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LETTER TO THE EDITOR

Dynamical group approach to the exponential cosine screened Coulomb potential

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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 to 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)

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

Introducing the operators $K_\pm = K_1 \pm iK_2$, the Hermitian representation is defined by

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

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

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

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

we obtain

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

The scaling variational method consists in setting the diagonal element $\langle lmn|\Omega(E, \theta)|lmn\rangle$ 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 be expressed each in terms of a Bargmann function (Bargmann 1947). One has

$$\langle lmn'| \exp[-(\lambda + i\mu)\, e^{-\theta}(K_3 - K_1)]|lmn\rangle$$
$$= \langle lmn| \exp[-(\lambda + i\mu)\, e^{-\theta}(K_3 - K_1)]|lmn'\rangle,$$

and

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

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:

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

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. Our results closely resemble the ones 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 first terms the truncated series development mentioned in their paper.

Table 1. Energy eigenvalues in atomic units for different values of the screening parameter λ of the ECSC potential

	$\lambda = \mu$				
(nl)	0.01	0.02	0.03	0.04	0.05
10	−0.490 0010	−0.480 0078	−0.470 0260	−0.460 0609	−0.450 1174
20	−0.115 0135	−0.105 1036	−0.095 3366	−0.085 7690	−0.076 4497
21	−0.115 0097	−0.105 0746	−0.095 2434	−0.085 5583	−0.076 0561
30	−0.045 6191	−0.036 0256	−0.027 0334	−0.018 8478	−0.011 6627
31	−0.045 6110	−0.035 9677	−0.026 8553	−0.018 4580	−0.010 9474
32	−0.045 5948	−0.035 8503	−0.026 4933	−0.017 6648	−0.009 4954
40	−0.021 4377	−0.012 5811	−0.005 3597	−0.001 0694	−0.000 7249
41	−0.021 4245	−0.012 4915	−0.005 0887	−0.000 4074	−0.000 0268
42	−0.021 3980	−0.012 3105	−0.004 5424		
43	−0.021 3578	−0.012 0347	−0.003 7143		

	$\lambda = \mu$			
(nl)	0.06	0.08	0.1	0.2
10	−0.440 2004	−0.420 4636	−0.400 8839	−0.306 2964
20	−0.067 4217	−0.050 3922	−0.034 9677	−0.002 3467
21	−0.066 7697	−0.048 9610	−0.032 3498	
30	−0.005 7194	−0.001 4821	−0.000 8951	
31	−0.004 5278			
32	−0.002 1307			
40	−0.000 4700			

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 algebraical 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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