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Short communication

MORSE'S RADIAL WAVE FUNCTION

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We show that the matrix elements $\langle m|\mathrm{e}^{\beta x}|n\rangle$ for the one-dimensional harmonic oscillator permit to resolve the vibrational Schrödinger equation for the Morse interaction.

Keywords: Morse potential, one-dimensional harmonic oscillator, matrix elements

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1. Introduction

In [1–3] were calculated the matrix elements

$$f(\beta) = \langle m|\mathrm{e}^{\beta x}|n\rangle = \int\limits_{-\infty}^{\infty} \psi_m^*(x)\,\mathrm{e}^{-\beta x}\,\psi_n(x)\,\mathrm{d}x \quad (1)$$

for the harmonic oscillator (HO) in one dimension, where $\beta \geq 0$ is an arbitrary parameter. Thus, it was obtained the following result for $m \geq n$:

$$f(b) = \sqrt{\frac{n!}{m!}}\left(-\frac{\beta}{\sqrt{2}}\right)^{m-n} \mathrm{e}^{-\beta/4}\,L_n^{m-n}\left(-\frac{\beta^2}{2}\right), \quad (2)$$

in terms of the associated Laguerre polynomials L_n^q.

It is interesting to observe that the 2th order differential equation defining to L_n^q (see [4] p. 781) permits to prove via (2) that $f(\beta)$ satisfies the equation

$$\frac{\mathrm{d}^2 f}{\mathrm{d}^2\beta} + \frac{1}{\beta}\frac{\mathrm{d}f}{\mathrm{d}\beta} - \frac{1}{4\beta^2}(\beta^4 + 4A\beta^2 + 4Q)f = 0\,, \quad (3)$$

where $A = m+n+1$ and $Q = (m-n)^2$; that is, (2) is a solution of (3).

In Sec. 2, $f(\beta)$ is employed to resolve the radial Schrödinger equation for the Morse potential.

2. Radial wave function for the Morse potential

Morse [5–7] proposed the potential

$$V(r) = D[\mathrm{e}^{-2ar-r_0} - 2\mathrm{e}^{-ar-r_0}] \quad (4)$$

as an approximation to vibrational motion of a diatomic molecule, where D is the dissociation energy (well depth), r_0 is the nuclear equilibrium separation, and a is a parameter associated with the well width, such that $a\sqrt{2}D/(2\pi)$gives the frequency of small classical vibrations around r_0. If we make the change of variable $u = r - r_0$ and we use natural units, then the corresponding Schrödinger equation is

$$\frac{\mathrm{d}^2}{\mathrm{d}\beta^2}\psi_\mathrm{M} + 2[E - D(\mathrm{e}^{-2au} - 2\mathrm{e}^{-au})]\psi_\mathrm{M} = 0\,, \quad (5)$$

where ψ_M/r is the Morse's radial wave function.

If now at (5) we introduce a new independent variable β given by

$$\beta = \mathrm{i}\sqrt{2K}\mathrm{e}^{-au/2}\,, \quad \mathrm{i} - \sqrt{-1}\,, \quad K = \frac{2}{a}\sqrt{2D}\,, \quad (6)$$

then (5) adopts the form

$$\frac{\mathrm{d}^2}{\mathrm{d}\beta^2}\psi_\mathrm{M} + \frac{1}{\beta}\frac{\mathrm{d}}{\mathrm{d}\beta}\psi_\mathrm{M} - \frac{1}{4\beta^2}\left(\beta^4 + 4K\beta^2 - \frac{32E}{a^2}\right)\psi_\mathrm{M} = 0\,, \quad (7)$$

with the same structure as (3)!

Therefore by formal comparison of (3) with (7) we have:

$$K = m+n+1\,,$$

$$E_n = -\frac{a^2}{8}(m-n)^2 = -\frac{a^2}{8}(K-2n-1)^2\,, \quad (8)$$

which implies that $m = n$ is not possible because in this case the value $E = 0$ is forbidden for bound

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states; then from (8) results $K > 1$ which is the condition [5] for the existence of a discrete spectrum energy. Besides, as $E_n \neq 0$ and $K > 1$, then (8) leads to $K - 2n - 1 > 0$, that is,

$$0 \leq 2n < K - 1\,, \tag{9}$$

this means [8] a finite number of bound states.

From (3) and (7) is clear that ψ_{M} is proportional to $f(\beta)$ given by (2) then:

$$\psi_{\mathrm{M}\,n}(r) = \sqrt{\frac{a\,b\,n!}{\Gamma(K-n)}\,q^b\,\mathrm{e}^{-q}}\,L_n^b(q)\,, \tag{10}$$

where $q = K\,\mathrm{e}^{-a(r-r_0)}$ and $b = m - n = K - 2n - 1$, in accordance with [9] for ψ_{M}/r normalized to unity.

Thus, we see that the Schrödinger equation was easily resolved, for the vibrational Morse oscillator, using the matrix elements $\langle m|\mathrm{e}^{\beta x}|n\rangle$ for the one-dimensional HO. This is a one more sample of the multiple correspondences [7, 10, 11] between the Morse and harmonic oscillators. Our results (8) and (10) can be interpreted as a very good approximation, because the associated Laguerre polynomials calculated in $K\,\mathrm{e}^{ar_0}$ generally speaking are not zero [12].

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Santrauka

Parodoma, kad vibracinius Šrėdingerio lygties su Morse sąveika sprendinius galima išreikšti vienmačio harmoninio osciliatoriaus matriciniais elementais.