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1986 J. Phys. A: Math. Gen. 19 L231

(http://iopscience.iop.org/0305-4470/19/5/003)

J. Phys. A: Math. Gen. 19 (1986) L231-L235. Printed in Great Britain

LETTER TO THE EDITOR

Dynamical group approach to the exponential cosine screened Coulomb potential

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Received 18 November 1985

Abstract. The bound state energies of the screened Coulomb potential $-\exp(-\lambda r)\cos(\mu r)/r$ can be approximated on account of a scaling variational principle and in such a way that no expansion in the screening parameters is required.

The exponential cosine screened Coulomb (ECSC) potential $V(r)=-\exp(-\lambda r)\cos(\lambda r)/r$, frequently encountered in solid state physics, has received much attention in recent years. The bound state energies of the ECSC potential have been studied using a variety of approximate methods, both numerical (Bonch-Bruevich and Glasko 1959, Singh and Varshni 1983) and analytical (Lam and Varshni 1972, Lai 1982, Dutt *et al* 1985). A non-perturbative dynamical group approach to screened Coulomb potentials has been formulated by Gerry and Laub (1984), whereas its application to the ECSC potential has been treated very recently by Roy and Choudhury (1985). More precisely, these authors have introduced two kinds of approximations. The first consists in a truncation of the series development of the potential in powers of λ; the second is inherent in the scaling variational method and consists in neglecting off-diagonal matrix elements of the transformed Hamiltonian. In the present letter we want to insist upon the fact that the former kind of approximation can be easily avoided. Moreover, we consider the extended ECSC potential

$$V(r)=-r^{-1}\,\mathrm{e}^{-\lambda r}\cos(\mu r)\qquad(\lambda,\mu>0)\tag{1}$$

to which we associate the energy functional $\Omega(E)$, defined by

$$\Omega(E)=r(\hat{H}-E)=r(\tfrac{1}{2}p^2+V(r)-E).\tag{2}$$

The SO(2, 1) Lie algebra is realised as follows (Bednar 1973):

$$\begin{aligned}K_1&=\tfrac{1}{2}(rp^2-r)\\K_2&=\boldsymbol{r}\cdot\boldsymbol{p}-\mathrm{i}\\K_3&=\tfrac{1}{2}(rp^2+r).\end{aligned}\tag{3}$$

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Introducing the operators $K_\pm = K_1 \pm \mathrm{i}K_2$, the Hermitian representation is defined by

$$\begin{aligned} &K_3|l\,m\,n\rangle = n|l\,m\,n\rangle \\ &K_\pm|l\,m\,n\rangle = [(l+1\pm n)(\pm n - l)]^{1/2}|l\,m\,n\pm 1\rangle \\ &(K_3^2 - K_1^2 - K_2^2)|l\,m\,n\rangle = l(l+1)|l\,m\,n\rangle \end{aligned} \tag{4}$$

where $n = n_r + l + 1$, n_r is the radial quantum number and l is the orbital angular momentum.

We now re-express the functional $\Omega(E)$ in terms of the generators K_1 and K_3 whereupon we carry out a tilting transformation $\Omega(E) \to \bar{\Omega}(E, \theta) = \exp(-\mathrm{i}\theta K_2)\Omega(E)\exp(\mathrm{i}\theta K_2)$. On account of the property

$$\mathrm{e}^{-\mathrm{i}\theta K_2}(K_3 \pm K_1)\,\mathrm{e}^{\mathrm{i}\theta K_2} = \mathrm{e}^{\pm\theta}(K_3 \pm K_1) \tag{5}$$

we obtain

$$\bar{\Omega}(E, \theta) = \tfrac{1}{2}\mathrm{e}^{\theta}(K_3 + K_1) - E\,\mathrm{e}^{-\theta}(K_3 - K_1) - \mathrm{Re}\{\exp[-(\lambda + \mathrm{i}\mu)\,\mathrm{e}^{-\theta}(K_3 - K_1)]\}. \tag{6}$$

The scaling variational method consists in setting the diagonal element $\langle l\,m\,n|\bar{\Omega}(E, \theta)|l\,m\,n\rangle$ equal to zero and solving the resulting equation with respect to E which now becomes a function $E(\theta)$ of the tilting parameter θ. The minimum attained by this function provides us with an approximation of the energy level $E_{n,l}$.

The matrix elements of the functional $\bar{\Omega}(E, \theta)$ can all be calculated in analytical closed form. Indeed, the matrix elements of the first two terms in the expression (6) follow immediately from the application of the properties (4), whereas the matrix elements of the remaining term can each be expressed in terms of a Bargmann function (Bargmann 1947). One has

$$\begin{aligned} &\langle l\,m\,n'|\exp[-(\lambda + \mathrm{i}\mu)\,\mathrm{e}^{-\theta}(K_3 - K_1)]|l\,m\,n\rangle \\ &\qquad = \langle l\,m\,n|\exp[-(\lambda + \mathrm{i}\mu)\,\mathrm{e}^{-\theta}(K_3 - K_1)]|l\,m\,n'\rangle \end{aligned}$$

and

$$\begin{aligned} &\langle l\,m\,n'|\exp[-(\lambda + \mathrm{i}\mu)\,\mathrm{e}^{-\theta}(K_3 - K_1)]|l\,m\,n\rangle \\ &\qquad = \frac{1}{\Gamma(1+n'-n)}\left(\frac{\Gamma(n'-l)\Gamma(n'+l+1)}{\Gamma(n-l)\Gamma(n+l+1)}\right)^{1/2}\left(1 + \frac{\lambda + \mathrm{i}\mu}{2}\mathrm{e}^{-\theta}\right)^{-n'-n} \\ &\qquad\quad \times \left(\frac{\lambda + \mathrm{i}\mu}{2}\mathrm{e}^{-\theta}\right)^{n'-n} {}_2F_1(l+1-n, -n-l; 1+n'-n; \tfrac{1}{4}(\lambda + \mathrm{i}\mu)^2\,\mathrm{e}^{-2\theta}) \\ &\qquad\quad (n' \geqslant n) \end{aligned} \tag{7}$$

all other matrix elements being zero.

Hence, it is straightforward to obtain an approximation to the energy levels $E_{n,l}$ by minimising the energy function

$$E_{n,l}(\theta) = \tfrac{1}{2}\mathrm{e}^{2\theta} - \frac{\mathrm{e}^{\theta}}{n}\mathrm{Re}\left[\left(1 + \frac{\lambda + \mathrm{i}\mu}{2}\mathrm{e}^{-\theta}\right)^{-2n} {}_2F_1(l+1-n, -l-n, 1; \tfrac{1}{4}(\lambda + \mathrm{i}\mu)^2\,\mathrm{e}^{-2\theta})\right] \tag{8}$$

with respect to θ. In table 1 we list the results obtained by minimising $E_{n,l}(\theta)$ for $1 \leqslant n \leqslant 4$, $l = 0, 1, \ldots, n-1$ and for the ECSC potential whereby $\mu = \lambda$ assumes certain typical values. Although we present only eight significant figures, the calculations have nevertheless been carried out in double precision by means of a FORTRAN 77 program.

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.

(n, l)		$\lambda=\mu$ 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 1035	−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).

(n, l)		$\lambda=\mu$			
		0.06	0.08	0.01	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			

Our results closely resemble those of Roy and Choudhury (1985), especially when λ is very small. In fact, one can verify that on expanding the RHS of (8) in powers of $\lambda=\mu$ one recovers as the first terms the truncated series development mentioned in their paper.

Finally, it should be remarked that, since the off-diagonal matrix elements of $\bar{\Omega}(E, \theta)$ can also be expressed in closed form, we could treat them as perturbation terms and perform an algebraic perturbation expansion. Then the tilting parameter θ can be utilised to increase as much as possible the rate of convergence of that expansion. Such an iterative perturbational scheme has been established already by us (Fack *et al* 1985) for the $\lambda x^2/(1+gx^2)$ potential. We hope to report soon on a similar treatment for the ECSC potential.

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