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J. Phys. A: Math. Gen. 17 (1984) L313–L315. Printed in Great Britain

LETTER TO THE EDITOR

Estimates of the ground states of the Yukawa potential from the Bogoliubov inequality

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Received 8 February 1984

Abstract. Using the SO(2, 1) dynamical group formulation of the Coulomb problem, we obtain estimates on the ground state energies of the Yukawa potential by employing the Bogoliubov inequality.

In this letter we present an application of the Bogoliubov inequality

$$\langle\psi|e^{X}|\psi\rangle \geqslant \exp\langle\psi|X|\psi\rangle, \tag{1}$$

where X is an operator, to the problems of bound states of the Yukawa potential $v(r) = -(a/r)\exp(-\lambda r)$. At first glance, such an application is not obvious due to the presence of the Coulomb factor $(-a|r)$. However in the SO(2, 1) dynamical group approach, the entire eigenvalue problem must be pre-multiplied from the left by the radial variable r. The resulting expression may then be expressed entirely in terms of the generators of SO(2, 1). We may thus employ the inequality of equation (1) to obtain upper bounds on the energy eigenvalues.

To demonstrate this explicitly we proceed as follows. The eigenvalue problem for the Hamiltonian

$$H = \tfrac{1}{2}p^2 - a\, e^{-\lambda r}/r \tag{2}$$

is written as

$$\tilde{\Omega}(E)|\tilde{\psi}\rangle = r(H-E)|\tilde{\psi}\rangle = 0 \tag{3}$$

where

$$\tilde{\Omega}(E) = \tfrac{1}{2}rp^2 - rE - a\, e^{-\lambda r}. \tag{4}$$

The generators of SO(2, 1) in the case of the Coulomb problem are realised as (Barut 1971)

$$k_0 = \tfrac{1}{2}(rp^2 + r) \qquad k_1 = \tfrac{1}{2}(rp^2 - r) \qquad k_2 = \boldsymbol{r}\cdot\boldsymbol{p} - i. \tag{5a, b, c}$$

Thus we may write equation (4) as

$$\tilde{\Omega}(E) = \tfrac{1}{2}(k_0 + k_1) - E(k_0 - k_1) - a\exp[-\lambda(k_0 - k_1)]. \tag{6}$$

The basis states for the relevant unitary irreducible representations of SO(2, 1) are

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labelled $|n, l\rangle$ such that

$$\langle nl|k_0|nl\rangle = n, \qquad n = 1, 2, \ldots, \tag{7a}$$

$$\langle nl|k_1|nl\rangle = 0. \tag{7b}$$

The quantum number n is identified with the usual principal quantum number and l is the angular momentum. However the states $|nl\rangle$ are not in fact the physical states, which we label $|\widetilde{nl}\rangle$, but are related to them by the tilting transformation

$$|\widetilde{nl}\rangle = e^{i\theta k_2}|nl\rangle. \tag{8}$$

The tilting angle θ is usually fixed by the requirement that the coefficients of the non-compact generator k_1, vanish. Here we shall treat it as a variational parameter (Gerry and Silverman 1983).

To obtain E as a function of θ we write

$$\langle\widetilde{nl}|\tilde{\Omega}(E)|\widetilde{nl}\rangle = 0 \tag{9}$$

and from equations (7) and (8) and the Baker–Hausdorff–Campbell formula obtain (Gerry and Laub 1983)

$$E_{nl}(\theta) = \tfrac{1}{2}\,e^{2\theta} - (a/n)\,e^{\theta}\langle\widetilde{nl}|\exp[-\lambda(k_0 - k_1)]|\widetilde{nl}\rangle. \tag{10}$$

As a special case for $\lambda = 0$, the minimum of $E_{nl}(\theta)$ is easily found to be at $\theta = \ln(a/n)$ yielding the usual point Coulomb energies $E_n = -a^2/(2n^2)$. For $\lambda \neq 0$ we apply the inequality of equation (1) to write

$$\begin{aligned}\langle\widetilde{nl}|\exp[-\lambda(k_0 - k_1)]|\widetilde{nl}\rangle &\geqslant \exp[-\lambda\langle\widetilde{nl}|(k_0 - k_1)|\widetilde{nl}\rangle]\\ &\geqslant \exp[-\lambda\, e^{-\theta}\langle nl|(k_0 - k_1)|nl\rangle]\\ &\geqslant \exp[-\lambda\, e^{-\theta} n].\end{aligned} \tag{11}$$

Then defining

$$E'_n(\theta) = \tfrac{1}{2}\,e^{2\theta} - (a/n)\,e^{\theta}\exp(-\lambda\, e^{-\theta} n) \tag{12}$$

we have inequality

$$E'_n(\theta) \geqslant E_n(\theta) \tag{13}$$

so that $E'_n(\theta)$ apparently provides an upper bound to $E_n(\theta)$. It should be pointed out that $E_n(\theta)$ itself is not exact and must be minimised according to the variational principle.)

We now minimise $E'_n(\theta)$ of equation (12) to obtain estimates on the ground state of the Yukawa potential and compare our results with the numerical results of McEnnan *et al* (1976). We follow these authors and take $a = Z\alpha$ and λ as the Thomas–Fermi radius $1.13\alpha Z^{1/3}$. Our results are displayed in table 1. Given the crudeness of the approximation, the results are surprisingly accurate especially for $Z = 36$ and 79.

Actually it is possible to use this dynamical group formulation to obtain very accurate results. This comes about from the fact that the left-hand side of equation (10) can be evaluated completely as an analytically continued finite SO(2,1) transformation matrix element. These matrix elements can be neatly expressed in terms of the Bargmann functions (Bargmann 1947). Using the variational method the energy eigenvalues are generally more accurate than the analytic perturbation calculations of McEnnan *et al.* This calculation will be presented elsewhere (Gerry and Laub 1983).

Table 1. Estimates of the energy eigenvalues from a variational calculation based on equation (1). The numerical values quoted are from McEnnan *et al* (1976).

Z	a	e^{θ}	E'	E (numerical)	Fractional error
13	0.094 86	0.093 07	−1.450 (0)	−1.488 (0)	0.0255
36	0.262 70	0.261 36	−1.416 (1)	−1.424 (1)	0.0056
79	0.576 47	0.575 43	−7.480 (1)	−7.495 (1)	0.0020

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