MATRIX ELEMENTS FOR THE ONE-DIMENSIONAL HARMONIC OSCILLATOR

José L. López-Bonilla & G. Ovando

Abstract. The properties of the Hermite polynomials are used to obtain the matrix elements $\langle m|e^{-\gamma x}|n\rangle$ for the harmonic oscillator in one dimension in an easy way.

1. Introduction

One month before E. Schrödinger published his famous equation, the Hungarian physicist C. Lanczos [1-6] wrote an integral equation as the first non-matricial version of quantum mechanics. If we transform the integral equation into a differential one, there results the Schrödinger equation for stationary states:

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2}+V(x)\right]\Psi_n(x)=E_n\Psi_n(x). \tag{1}$$

The harmonic oscillator (HO), with potential $V(x)=\frac{M}{2}\omega^2x^2$, was one of the first cases solved on in an exact way [7]. The corresponding solution appears in any book on quantum mechanics. It is given by (we will employ natural units such that $\hbar=M=\omega=1$):

$$\Psi_n(x)=\frac{1}{\sqrt{2^n n!\sqrt{\pi}}}e^{-\frac{x^2}{2}}H_n(x),\quad -\infty<x<\infty, \tag{2.a}$$

$$E_n=n+\frac{1}{2},\quad n=0,1,2,\ldots$$

where the $H_n(x)$ stands for the Hermite polynomials [8]:

$$H_n(x)=(-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2} \tag{2.b}$$

satisfying the orthonormality property

$$\int_{-\infty}^{+\infty} e^{-x^2} H_p(x) H_q(x)\, dx = 2^p p! \sqrt{\pi} \delta_{p,q}. \qquad (2.c)$$

The goal of this paper is to use an analytical method to calculate the following matrix elements for the HO:

$$\langle m|e^{-\gamma x}|n\rangle \equiv \int_{-\infty}^{+\infty} \Psi_m(x)\, e^{-\gamma x}\, \Psi_n(x)\, dx, \quad \gamma \geq 0 \qquad (3)$$

in an alternative procedure compared to other methods presented in the literature [9-13]. In [10] it is shown how with equation (3) it is easy to obtain $\langle m|x^k|n\rangle$, $k = 0, 1, 2, \ldots$, which leads to closed formulas for $\langle m|f(x)|n\rangle$ using the Taylor series of $f(x)$.

In the next section we will determine (3) explicitly; our procedure is very simple and follows known mathematical relations involving the Hermite polynomials. We hope that this technique may be useful for those people interested in quantum mechanics.

2. Matrix elements for the HO

Because expression (3) is symmetrical in the indices m and n, we can take $m \geq n$ without loss of generality. The H_n are a basis because any function is a series expansion of them, in particular from [8] we have

$$e^{-\gamma x} = e^{\frac{\gamma^2}{4}} \sum_{r=0}^{\infty} \frac{(-\gamma)^r}{2^r r!} H_r(x) \qquad (4.a)$$

which in conjunction with (2.a) and (3) implies

$$\langle m|e^{-\gamma x}|n\rangle = (2^{n+m} \pi n! m!)^{-1/2} e^{\frac{\gamma^2}{4}} \sum_{r=0}^{\infty} \frac{(-\gamma)^r}{2^r r!} I(r, n, m), \qquad (4.b)$$

where $\quad I(r, n, m) = \int_{-\infty}^{\infty} e^{-x^2} H_r(x) H_n(x) H_m(x) dx.$

But the product of two Hermite polynomials is another polynomial admitting an expansion in terms of H_n, see [8]:

$$H_n(x)H_m(x) = 2^n n!m! \sum_{k=0}^{n} \frac{H_{2k+m-n}(x)}{2^k k!(k+m-n)!(n-k)!} \tag{4.c}$$

whose insertion into (4.b) leads to

$$\langle m|e^{-\gamma x}|n\rangle = (2^{n-m}\frac{n!m!}{\pi})^{1/2} e^{\frac{\gamma^2}{4}} \sum_{r=0}^{\infty} \frac{(-\gamma)^r}{2^r r!} J(r,n,m), \tag{5.a}$$

where

$$J(r,n,m) =$$
$$\sum_{k=0}^{n} \frac{1}{2^k k!(k+m-n)!(n-k)!} \int_{-\infty}^{\infty} e^{-x^2} H_r(x) H_{2k+m-n}(x) dx.$$

This allows us to use (2.c) to obtain

$$\langle m|e^{-\gamma x}|n\rangle = (2^{n-m}\frac{n!}{m!})^{1/2} e^{\frac{\gamma^2}{4}} (-\gamma)^{m-n} f(n,m), \tag{5.b}$$

where $$f(n,m) = \sum_{k=0}^{n} \frac{m!\gamma^{2k}}{2^k k!(k+m-n)!(n-k)!}.$$

On the other hand, the associated Laguerre polynomials $L_n^q(x)$, see [14], are defined by

$$L_n^q(x) = \sum_{k=0}^{n} \frac{(-1)^k (n+q)!}{k!(k+q)!(n-k)!} x^k, \tag{6.a}$$

Evaluating this polynomial when $q = m-n$ and $x = -\frac{\gamma^2}{2}$ gives

$$L_n^{m-n}\left(-\frac{\gamma^2}{2}\right) = \sum_{k=0}^{n} \frac{m!\gamma^{2k}}{2^k k!(k+m-n)!(n-k)!} x^k \tag{6.b}$$

and leads to an expression of (5.b) as

$$\langle m|e^{-\gamma x}|n\rangle = (2^{n-m}\frac{n!}{m!})^{1/2}\,(-\gamma)^{m-n}\,e^{\frac{\gamma^2}{4}}L_n^{m-n}\left(-\frac{\gamma^2}{2}\right), \quad (7)$$

in complete accordance with the expressions of other authors [10,12,15].

It is known from [10] that with equation (7) we are able to determine the matrix elements

$$\langle m|x^q|n\rangle \equiv \int_{-\infty}^{+\infty} \Psi_m(x)x^q\Psi_n(x)\,dx, \quad q = 0,1,2,\ldots; \quad (8.a)$$

however, if we desire to calculate (8.a) directly (for q even or odd), we would employ the following expansions (see [8])

$$x^{2p} = \frac{(2p)!}{2^{2p}}\sum_{k=0}^{p}\frac{H_{2k}(x)}{(2k)!(p-k)!} \quad (8.b)$$

and $$x^{2p+1} = \frac{(2p+1)!}{2^{2p+1}}\sum_{k=0}^{p}\frac{H_{2k+1}(x)}{(2k+1)!(p-k)!}, \quad p = 0,1,2,\ldots (8.c)$$

and then repeat the process shown in this paper. This results in the formulas for (8.a) reported in the literature, see [9-11,13].

References

[1] C. Lanczos, *On a field theoretical representation of the new quantum mechanics*, Z. Phys. **35** (1926), 812.

[2] J. Mehra, Aspects of Quantum Theory, ed. A. Salam, E. Wigner. Cambridge University Press, 1972.

[3] J. Mehra, The Physicist's Conception of Nature. Academic Press, 1974.

[4] B. K. P. Scaife, Studies in Numerical Analysis. Academic Press, 1974.

[5] B. Gellai, *Cornelius Lanczos*, Comp. Maths. Appls. **1** (1975), 260.

[6] I. Rhodes, *Reminicences of a cherished friend*, Comp. Maths. Appls. **1**(1975), 267.

[7] C. Eckart, *The solution of the problem of the simple oscillator by a combination of the Schrödinger and Lanczos theories*, Proc. Nat. Acad. Sc. **12** (1926), 473.

[8] N. N. Lebedev, Special Functions and their Applications. Dover: New York, 1965.

[9] J. Morales, A. Palma and L. Sandoval, *Hypervirial theorem and ladder operators. Recurrence relations for harmonic oscillator integrals*, Int. J. Quantum Chem. **29** (1986), 211.

[10] J. López-Bonilla, J. Morales and A. Palma, *Hypervirial theorem and parameter differentiation: closed formulation for harmonic oscillator integrals*, J. Math. Phys. **28**(1987), 1032.

[11] A. Palma, L. Sandoval and J. Morales, *Closed formulas for one and two center harmonic oscillator integrals*, Int. J. Quantum Chem. **S21**(1987), 729.

[12] V. Gaftoi, J. López-Bonilla, J. Morales and D. Navarrete, *Integral representation of the Laguerre polynomials*, Rev.Mex.Fis **36** (1990), 310

[13] O. L. de Lange and R. E. Raab, Operators Methods in Quantum Mechanics. Clarendon Press: Oxford, 1991.

[14] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. John Wiley and Sons: New York, 1972.

[15] J. López-Bonilla, D. Navarrete, H. N. Núñez-Yépez and A. L. Salas-Brito, *Oscillators in one and two dimensions and ladder operators for the Morse and the Coulomb problems*, Int. J. Quantum Chem. **62** (1997), 177.

José L. López-Bonilla
The International Institute of Integral Human Sciences
1974 de Maisonneuve West
Montréal, Québec
Canada H3H 1K5

G. Ovando
Departamento de Ciencias Básicas
Universidad Autónoma Metropolitana-Azcapotzalco
Apdo. Postal 16-306
02200 México D.F.
e-mail: gaoz@hp9000a1.uam.mx