) energies of a two-dimensional D<sup>-</sup> centre. *N<sub>GLP</sub>* is the number of generalized Laguerre polynomials, *N<sub>HH</sub>* is the number of hyperspherical harmonics, and *λ<sub>m</sub>* is the corresponding maximum *λ*-value. The first line in each entry gives the results calculated with the correlation factor  $\chi = \exp[-\sqrt{|E|}(r_1 + r_2)]$ , while the second line in each entry gives the results calculated with  $\chi = \exp[-\sqrt{|E|}(r_1^2 + r_2^2)^{1/2}]$ .

<i>N<sub>HH</sub></i> ( <i>λ<sub>m</sub></i> )	<i>N<sub>GLP</sub></i>					
	3	4	5	6	7	8
4(4)	-2.1222555	-2.1214801	-2.1212673	-2.1212001	-2.1211757	-2.1211657
	-1.9906250	-1.9905223	-1.9904967	-1.9904886	-1.9904856	-1.9904843
16(12)	-2.1979780	-2.1971270	-2.1969432	-2.1968854	-2.1968645	-2.1968560
	-2.1490957	-2.1491899	-2.1491722	-2.1491661	-2.1491638	-2.1491629
36(20)	-2.2193228	-2.2183587	-2.2181942	-2.2181401	-2.2181205	-2.2181126
	-2.1920478	-2.1930192	-2.1930653	-2.1930620	-2.1930600	-2.1930591
64(28)	-2.2281474	-2.2271354	-2.2269843	-2.2269315	-2.2269126	-2.2269050
	-2.2093718	-2.2112460	-2.2114402	-2.2114511	-2.2114500	-2.2114493
100(36)	-2.2326000	-2.2315791	-2.2314386	-2.2313865	-2.2313679	-2.2313604
	-2.2179318	-2.2204752	-2.2208324	-2.2208698	-2.2208716	-2.2208711

**Table 2.** Ground-state (<sup>1</sup>S<sub>1</sub>) energies of a two-dimensional D<sup>-</sup> centre calculated with the correlation factor  $\chi = \exp[-2(r_1+r_2)]$ . The last line gives the expectation values of the total Coulomb potential *V* divided by 2.

<i>N<sub>HH</sub></i> ( <i>λ<sub>m</sub></i> )	<i>N<sub>GLP</sub></i>					
	16	17	18	19	20	21
4(4)	-2.2564182	-2.2564196	-2.2564191	-2.2564193	-2.2564192	-2.2564192
16(12)	-2.2416867	-2.2417024	-2.2416951	-2.2416985	-2.2416969	-2.2416976
36(20)	-2.2404820	-2.2404984	-2.2404907	-2.2404943	-2.2404926	-2.2404934
64(28)	-2.2402793	-2.2402956	-2.2402879	-2.2402915	-2.2402898	-2.2402906
100(36)	-2.2402365	-2.2402528	-2.2402451	-2.2402488	-2.2402470	-2.2402479
144(44)	-2.2402286	-2.2402449	-2.2402372	-2.2402408	-2.2402391	-2.2402399
<i>⟨V⟩</i> /2	-2.2402312	-2.2402451	-2.2402401	-2.2402496	-2.2402408	-2.2402409

is further improved but the convergence in the expansion of Laguerre polynomials shows significant further deterioration.

Presented in the last line of table 2 are the expectation values of the total Coulomb interaction energy in the ground state divided by 2, which should be equal to the expectation values of the full Hamiltonian with a true eigenfunction, according to the virial theorem:

$$2\langle\hat{T}\rangle = -\langle V \rangle \tag{26}$$

for a system governed by (1/*r*)-type interactions, where  $\hat{T}$  is the kinetic energy operator. However, when an approximate eigenfunction is used, the virial theorem does not hold automatically. Therefore, besides the convergence pattern, the difference between the eigenenergies obtained from solving the secular equation of equation (24) and the eigenenergies derived from the virial theorem can serve as an independent check of the accuracy of the calculated results (note that the direct evaluation of  $\langle H \rangle$  is computationally very tedious). From table 2, we see that the ground-state energies derived from the two methods are in agreement up to the fifth significant figure when 144 hyperspherical harmonics and 21 Laguerre polynomials are used.

Table 3 presents the eigenenergies of the first excited state (denoted by  $^1S_2$ ). For this state, the inclusion of 38 generalized Laguerre polynomials and 64 hyperspherical harmonics produces an eigenenergy of  $-1.997\,3418$  au, which is converged to an error in the fourth significant figure. It is interesting to notice that this value is very close to the ground-state energy of a neutral donor,  $-2.0$  au.

**Table 3.** Eigenenergies of the first excited state ( $^1S_2$ ) of a two-dimensional  $D^-$  centre calculated with the correlation factor  $\chi = \exp[-2(r_1 + r_2)]$ .

$N_{HH}(\lambda_m)$	$N_{GLP}$					
	26	30	32	34	36	38
16(12)	-1.9769251	-1.9764876	-1.9764208	-1.9763914	-1.9763791	-1.9763740
25(16)	-1.9896599	-1.9888930	-1.9886679	-1.9885271	-1.9884447	-1.9883989
36(20)	-1.9943256	-1.9943743	-1.9942480	-1.9940975	-1.9939578	-1.9938450
49(24)	-1.9950413	-1.9959417	-1.9961986	-1.9963505	-1.9964189	-1.9964273
64(28)	-1.9951115	-1.9961790	-1.9965752	-1.9968959	-1.9971491	-1.9973418

To summarize, in this paper we have shown that the inclusion of a simple correlation factor of equation (4) hastens the convergence of the hyperspherical expansion to some extent depending on the  $a$ -value chosen. With  $a = \sqrt{|E|}$ , the correlation factor correctly represents the asymptotic behaviour of the full ground-state wavefunction as  $\rho \rightarrow \infty$ , such that the convergence of the radial expansion is rapid, but fails to capture the full features of the wavefunction near the coalescence points (i.e.,  $r_i = 0$ ,  $i = 1, 2$ ); many hyperspherical harmonics are still required to obtain an accurate ground-state energy. With  $a = 2$ , the correlation factor captures the full features of the wavefunction near the coalescence points, but decays too fast as  $\rho \rightarrow \infty$ ; many Laguerre polynomials are required to compensate for this. Since the inclusion of hyperspherical harmonics associated with higher- $\lambda$  quanta makes computation more difficult, taking  $a = 2$  is computationally more favourable. It is possible that the hyperspherical and radial expansions can both be accelerated by using a more sophisticated correlation factor. But the evaluation of matrix elements must then become more complicated.

Finally we would like to point out the difficulty of generalizing the present method to a three-body system with finite masses (e.g., charged excitons). The transformed Hamiltonian  $H'$  will have some additional three-body terms which cannot be calculated analytically. The evaluation of the numerous matrix elements of the Hamiltonian then becomes computationally difficult.

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