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LETTER TO THE EDITOR

The exponential cosine screened Coulomb potential in the framework of algebraic perturbation theory†

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Abstract. High accuracy approximations for the bound state energies of the exponential cosine screened Coulomb potential are obtained by means of algebraic perturbation calculations.

In a previous letter (De Meyer *et al* 1985), we have shown how the bound state energies of the screened Coulomb potential

$$V(r) = -(1/r)\,\mathrm{e}^{-\lambda r}\cos(\mu r) \tag{1}$$

are approximated by the application of a scaling variational principle. In contrast to the previous treatment by Roy and Choudhury (1985), we have been able to avoid any truncation of the series development of the potential in powers of the screening parameters λ and μ. Indeed, from a dynamical group approach to this problem we have established a scaled functional $\bar{\Omega}(E, \theta)$, where θ is a scaling parameter of which the value attributed should in principle not affect the energy eigenvalue E.

We introduce the SO(2, 1) group states $|lmn\rangle$ labelled by the orbital angular momentum l, its projection m and a positive integer n which is related to the radial quantum number n_r by $n = n_r + l + 1$. Then the matrix elements of $\bar{\Omega}(E, \theta)$ with respect to this group basis are given by(De Meyer *et al* 1985)

$$\begin{aligned}
&\langle lmn'|\bar{\Omega}(E,\theta)|lmn\rangle \\
&\quad = \langle lmn|\bar{\Omega}(E,\theta)|lmn'\rangle \\
&\quad = \frac{1}{\Gamma(1+n'-n)}\left|\frac{\Gamma(n'-l)\Gamma(n'+l+1)}{\Gamma(n-l)\Gamma(n+l+1)}\right|^{1/2}\Bigg\{\tfrac{1}{4}n(\mathrm{e}^{\theta}-2E\,\mathrm{e}^{-\theta})\delta_{n'n} \\
&\qquad + \tfrac{1}{4}(\mathrm{e}^{\theta}+2E\,\mathrm{e}^{-\theta})\delta_{n'n+1} - \mathrm{Re}\Bigg[\left(1+\frac{\lambda+\mathrm{i}\mu}{2}\mathrm{e}^{-\theta}\right)^{-n'-n}\left(\frac{\lambda+\mathrm{i}\mu}{2}\mathrm{e}^{-\theta}\right)^{n'-n} \\
&\qquad \times {}_2F_1(l+1-n, -n-l; 1+n'-n; \tfrac{1}{4}(\lambda+\mathrm{i}\mu)^2\,\mathrm{e}^{-2\theta})\Bigg]\Bigg\} \qquad (n' \geqslant n).
\end{aligned} \tag{2}$$

† *Editor's note.* Due to an error, the wrong text was printed earlier (De Meyer H, Fack V and Vanden Berghe G 1986 *J. Phys. A: Math. Gen.* **19** L231) and this reference should be ignored. The following is the correct version.

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The scaled variational method consists in minimising with respect to θ the E value obtained by setting the diagonal element $\langle lmn|\bar{\Omega}(E,\theta)|lmn\rangle$ equal to zero. The minimal E value is clearly an approximation to the bound state energy $E_{n,l}$.

Also, since the off-diagonal matrix elements of $\bar{\Omega}(E,\theta)$ can be expressed in closed form, we shall treat them here as perturbation terms and we shall perform an algebraic perturbation expansion. Let us first notice that all matrix elements (2) are linear with respect to E. Hence we introduce the shorthand notation

$$\langle lmn+i|\bar{\Omega}(E,\theta)|lmn\rangle = a_{n+i,n}+b_{n+i,n}E \qquad (i\geqslant l+1-n) \tag{3}$$

whereby for fixed n, l and m the coefficients a and b are easily obtained from (2). Since $\bar{\Omega}(E,\theta)$ leaves the l and m value invariant we develop its eigenstate $|\bar{\psi}_{l,m,n}\rangle$ in terms of the SO(2, 1) group states as follows:

$$|\bar{\psi}_{l,m,n}\rangle = \sum_{i=l+1}^{\infty} c_i|lmi\rangle \tag{4}$$

where the c coefficients remain to be determined. Substituting (4) into the eigenvalue equation $\bar{\Omega}(E_{n,l},\theta)|\bar{\psi}_{n,l,m}\rangle = 0$ we obtain

$$\sum_{j=l+1}^{\infty}\sum_{i=l+1}^{\infty}(a_{ji}+b_{ji}E_{n,l})c_i|lmj\rangle = 0. \tag{5}$$

For $j=n$ we solve the resulting secular equation with respect to $E_{n,l}$, whereas for $j\neq n$ we solve that equation with respect to c_j. This yields

$$E_{n,l} = -\frac{a_{nn}c_n+\Sigma_{i\neq n}\,a_{ni}c_i}{b_{nn}c_n+\Sigma_{i\neq n}\,b_{ni}c_i} \tag{6}$$

$$c_j = -\frac{\Sigma_{i\neq j}\,a_{ji}c_i+\Sigma_{i\neq j}\,b_{ji}c_iE_n}{a_{jj}+b_{jj}E_{n,l}} \qquad (j\neq n). \tag{7}$$

These expressions have the appropriate form to establish an iteration algorithm for the calculation of $E_{n,l}$. More precisely, denoting by $E_{n,l}^{(k)}$ and $c_j^{(k)}$ the kth order approximations to $E_{n,l}$ and c_j respectively, we prescribe the following Gauss-Seidel iteration scheme (Fernandez *et al* 1985, Fack *et al* 1986):

$$\begin{aligned}
&E_{n,l}^{(k)} = -\frac{a_{nn}+\Sigma_{i\neq n}\,a_{ni}c_i^{(k)}}{b_{nn}+\Sigma_{i\neq n}\,b_{ni}c_i^{(k)}} \qquad (k\geqslant 0)\\
&c_j^{(k)} = -\frac{\begin{array}{l}\Sigma_{i<j}\,a_{ji}c_i^{(k)}+\Sigma_{i<j}\,b_{ji}c_i^{(k)}E_{n,l}^{(k-1)}\\ +\Sigma_{i>j}\,a_{ji}c_i^{(k-1)}+\Sigma_{i>j}\,b_{ji}c_i^{(k-1)}E_{n,l}^{(k-1)}\end{array}}{a_{jj}+b_{jj}E_{n,l}^{(k-1)}} \qquad (j\neq n,\ k\geqslant 1)\\
&c_n^{(k)} = 1 \qquad (k\geqslant 1)
\end{aligned} \tag{8}$$

where the initial c values are determined by $c_i^{(0)}=\delta_{in}$.

Although the scheme (8), when it is convergent, theoretically produces the correct eigenvalue $E_{n,l}$ in the limit $k\to\infty$, we have to introduce in practice one additional constraint. From the closed form expression (2) we recognise that $b_{ij}=0$ if $|i-j|\geqslant 2$, but a similar restriction upon the a_{ij} coefficients does not hold. Hence, for calculational purposes, since it is impossible to evaluate to all orders k an infinity of $c_j^{(k)}$ coefficients, we have built in a cutoff on the a_{ij} coefficients such that the matrix of these coefficients reduces to a band matrix. Setting, in particular, $a_{ij}=b_{ij}=0$ for all $i\neq j$, we clearly

Table 1. Energy eigenvalues in atomic units for different values of the screening parameter λ of the ECSC potential, obtained from a five-band matrix (F) and a nine-band matrix (N). Under (D) are listed the corresponding eigenvalues obtained by the scaling variational method, whereas under (O) are given the values of $\exp(-\theta)$, where θ is the tilting parameter.

		$\lambda = \mu$			
(n, l)		0.01	0.02	0.03	0.04
10	D	−0.490 0010	−0.480 0078	−0.470 0260	−0.460 0609
	F	−0.490 0010	−0.480 0078	−0.470 0260	−0.460 0609
	N	−0.490 0010	−0.480 0078	−0.470 0260	−0.460 0609
	O	1.000 0623	1.000 1360	1.000 1969	1.000 2660
20	D	−0.115 0135	−0.105 1036	−0.095 3366	−0.085 7690
	F	−0.115 0135	−0.105 1036	−0.095 3366	−0.085 7690
	N	−0.115 0135	−0.105 1036	−0.095 3366	−0.085 7690
	O	2.000 3912	2.001 6340	2.004 8297	2.011 3276
21	D	−0.115 0097	−0.105 0746	−0.095 2434	−0.085 5583
	F	−0.115 0097	−0.105 0746	−0.095 2436	−0.085 5591
	N	−0.115 0097	−0.105 0746	−0.095 2436	−0.085 5591
	O	2.000 2674	2.001 1639	2.004 1965	2.008 0199
30	D	−0.045 6191	−0.036 0256	−0.027 0334	−0.018 8478
	F	−0.045 6191	−0.036 0251	−0.027 0283	−0.018 8226
	N	−0.045 6191	−0.036 0251	−0.027 0283	−0.018 8228
	O	3.002 9758	3.023 4643	3.074 4943	3.170 6808
31	D	−0.045 6110	−0.035 9677	−0.026 8553	−0.018 4580
	F	−0.045 6110	−0.035 9676	−0.026 8544	−0.018 4530
	N	−0.045 6110	−0.035 9676	−0.026 8545	−0.018 4532
	O	3.002 6059	3.020 6535	3.065 6588	3.150 0355
32	D	−0.045 5948	−0.035 8503	−0.026 4933	−0.017 6648
	F	−0.045 5948	−0.035 8507	−0.026 4969	−0.017 6819
	N	−0.045 5948	−0.035 8507	−0.026 4970	−0.017 6821
	O	3.001 8480	3.015 0901	3.211 9346	3.211 9346
40	D	−0.021 4377	−0.012 5811	−0.005 3597	
	F	−0.021 4375	−0.012 5716	−0.005 2692	
	N	−0.021 4375	−0.012 5717	−0.005 2701	
	O	4.022 3166	4.160 6630	4.576 1110	
41	D	−0.021 4245	−0.012 4915	−0.005 0887	
	F	−0.021 4244	−0.012 4856	−0.005 0321	
	N	−0.021 4244	−0.012 4857	−0.005 0327	
	O	4.020 0457	4.150 2941	4.530 7707	
42	D	−0.021 3980	−0.012 3105	−0.004 5424	
	F	−0.021 3980	−0.012 3102	−0.004 5390	
	N	−0.021 3980	−0.012 3102	−0.004 5393	
	O	4.017 7774	4.128 3230	4.443 9450	
43	D	−0.021 3578	−0.012 0347	−0.003 7143	
	F	−0.021 3578	−0.012 0382	−0.003 7480	
	N	−0.021 3578	−0.012 0382	−0.003 7481	
	O	4.012 2692	4.095 7429	4.323 9350	

Table 1. (continued)

		$\lambda = \mu$			
(n, l)		0.06	0.08	0.1	0.2
10	D	−0.440 2004	−0.420 4636	−0.400 8839	−0.306 2964
	F	−0.440 2005	−0.420 4639	−0.400 8447	−0.306 3338
	N	−0.440 2005	−0.420 4639	−0.400 8448	−0.306 3340
	O	1.000 3111	1.000 8965	1.001 7150	1.011 3295
20	D	−0.067 4217	−0.050 3922	−0.034 9677	
	F	−0.067 4209	−0.050 3858	−0.034 9401	
	N	−0.067 4210	−0.050 3862	−0.034 9410	
	O	2.036 2238	2.080 9071	2.155 3547	
21	D	−0.066 7697	−0.048 9610	−0.032 3498	
	F	−0.066 7774	−0.048 9968	−0.032 4682	
	N	−0.066 7774	−0.048 9970	−0.032 4687	
	O	2.026 5355	2.058 8019	2.112 2840	
30	D	−0.005 7194			
	F	−0.005 4575			
	N	−0.005 4615			
	O	3.679 4460			
31	D	−0.004 5278			
	F	−0.004 4743			
	N	−0.004 4748			
	O	3.570 2375			
32	D	−0.002 1307			
	F	−0.002 3151			
	N	−0.002 3137			
	O	3.388 3419			

reconvert the iteration scheme into a single step formula for $E_{n,l}$ which is in complete agreement with the scaled variational prescription (De Meyer *et al* 1985). By extending the matrix to a non-diagonal band matrix we can choose the value of the scaling parameter θ such that the rate of convergence of the iteration calculation is as high as possible. We have verified that the convergence is assured and is of nearly maximal rate if we take for θ the value obtained from the variational treatment, i.e. the value which minimises $E_{n,l}^{(0)}$ considered as a function of θ. Next, for certain typical values of the screening parameters, we have repeatedly carried out the iteration calculations based upon (10) for a five- and nine-band matrix, respectively.

In table 1 our results for some equal values of the two screening parameters are listed. Comparing them with our previous results (De Meyer *et al* 1985) we notice that for small values of $\lambda = \mu$ and for the lowest energy levels, there is almost complete agreement already. With increasing λ or by considering the higher energy levels, the newly obtained eigenvalues correct the previous ones. For the particular cases treated here, the correction takes place from the fifth decimal place onwards. Furthermore, in the extension from the five-band matrix to the nine-band matrix the first five decimals

remain unaffected. It is clear that by further extending the coefficient matrix, we can generate approximations by the algebraic perturbation technique which are even more accurate.

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