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Matrix Elements for the One–Dimensional Harmonic Oscillator and Morse's Radial Wave Function

J. LÓPEZ–BONILLA , V. GAFTOI AND G. OVANDO

Abstract: We determine in a simple form the matrix elements for the one-dimensional harmonic oscillator and the radial wave functions of the Morse potential. The approach is performed using the known expression of the associated Laguerre polynomials in terms of an integral over the Hermite polynomials.

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1. Introduction

We will use the notation and quantities of refs. [1,2,3]. In the literature [3,4] there is a direct integral relation between the associated Laguerre L_b^a and Hermite H_c Polynomials, given by $(m \geq n)$:

$$(1) \qquad L_n^{m-n}(-z) = \frac{(-1)^{m-n}}{(2z)^{\frac{m-n}{2}}\, 2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} e^{-(x+\sqrt{\frac{z}{2}})^2} H_m(x)\, H_n(x) dx$$

Now we show that this integral representation is useful in quantum mechanics to calculate in a very simple way the matrix elements

$$(2) \qquad f(\beta) \equiv \left\langle m \left| e^{-\beta x} \right| n \right\rangle = \int_{-\infty}^{\infty} \psi_m^*(x)\, e^{-\beta x} \psi_n(x)\, dx$$

for the one-dimensional harmonic oscillator (HO), $\beta \geq 0$ is an arbitrary parameter. This is accomplished in section 2, and in section 3 we show that $f(\beta)$ allows to resolve the Schrödinger radial equation for the Morse potential.

2. Determination of $f(\beta)$.

In [2,5–8] are reported special methods to evaluate integrals over HO quantum states ; this type of calculations are improved with the use of eq. (1), thus avoiding the requirement of special techniques.

We employ natural units such that $\hbar = m = w = 1$. The normalized wave functions of the HO are [7,9]:

$$\psi_n(x) = \left(2^n \sqrt{\pi}\, n!\right)^{-1/2} e^{-x^2/2} H_n(x), \quad n = 0, 1, 2, \ldots \tag{3}$$

We select $m \geq n$ without loss of generality, following the symmetry of eq. (2) in indices m and n. The substitution of (3) into (2) with the use of (1) implies immediately that:

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

which is an expression in accordance with the ones reported [2,5,6].
In ref. [2] it is shown that with eq. (4) it is a simple matter to obtain the matrix elements for the x^k, $k = 0, 1, 2, \ldots$, for $x^{-\gamma x^2}$, etc.
We now need to mention that the 2th order differential equation defining to L_q^p (see [1] page 781) can be used to prove that $f(\beta)$, as given in eq. (4), satisfies the differential equation :

$$\frac{d^2 f}{d\beta^2} + \frac{1}{\beta}\frac{df}{d\beta} - \frac{1}{4\beta^2}(\beta^4 + 4A\beta^2 + 4Q) f = 0 \tag{5}$$

where $A = m + n + 1$ and $Q = (m-n)^2$; that is, (4) is a solution of (5). It is also possible to deduce (5) using the hypervirial theorem [2, 7, 10 –12] and parametric differentiation.

3. Morse's Radial Wave Function.

Morse [3, 7, 13–20] proposed the potential :

$$V(r) = D\left[\, e^{-2a(r-r_0)} - 2e^{-a(r-r_0)} \,\right] \tag{6}$$

as an approximation to the 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 to the well width. The combination $a\sqrt{2D}/2\pi$ gives the frequency of the small classical vibrations around r_0. If we make the change of variable $u = r - r_0$ and use natural units, the corresponding Schrödinger equation is

$$\frac{d^2}{du^2}\underset{M}{\psi} + 2\left[E - D\left(e^{-2au} - 2e^{-au}\right)\right]\underset{M}{\psi} = 0 \tag{7}$$

where $\frac{1}{r}\underset{M}{\psi}$ is the Morse radial wave function. If now we introduce a new independent variable β at (7), given by :

$$\beta = i\sqrt{2K}e^{-\frac{au}{2}},\ \ i=\sqrt{-1},\ \ K=\frac{2}{a}\sqrt{2D} \tag{8}$$

and note that the constant $K > 0$ is not necessarily an integer, then we see that (7) acquires the form

$$\frac{d^2}{\beta^2}\underset{M}{\psi}+\frac{1}{\beta}\frac{d}{d\beta}\underset{M}{\psi}-\frac{1}{4\beta^2}\left(\beta^4+4K\beta^2-\frac{32E}{a^2}\right)\underset{M}{\psi}=0 \tag{9}$$

with the same structure that (5)!

Therefore, by formal comparison of (5) with (9) we have :

$$K=m+n+1,\ \ E_n=-\frac{a^2}{8}(m-n)^2=-\frac{a^2}{8}(k-2n-1)^2 \tag{10}$$

which implies that $m = n$ is not a possible choice, because it is forbidden the energy value $E = 0$ for the bounded states of the Morse's potential. From eq. (10) it results the condition $K > 1$ for the existence of a discrete spectrum energy [13]. Besides, the conditions $E_n \neq 0$ and $K > 1$ give from (10) the inequality $(k-2n-1) > 0$, that is :

$$0 \leq 2n < (k-1) \tag{11}$$

which means a finite number of bounded states [16].

From (5) and (9) it is clear that $\underset{M}{\psi}$ is proportional to the $f(\beta)$ given by (4), therefore :

$$\underset{M}{\psi_n}(r)=\left[\frac{abn!}{\Gamma(k-n)}\right]^{\frac{1}{2}} q^{b/2}\, e^{-q/2}\, L_n^b(q) \tag{12}$$

where $\underset{M}{\psi}$ is normalized to unity.

$$q=Ke^{-a(r-r_0)},\ \ b=\ m-n=\ k-2n-1$$

Thus we see that the Schrödinger equation has been easily resolved for the vibrational Morse oscillator thanks to the matrix elements $\langle\, m|e^{-\beta x}|n\,\rangle$ for the one dimensional HO. The exhibited scheme is another example of the multiple correspondences between the Morse and harmonic oscillators [3,18,21].

REFERENCES

[1] Abramowitz, M., Stegun, I.A., *Handbook of mathematical functions*, Wiley and Sons, New York (1972) Chap. 22.

[2] Berrondo, M., Palma, A., and López–Bonilla, J., Int. J. Quantum Chem, **31** (1987) 243.

[3] Childs, D.R., J. Quant. Spectros. Radiat. Transfer, **4** 1964 283
[4] Cooper, F., Khare, A., and Sukhatme, U., Phys. Rev. **251** (1995) 265.
[5] Drigo Filho, E., J. Phys. A. : Math. Gen,, **21**(1988) L1025.
[6] Glassgold, A.E., and Holliday, D., Phys, Rev., **A138** (1965) 1717.
[7] Goswami, A., *Quanturn Mechanics*, Brown Pub., USA (1992).
[8] Holstein, B.R., *Topics in advanced quanturn mechanics*, Addison-Wesley, California (1992).
[9] Huffaker, J.N., and Dwivedi, P.H., J. Math. Phys., **16** (1975) 862
[10] Infeld, L., and Hull, T.E., Rev. Mod. Phys., **23** (1951) 21.
[11] De Lange, O.L. and Raab, R. E.,*Operators methods in quanturm mechanics*, Clarendon Press-Oxford (1991).
[12] Lee, S.Y., Am. J. Phys., **53** (1985) 753.
[13] López–Bonilla, J., Navarrete, D., Núñez-Yépez, H. N., and Salas-Brito, A., Int. J.Quantum Chem., **62** (1997) 177.
[14] López–Bonilla, J., Núñez-Yépez, H. N. and Salas-Brito, A.L., J. Phyus. B: At. Mol. Opt. Phys., **28** (1995) L525.
[15] López–Bonilla, J., Morales, J., and Rosales, M.A., Int. J. *Quanturn Chem.*, **53** (1995) 3.
[16] Morales, J., and Flores-Riveros, A., J. Math. Phys., **30** (1989) 393.
[17] Morales, J. López–Bonilla, J., and Palma, A., J. Math. Phys., **28** (1987) 1032
[18] Morales, J. López–Bonilla and Peña, J.J., Mol, J., Struct. (Teochem), **330** (1995) 63.
[19] Morales, J., Peña, J.J., Gaftoi,V., and Ovando, G., Int. J. Quantum Chem ., **71** (1999) 465
[20] Morse, P. M., Phys. Rev. **34** (1929) 57.
[21] Prudnikov, A.P., Brychkov, Yu. and Marichev, O.J. Integrals and series, Vol. 2 : *Special Functions*, Gordon breach (1986)

J. LÓPEZ–BONILLA
Seceión de estudios de Posgrado e Investigacion
Escuela Superior de Ingeniería Mecánica y Eléctrica
Instituto Politécnico Nacional
Edif. Z-4, 3er Piso, Col. Lindavista, 07738 México, D.F.
E-mail address: lopezbjl@hotmai.com

V. GAFTOI AND G. OVANDO
Area de Física AMA, División de CBI
Universidad Autónoma Metropolitana-Azcapotzalco
Apdo. Postal 16–306, 02200 Mexico, D.F.
E-mail address : gaoz@correo.azc.uam.mx