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Matrix elements of x^k and $e^{\alpha x}x^k$ in the harmonic oscillator basis

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Abstract. General and compact formulae for matrix elements of x^k and $x^k\,e^{\alpha x}$ are derived using the second quantisation technique.

1. Introduction

The harmonic oscillator is a classical textbook example (Dirac 1958) of a problem that can be solved exactly. One may expect that all useful formulae for the matrix elements of various operators in the harmonic oscillator basis were derived half a century ago. Therefore it is surprising to find that a formula for the matrix element $\langle n|x^k|m\rangle$ was given in a general form not sooner than 1975 (Reid and Brandas 1975). The derivation was based on the properties of Hermite polynomials and requires some knowledge of the theory of special functions. Even more surprising is the fact that matrix elements of the type $\langle n|x^k\,e^{\alpha x}|m\rangle$ frequently appearing in various vibrational problems are still calculated by numerical integration (Thompson and Truhlar 1982).

It is the purpose of this note to show how the second quantisation method may be used to derive general formulae for matrix elements of the functions of x. The algebra used is very simple and only the most basic knowledge of second quantisation is required.

2. Matrix elements $\langle n|x^k|m\rangle$

The Harmonic oscillator Hamiltonian is

$$H = P^2/2m + \tfrac{1}{2}m\omega^2X^2 = \tfrac{1}{2}\hbar\omega(-\partial^2/\partial x^2 + x^2) \tag{1}$$

where $x = (m\omega/\hbar)^{1/2}X$. Introducing annihilation and creation operators

$$a = (1/\sqrt{2})(x + \partial/\partial x), \qquad a^+ = (1/\sqrt{2})(x - \partial/\partial x), \tag{2}$$

the familiar commutation relations are found:

$$[a, a^+] = 1. \tag{3}$$

The Hamiltonian takes a simple form:

$$H = \hbar\omega(a^+a + \tfrac{1}{2}). \tag{4}$$

The solution of an eigenproblem for this Hamiltonian defines a basis set $\{|n\rangle\}$

$$H|n\rangle = \hbar\omega(n+\tfrac{1}{2})|n\rangle, \qquad n=0,1,2,\ldots, \tag{5}$$

and does not require specification of the kets $|n\rangle$ or solution of the pertinent differential equations. Further, operating with a and a^+ operators on the ket $|n\rangle$ we get

$$a|n\rangle = \sqrt{n}|n-1\rangle, \qquad a^+|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{6}$$

This is all we need to calculate any matrix element of the functions of x. From the definition of the annihilation and creation operators,

$$x = (1/\sqrt{2})(a^+ + a). \tag{7}$$

To find the expression for x^k we have to expand $(a^+ + a)^k$ preserving the normal order of the operators, i.e. a^+ should be to the left of a. First let us calculate the commutator:

$$[a,(a^+ + a)^k] = (a^+ + a)^{k-1} + (a^+ + a)[a,(a^+ + a)^{k-1}] = \ldots = n(a^+ + a)^{k-1}. \tag{8}$$

Although the operators a and a^+ do not commute it is useful to introduce a symbol $(a^+ + a)^k_N$ defined as

$$(a^+ + a)^k_N = \sum_{l=0}^{k} \binom{k}{l} (a^+)^{k-l} a^l \tag{9}$$

which will be called a Newton binomial. It has a nice property:

$$a^+(a^+ + a)^k_N + (a^+ + a)^k_N a = (a^+ + a)^{k+1}_N \tag{10}$$

which may be easily proved noting that $\binom{k}{l} + \binom{k}{l-1} = \binom{k+1}{l}$. The binomial expansion $(a^+ + a)^k$ expressed through the Newton binomials has the form

$$(a^+ + a)^k = A^k_k (a^+ + a)^k_N + A^k_{k-2}(a^+ + a)^{k-2}_N + \ldots + A^k_p (a^+ + a)^p_N \tag{11}$$

where $p=0$ for k even and $p=1$ for k odd. Using mathematical induction we shall prove that this is a correct form and the coefficients A^k_n will be obtained. Using (8) and (10), assuming that (11) is valid for $k-1$, we have

$$\begin{aligned}(a^+ + a)^k &= a^+(a^+ + a)^{k-1} + (a^+ + a)^{k-1}a + (k-1)(a^+ + a)^{k-2} \\ &= A^{k-1}_{k-1}(a^+ + a)^k_N + A^{k-1}_{k-3}(a^+ + a)^k_N + \ldots (k-1)A^{k-2}_{k-2}(a^+ + a)^{k-2}_N \\ &\quad + (k-1)A^{k-2}_{k-4}(a^+ + a)^{k-4}_N + \ldots \\ &= A^{k-1}_{k-1}(a^+ + a)^k_N + (A^{k-1}_{k-3} + (k-1)A^{k-2}_{k-2})(a^+ + a)^{k-2}_N \\ &\quad + (A^{k-1}_{k-5} + (k-1)A^{k-2}_{k-4})(a^+ + a)^{k-4}_N + \ldots.\end{aligned} \tag{12}$$

Comparing the coefficients in (11) and (12) we find a recurrence relation for A^k_n:

$$A^k_n = A^{k-1}_{n-1} + (k-1)A^{k-2}_n, \qquad A^1_1 = 1, \tag{13}$$

which leads to

$$A^k_n = (k-n-1)!!\binom{k}{k-n} \tag{14}$$

where $l!! = l(l-2)(l-4)\ldots$ and $(-1)!! = 1$.

Now we can express the binomial expansion through the Newton binomials:

$$(a^+ + a)^k = \sum_{l=0}^{[k/2]} (2l-1)!!\binom{k}{2l}(a^+ + a)_N^{k-2l} \tag{15}$$

where $[k/2]$ is the integer part of $k/2$. The operators in this expansion are in the normal order so it is easy to calculate their matrix elements. The element of a single Newton binomial is

$$\begin{aligned}\langle n|(a^+ + a)_N^l|m\rangle &= \sum_{j=0}^{l}\binom{l}{j}\left(\frac{m!}{(m-j)!}\right)^{1/2}\left(\frac{(m+l-2j)!}{(m-j)!}\right)^{1/2}\langle n|m+l-2j\rangle \\ &= \begin{cases}\dbinom{l}{\frac{n-m+l}{2}}\left[(m!n!)^{1/2}\Big/\left(\dfrac{n+m-l}{2}\right)!\right], & (l+n+m)\text{ even, } l \geqslant |n-m|,\\ 0 & \text{otherwise.}\end{cases}\end{aligned} \tag{16}$$

The matrix element of x^k is now easily calculated:

$$\begin{aligned}\langle n|x^k|m\rangle &= 2^{-k/2}\sum_{i=0}^{[k/2]}(2i-1)!!\binom{k}{2i}\binom{k-2i}{\frac{1}{2}(n-m+k)-i}\frac{m!n!}{(\frac{1}{2}(n+m-k)+i)!} \\ &= 2^{-k/2}(m!n!)^{1/2}k! \\ &\quad\times\sum_i\frac{2^{-i}}{i!(\frac{1}{2}(n-m+k)-i)!(\frac{1}{2}(m-n+k)-i)!(\frac{1}{2}(n+m-k)+i)!}, \\ &\quad\max(0, \tfrac{1}{2}(k-m-n)) \leqslant i \leqslant \tfrac{1}{2}(k-|m-n|).\end{aligned} \tag{17}$$

Changing the summation index to $l = i-(k-n-m)/2$ simplifies this formula:

$$\begin{aligned}\langle n|x^k|m\rangle &= 2^{1/2(m+n)-k}k!(m!n!)^{1/2}\sum_l\frac{2^{-l}}{l!(n-l)!(m-l)!(\frac{1}{2}(k-m-n)+l)!} \\ &= 2^{\nu-k/2}\left(\frac{m!}{n!}\right)^{1/2}k!\sum_l\frac{\binom{n}{l}}{2^l(m-l)!(l-\nu)!}, \qquad \nu \leqslant l \leqslant \min(n, m) \\ &\quad \nu = \tfrac{1}{2}(n+m-k).\end{aligned} \tag{18}$$

The number of terms in this sum is of the order of $k/2$. The formula above was obtained for the first time by Reid and Brandas (1975). Their technique of using generating functions of Hermite polynomials may also be used in case of more general operators than x^k, but not so easily as the technique of second quantisation.

3. Matrix elements $\langle n|x^k e^{\alpha x}|m\rangle$

The advantages of second quantisation are evident in the calculation of matrix elements involving $e^{\alpha x}$. To get the normal product expansion of the exponent we shall use the Baker–Hausdorff formula:

$$e^{x+y} = e^{-[x,y]/2}e^x\, e^y \qquad \text{if } [x,[x,y]] = [y,[x,y]] = 0. \tag{19}$$

Thus we have

$$\langle n|x^k\,e^{\alpha x}|m\rangle = \exp(\alpha^2/4)\,\langle n|x^k \exp(\alpha a^+/\sqrt{2})\exp(\alpha a/\sqrt{2})|m\rangle$$

$$= \exp(\alpha^2/4)\sum_{i=0}\sum_{j=0}^{m}\left(\frac{\alpha}{\sqrt{2}}\right)^{i+j}\frac{(m!(m-j+i)!)^{1/2}}{i!j!(m-k)!}\langle n|x^k|m-j+i\rangle. \qquad (20)$$

Introducing a new summation index $l = m - j + i$ and noting that the matrix element $\langle n|x^k|l\rangle$ is non-zero only if $l = n-k, n-k+2, \ldots, n+k$, the final formula is obtained:

$$\langle n|x^k\,e^{\alpha x}|m\rangle = \exp(\alpha^2/4)\left(\frac{\alpha}{\sqrt{2}}\right)^{-m}\sqrt{m!}\sum_{\substack{l=n-k\\ l>0}}^{n+k}{}'\left(\sum_{j=0}^{m}\frac{(\alpha/\sqrt{2})^{2j+l}\sqrt{l!}}{j!(m-j)!(j+l-m)!}\right)\langle n|x^k|l\rangle \qquad (21)$$

where the prime over the first sum should remind one that only the values of l which have the same parity as $n+k$ should be taken, other terms giving no contributions.

The formulae (18) and (21) are easy to program and involve simple sums with a small number of terms. Their derivation illustrates the simplicity and potential of the second quantisation technique in calculations of a similar kind.

The method used here is closely related to the operator ordering technique (Heffner and Louisell 1965, Wilcox 1967, Louisell 1973).

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