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Abstract
We calculate accurate eigenvalues and eigenfunctions of the Schrödinger equation for a
two-dimensional quantum dipole. This model proved useful for the study of elastic effects of a
single edge dislocation. We show that the Rayleigh–Ritz variational method with a basis set of
Slater-type functions is considerably more efficient than the same approach with the basis set
of point-spectrum eigenfunctions of the two-dimensional hydrogen atom used in earlier
calculations.

(Some figures may appear in colour only in the online journal)

1. Introduction

In a recent paper, Dasbiswas *et al* [1] discussed the bound-state
spectrum for a straight edge dislocation oriented along the *z*
axis. Within the continuum model, the authors reduced the
problem to the two-dimensional Schrödinger equation for a
quantum dipole. They obtained very accurate eigenvalues and
eigenfunctions by means of a discretization of the *x*–*y* space.
Since this real-space diagonalization method (RSDM) is not
so practical for highly excited states, those authors also carried
out a Rayleigh–Ritz (RR) variational calculation with the
basis set of eigenfunctions of the two-dimensional Coulomb
problem [2].

   The variational RR eigenvalues are known to approach
the exact ones from above. However, in the present case
the ground-state energy $\epsilon_1^{\mathrm{RR}} = -0.0970$ calculated with
as many as 400 basis functions exhibits a considerable
discrepancy with respect to the same eigenvalue obtained by
RSDM $\epsilon_1^{\mathrm{RSDM}} = -1.39$. Later on, Amore [3] carried out a
more accurate calculation with 3600 hydrogen eigenfunctions
and obtained $\epsilon_1^{\mathrm{RR}} = -0.128$ as well as $\epsilon_1^{\mathrm{RRS}} = -0.132$
by fitting and extrapolating the outcome of a Shanks
transformation. The authors of both papers resorted to a
variational parameter (decaying parameter [1] or the length
scale [3]) that considerably improves the result. The remaining
disagreement between RR and RSDM is probably due to the

well-known fact that the basis set used in those calculations
is not complete because it does not include the continuous
spectrum [2] (see, for example, [4] and the references therein).
For this reason, the RR calculation proposed by those authors
[1, 3] is expected to have a limited accuracy no matter
how large the dimension of the basis set of discrete states.
It is surprising, however, that the lack of the continuous
wavefunctions appears to be more notable for the ground state.
In addition to it, at first sight it seems that there is better
agreement for the odd states [1].

   The purpose of this paper is to carry out an RR calculation
with a nonorthogonal basis set of square-integrable functions
that in principle does not require the continuous spectrum. In
section 2, we describe the RR variational method with such an
improved basis set. In section 3, we compare present results
with those obtained earlier by Dasbiswas *et al* [1] and Amore
[3]. Finally, in section 4, we summarize the main results and
draw conclusions.

2. The Rayleigh–Ritz variational method

The linearized model for the Ginzburg–Landau theory leads
to the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + p\frac{\cos\theta}{r}\psi = E\psi, \tag{1}$$

where $r = \sqrt{x^2 + y^2}$, $0 \leqslant \theta = \arctan(y/x) < 2\pi$ and p is the
strength of the dipole potential [1]. Choosing the units of length

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$\hbar^2/(2mp)$ and energy $2mp^2/\hbar^2$, we obtain the dimensionless eigenvalue equation

$$-\nabla^2\psi + \frac{\cos\theta}{r}\psi = \epsilon\psi, \tag{2}$$

where $\epsilon = \hbar^2 E/(2mp^2)$. Since the potential $V(r,\theta) = \cos\theta/r$ is invariant under reflection about the x axis $V(r,-\theta) = V(r,\theta)$, then the wavefunctions are either even $\psi(r,-\theta) = \psi(r,\theta)$ or odd $\psi(r,-\theta) = -\psi(r,\theta)$ under such coordinate transformation.

Dasbiswas *et al* [1] and Amore [3] resorted to the RR variational method with the basis set of eigenfunctions of the planar hydrogen atom:

$$\psi_{n,l}^H(r,\theta) = \frac{1}{\sqrt{\pi}}R_{n,l}(r) \times \begin{cases} \cos(l\theta), & 1 \leqslant l \leqslant n \\ \frac{1}{\sqrt{2}}, & l = 0 \\ \sin(l\theta), & -n \leqslant l \leqslant -1, \end{cases} \tag{3}$$

where $n = 1, 2, \ldots$ and $R_{n,l}(r)$ is the normalized solution to the radial equation [2]. However, this basis set is incomplete if one does not include the eigenfunctions for the continuous spectrum (see, for example, [4] and references therein).

If, on the other hand, the chosen basis set of square-integrable functions does not require the continuous spectrum to be complete, then one expects the accuracy of the RR variational results to be determined only by the basis dimension. Here we propose the nonorthogonal set of functions

$$\left\{\phi_j^e, \ j = 1, 2, \ldots\right\} = \{e^{-\alpha r}, r^{i+1}\cos^j\theta e^{-\alpha r}, \ i, j = 0, 1, \ldots\} \tag{4}$$

for the even states and

$$\left\{\phi_j^o, \ j = 1, 2, \ldots\right\} = \{r^{i+1}\sin\theta\cos^j\theta e^{-\alpha r}, \ i, j = 0, 1, \ldots\} \tag{5}$$

for the odd ones, where $\alpha > 0$ is a variational parameter. This basis set resembles the Slater orbitals commonly used in quantum chemistry calculations of atomic and molecular electronic structure [4].

The RR method with the variational ansatz

$$\psi = \sum_{j=m}^{N} c_m\phi_m \tag{6}$$

leads to the generalized eigenvalue problem

$$\mathbf{HC} = \epsilon\mathbf{SC}, \tag{7}$$

where $H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$ and $S_{ij} = \langle\phi_i|\phi_j\rangle$. Note that it is possible to obtain explicit expressions for both kinds of matrix elements in terms of the variational parameter α; even more important is the fact that, with the help of a computer algebra software package, like Mathematica, we can obtain the inverse of $\mathbf{S}$ explicitly for all the cases considered in this paper. In this way, the inversion does not introduce any round-off errors and the original generalized eigenvalue problem is converted to the ordinary eigenvalue problem

$$\mathbf{S}^{-1}\mathbf{HC} = \epsilon\mathbf{C} \tag{8}$$

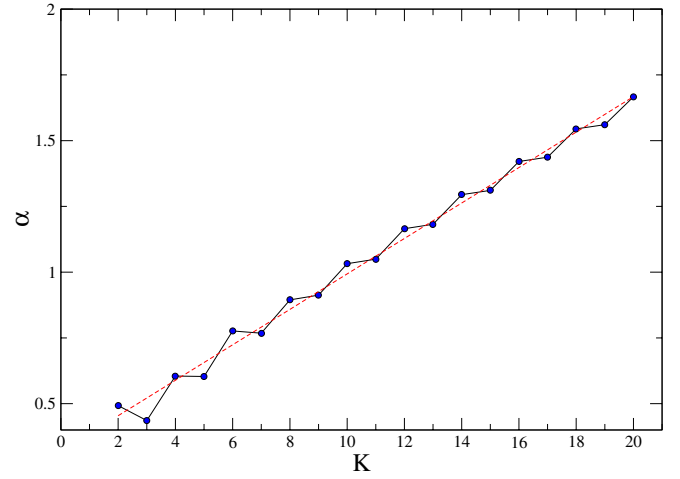for the nonsymmetric matrix $\mathbf{S}^{-1}\mathbf{H}$.

Figure 1. Optimal value of α for the ground state as a function of K.
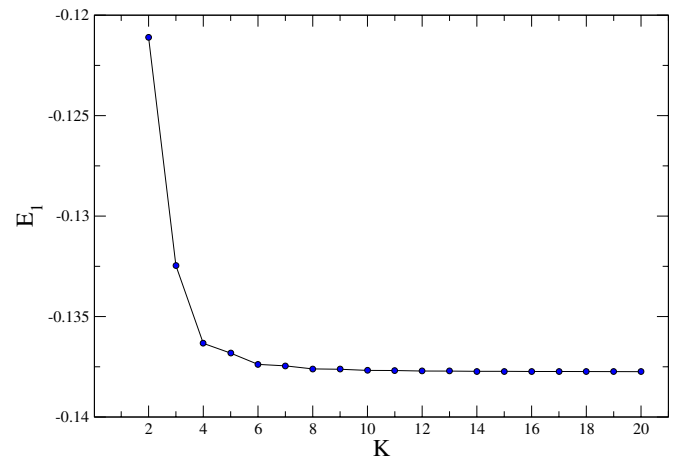

Figure 2. Convergence of ϵ_1 in terms of K for the optimal value of α.

3. Results

For brevity, we write both the exact and approximate RR eigenvalues and eigenfunctions as $\epsilon_1 < \epsilon_2 < \ldots$ and $\psi_1, \psi_2, \ldots$, respectively. We express the rate of convergence of the RR results in terms of the largest parameter $K = i+j$ in the wavefunction expansion (6), where i and j are the exponents of r and $\cos\theta$ in either equation (4) or (5). Thus, for a given value of K there are $N = (K^2 + K + 2)/2$ basis functions of either even or odd symmetry. The optimal value of the nonlinear variational parameter α depends on both the chosen eigenvalue and the number of terms N in the wavefunction expansion (6). For example, figure 1 shows that for the ground state α increases with K oscillating about a straight line. Figure 2 shows the RR eigenvalue ϵ_1 for a range of values of K. The rate of convergence is remarkably greater than the one for the Coulomb basis set [3].

Table 1 shows the RR eigenvalues obtained with the nonorthogonal basis sets (4) and (5) $\left(\epsilon_n^{NB}\right)$ on the one side and with the basis sets of even and odd Coulomb functions (3) $\left(\epsilon_n^{CB}\right)$ on the other. We appreciate the following facts: the accuracy of the present nonlinear basis set is always greater $\left(\epsilon_n^{NB} \leqslant \epsilon_n^{CB}\right)$ in spite of the fact that the RR calculations
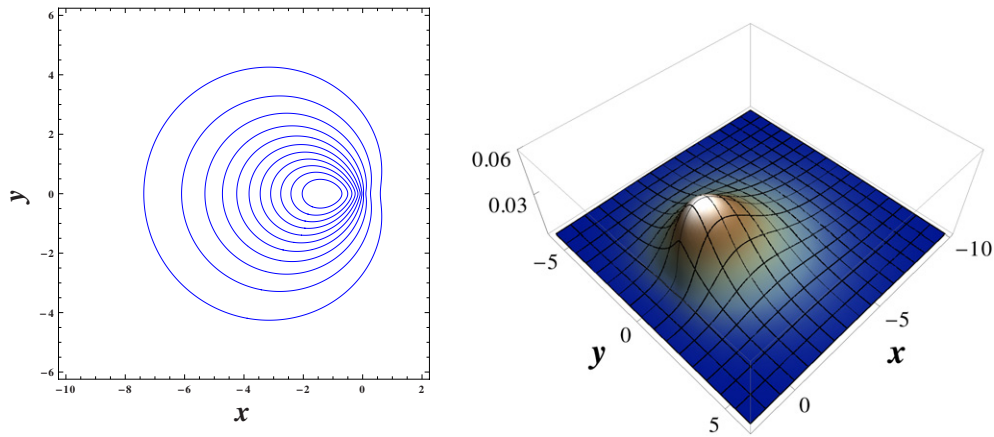
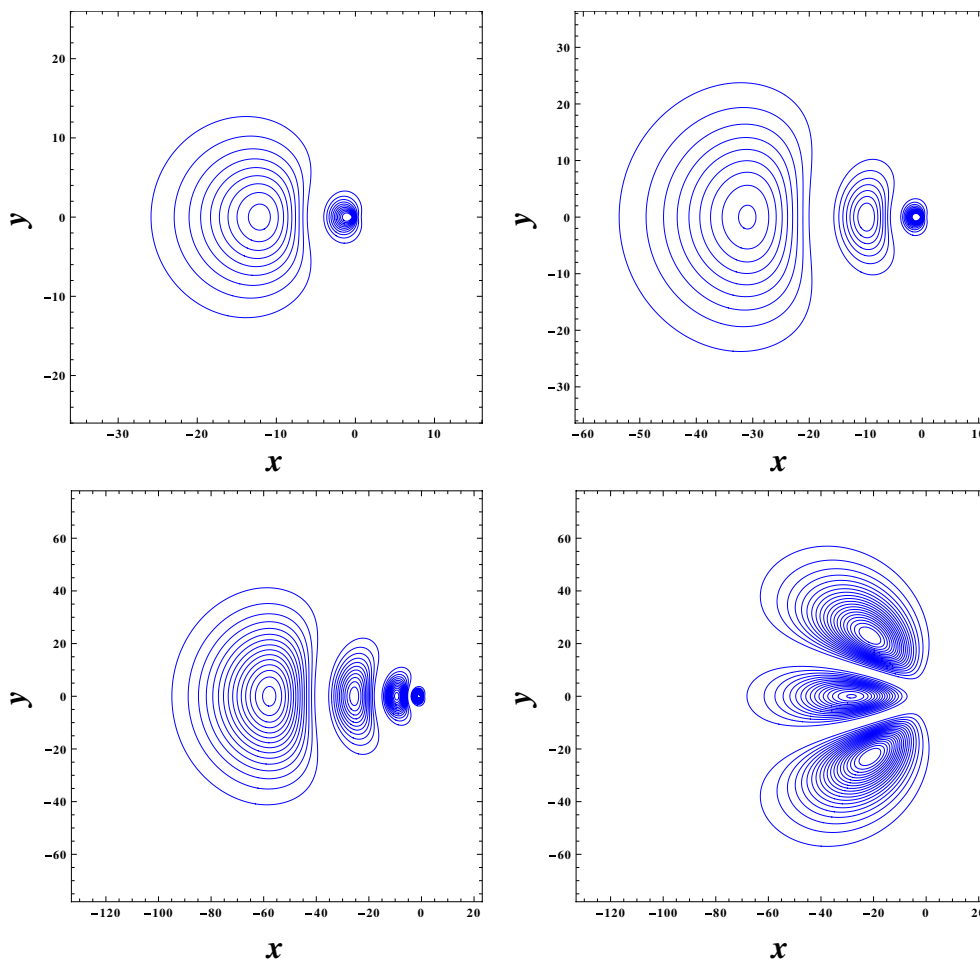**Figure 3.** Contour and 3D plot for $|\psi_1|^2$.

Figure 4. Contour plots for the squares of the second, third, fourth and fifth even states.

Table 1. Optimal α and energies for the first five even and odd states for $K = 20$.

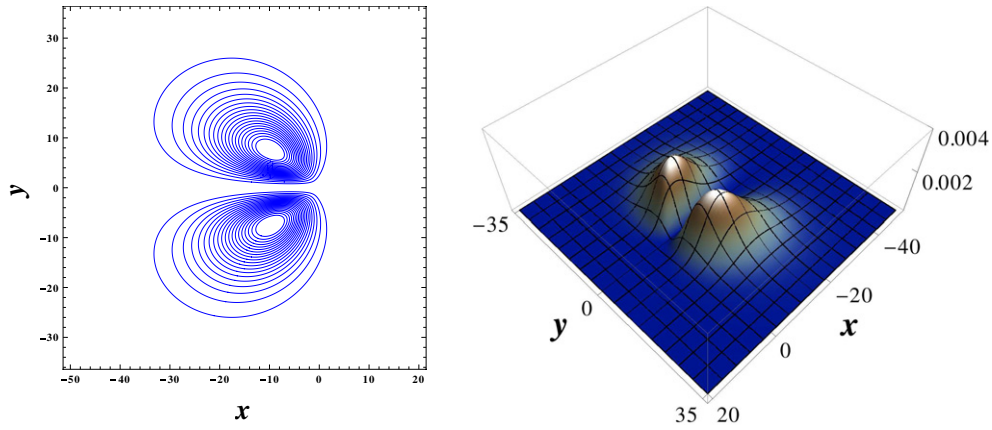| n	α	$\epsilon_n^{\text{NB even}}$	$\epsilon_n^{\text{CB even}}$	α	$\epsilon_n^{\text{NB odd}}$	$\epsilon_n^{\text{CB odd}}$
1	1.667	−0.137 7416	−0.127 9886	0.3984	−0.023 2932	−0.023 2932
2	0.7002	−0.041 1524	−0.039 4579	0.2469	−0.012 5862	−0.012 5862
3	0.4273	−0.019 9679	−0.019 3729	0.1773	−0.007 9918	−0.007 991 86
4	0.2676	−0.011 8525	−0.011 5734	0.1239	−0.005 5643	−0.005 564 35
5	0.1515	−0.009 7472	−0.009 7472	0.0997	−0.005 3312	−0.005 331 16

3

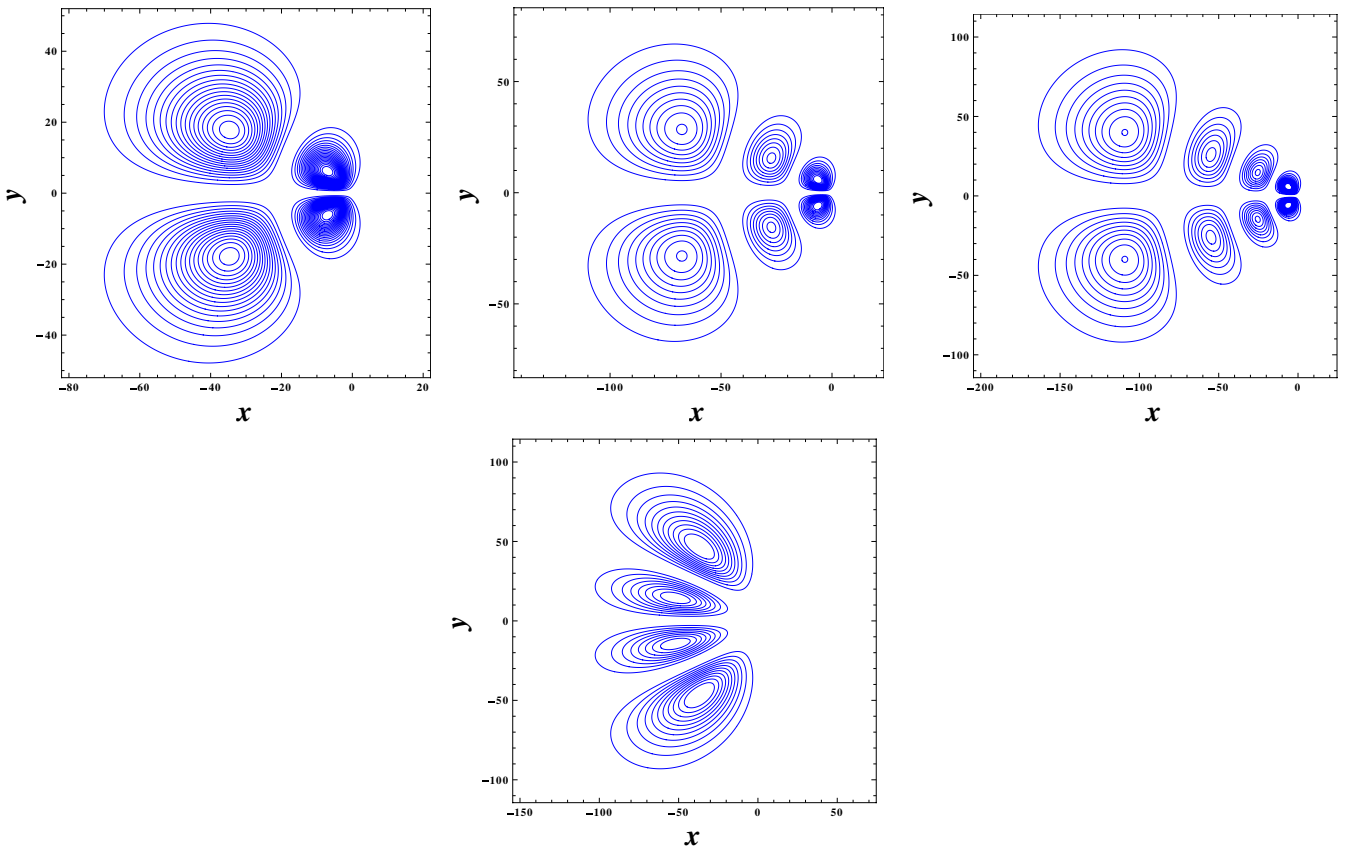**Figure 5.** Contour and 3D plot for the square of the first odd state.

Figure 6. Contour plots for the squares of the second, third, fourth and fifth odd states.

have been carried out with $N = 211$ nonorthogonal basis functions ($K = 20$) and $N = 3600$ Coulomb functions [3]. The discrepancy is greater for the lowest states and it is less notable for the odd ones. We are presently unable to provide a rigorous proof for the last two facts; however, we may conjecture that the omitted continuous spectrum is not so relevant in those cases where there is agreement between the NB and CB variational results. The number of digits in the entries of this table is dictated by comparison purposes and does not reflect the estimated accuracy of the calculation.

Both the analytical calculation of the matrix elements and the analytical inversion of the matrix **S** are time consuming, but we do them only once for all the states. On the other hand,

the optimization of the variational parameter α for each state is a time consuming calculation that we should repeat several times. Earlier and present calculations suggest that the RR variational method is less efficient for the ground state. For this reason, we have attempted variational calculations with considerably greater basis sets only for this state. For example, we have obtained $\epsilon_1^{\text{NB even}} = -0.137\,746\,772\,27$ with $N = 466$ NB functions ($K = 30$) and $\epsilon^{\text{NB even}} = -0.137\,747\,782\,05$ with the $N = 821$ ones ($K = 40$). These results suggest that the first six digits remain stable and, consequently, that the RR calculation with the Slater-type basis functions no longer appears to approach the RSDM results closely. However, it is worth noting that the present RR eigenvalues agree with

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the RSDM ones within the 2% error estimated by Dasbiswas *et al* [1].

By means of the approximate ground-state wavefunction $\psi_1(x, y)$ in terms of the Slater-like orbitals, we have also calculated the effective dimensionless coupling constant [1]

$$g = \int dx\, dy |\psi_1(x, y)|^4. \tag{9}$$

Dasbiswas *et al* [1] obtained $g = 0.017$ by means of a simple variational function constructed from the first three elements of the even nonorthogonal basis set (4): $\{e^{-\alpha r}, re^{-\alpha r}, r\cos\theta\, e^{-\alpha r}\}$ and $g = 0.0194$ by means of the RSDM. Amore [3] obtained $g = 0.017$ by means of a reduced RR basis set of Coulomb functions ($N = 345$). Note that just $N = 3$ NB functions yield the same result as the $N = 345$ Coulomb ones. The RR method with $N = 211$ functions ($K = 20$) of the basis set (4) yields $g = 0.0193$, which is quite close to the RSDM result.

Figures 3 (left panel), 4, 5 (left panel) and 6 show the contour plots for $\psi(x, y)^2$ for the first five even and odd states obtained by means of the $N = 211$ NB functions. One clearly realizes that there are two types of nodal lines $\psi(x, y)^2 = 0$ and that the energy depends differently on each of them. The right panels of figures 3 and 5 show 3D plots of the probability densities of the first even and odd states.

4. Conclusions

The present results clearly show that the basis set of Slater-type orbitals is preferable to the Coulomb basis set. With just a few functions of the former set, one obtains results that are considerably more accurate than those arising from much larger sets of the latter. As argued above, the reason is that any linear combination of discrete-spectrum Coulomb eigenfunctions is orthogonal to the continuous-spectrum eigenfunctions. On the other hand, no continuous-spectrum functions are required when using the Slater-type basis set. The contribution of the continuous spectrum appears to be more relevant for the lowest states and for the even ones. However, we have not proved that the RR variational method with the Slater-type functions converges towards the actual eigenvalues as K increases. The present variational eigenvalues converge to limits that are slightly larger than the RSDM ones and we cannot safely state that all the stable digits of our results agree with those of the exact eigenvalues. Accurate lower bounds are required for that purpose and we have not yet been able to obtain them. In spite of this fact, it is encouraging that the present RR results agree with the RSDM

ones within the reported 2% accuracy of the latter [1]. If, as argued by Dasbiswas *et al* [1], the RR variational method is more convenient than the RSDM for highly excited states, then the present contribution is relevant because there is no doubt that the basis set proposed in this paper is preferable to the Coulomb one.

Finally, we mention an alternative approach based on the Sturmian functions that are solutions to the Sturm–Liouville equation [5]

$$\left(-\frac{1}{2}\nabla^2 + \frac{1}{2}p_0^2 - \frac{np_0}{r}\right) f_a = 0, \tag{10}$$

where p_0 is a fixed parameter, n the principal quantum number and a the set of two quantum numbers that specify the state of the two-dimensional hydrogen atom. The Sturmian eigenfunctions satisfy the orthogonality condition

$$\frac{n}{p_0} \int f_a^* \frac{1}{r} f_{a'}\, d\mathbf{r} = \delta_{aa'}. \tag{11}$$

The Sturm–Liouville equation (10) can be solved in terms of polar coordinates (r, θ) or parabolic ones $\left(x = \mu\nu,\ y = \frac{1}{2}\left(\mu^2 - \nu^2\right)\right)$. The two sets of eigenfunctions $u_{n,l}(r, \theta)$ and $U_{n_1, n_2}(\mu, \nu)$ are related by a unitary transformation [6]. The complete set of Sturmian functions (in either set of coordinates) is discrete and it is therefore suitable for the calculation of the energies of the quantum dipole. It has the additional advantage of being orthogonal. However, in this paper we resorted to the Slater-type functions because the calculation of the necessary integrals is quite straightforward and the overlap matrix in the generalized eigenvalue equation can be inverted explicitly.

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