Classical mnemonic approach for obtaining hydrogenic expectation values of r^P

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A recent paper by Drake and Swainson [Phys. Rev. A **42**, 1123 (1990)] presents a recursion relation that generates a set of coefficients needed to obtain general closed-form expressions for hydrogenic expectation values for r^P. By combining this recursion relation with an earlier semiclassical formulation of this calculation [J. Phys. B **14**, 1373 (1981)], it is shown that the correct expectation values can also be obtained by a simple substitution of prescribed angular momentum operators into the classical Kepler formula, which provides a transparent connection to the correspondence limit.

A recent paper by Drake and Swainson[1] presents a general method for obtaining a closed-form symbolic expression for the hydrogenic expectation value of any power of the radial coordinate r^P. This formulation was made possible by their derivation of a recursion relation which permits a crucial set of coefficients to be sequentially generated. It is interesting to note that the need for these same coefficients occurred earlier in the context of a semiclassical formulation[2] of this problem. In the formulation of Ref. 2, it was shown that the exact quantum-mechanical expression can be obtained directly from the corresponding classical formula by a simple mnemonic, provided these coefficients are known. By combining the recursion formula of Ref. 1 with the semiclassical formulation of Ref. 2, the correct quantum-mechanical expressions can now be obtained from the classical formula by a simple substitutional prescription for the angular momentum operators. This method of embedding the quantum-mechanical dependences directly into the classical formulation offers some conceptual advantages; for example, by providing a smooth transition between the predictions of quantum-mechanical and classical Hamilton-Jacobi perturbation theories.[3]

The average value for a power of the radial coordinate r for a classical planetary Kepler orbit of semimajor axis a and semiminor axis b can be written[3] as an integral over the angular coordinate ϑ

$$\langle r^s \rangle = a^s (b/a)^{2s+3} \times \int_0^\pi d\vartheta [1+(1-b^2/a^2)^{1/2}\cos\vartheta]^{-s-2}/\pi \; . \quad (1)$$

This integration can be performed in closed form[4] to obtain

$$\langle r^s \rangle = a^s (b/a)^{s+1} P_\lambda(a/b) \; . \quad (2)$$

Here P_λ is the Legendre polynomial of order $\lambda = |s+3/2| - 1/2$, where λ has been constructed so that both positive and negative powers are described by a Legendre polynomial of positive index ($\lambda = s+1$ for $s \geq -1$, $\lambda = -s-2$ for $s \leq -2$). (Notice that this is an unusual application of the Legendre polynomial with an argument greater than unity.) For a semiclassical system[2] with semimajor axis $a = n^2/Z$ and a semiminor-to-semimajor axis ratio $b/a = k/n$, this can be written as [Eq. (10) of Ref. 2]

$$\langle r^s \rangle = (n^2/Z)^s (n/k_o)^{\lambda-s-1} [(k_e/n)^\lambda P_\lambda(n/k_e)] \; . \quad (3)$$

Here the quantity k is associated with the angular momentum, and has been factored into two contributions: k_e leads to even powers; k_o leads to odd or noncontributing powers [$n^{2s}(n/k_o)^{\lambda-s-1}$ reduces to $n^{-3}k_o^{2s+3}$ for $s \leq -2$ and to n^{2s} for $s \geq -1$]. In the classical and semiclassical cases these two quantities are equal: in the semiclassical case $k_o = k_e = l + \frac{1}{2}$, where $\frac{1}{2}$ is the contribution from the Maslov index.[5]

To obtain the quantum-mechanical result, Eq. (2) was compared in Ref. 2 with the explicit formulas presented by Bockasten.[6] This comparison revealed that, with the exception of these angular momentum operators, all factors agree exactly in the classical and quantum-mechanical expressions. For these operators, the comparison indicated that different substitutions should be made for the odd and even powers, which were shown [Eqs. (17) and (18) of Ref. 2] to be given by

$$k_o^{2q+1} = (2l+q+1)!/(2l-q)! 2^{2q+1} \; , \quad (4)$$

$$k_e^{2q} = \sum_{r=0}^{q} (-1)^{q+r} C_{\lambda,q,r} (l+r)!/(l-r)! \; . \quad (5)$$

The closed-form quantum-mechanical expression for $\langle r^s \rangle$ can thus be obtained for arbitrary s by substituting Eqs. (4) and (5) into Eq. (3), provided the coefficients $C_{\lambda,q,r}$ are known. However, no general formula for specifying this quantity was available at the time of Ref. 2, and a table of specific numerical values for $C_{\lambda,q,r}$ for $\lambda \leq 6$ (obtained by comparison with Ref. 6) was presented. The paper by Drake and Swainson[1] contains this needed relationship, in the form of a recursion relation for the quantity they denote as $d_{q,r}^{(\lambda)}$, which is related to $C_{\lambda,q,r}$ by

$$(-1)^{q+r} C_{\lambda,q,r} = d_{q,r}^{(\lambda+2)} \; . \quad (6)$$

With this correspondence, Ref. 1 completes the specification of these quantities by the use of the recursion formula [Eq. (7) of Ref. 1]

TABLE I. The coefficients $C_{\lambda,q,i}$ of Eq. (5), tabulated for $7 \le \lambda \le 10$. Values for $\lambda \le 6$ are tabulated in Ref. 2.

		$C_{\lambda,q,i}$					
λ	q	$i=0$	$i=1$	$i=2$	$i=3$	$i=4$	$i=5$
7	1	10/3	1				
7	2	101/15	5	1			
7	3	36/7	36/5	3	1		
8	1	9/2	1				
8	2	27/2	22/3	1			
8	3	761/35	332/15	13/2	1		
8	4	0	0	0	0	1	
9	1	35/6	1				
9	2	145/6	10	1			
9	3	1315/21	48	21	1		
9	4	64	576/7	144/5	16/3	1	
10	1	22/3	1				
10	2	119/3	13	1			
10	3	3124/21	177/2	15	1		
10	4	10736/35	2124/7	84	34/3	1	
10	5	0	0	0	0	0	1

$$d_{q,r}^{(\lambda+2)}=\frac{1}{\lambda(2\lambda-2q-1)} \times((\lambda-2q)(2\lambda-1)d_{q,r}^{(\lambda+1)} +2q(\lambda-1)\{d_{q-1,r-1}^{(\lambda)} +[r(r+1)-\lambda(\lambda-2)/4]d_{q-1,r}^{(\lambda)}\}) , \quad (7)$$

and the starting values

$$d_{0,0}^{(2)}=1, \quad d_{0,0}^{(3)}=1 . \quad (8)$$

These formulas reproduce the values listed in the table in Ref. 2 for $\lambda \le 6$, and those results are supplemented for $7 \le \lambda \le 10$ in Table I. By combining these values for $C_{\lambda,q,r}$ with Eqs. (3)–(5) above, the exact expressions for $\langle r^P \rangle$ can be obtained.

The use of these three equations is equivalent to the use of Eqs. (2)–(5) in Ref. 1, but explicit expressions for all powers in the range $-16 \le P \le 13$ have already been presented there, and need not be duplicated. However, the identity of the Legendre functions and the role of the angular momentum operators in its arguments is not immediately apparent from the purely quantum-mechanical formulation, and some insights can be gained from comparing the semiclassical equations presented here with the explicit expressions in Ref. 1.

In this formulation, the extension from the classical to the quantum-mechanical case is achieved when the Legendre polynomial is replaced by a Legendre function, in which the order of successive terms in the series becomes a factorial relationship rather than one of successive multiplication. In the classical case, Hamilton-Jacobi theory treats a perturbation proportional to $\langle r^p \rangle$ by formally differentiating this quantity with respect to the angular momentum[3] to obtain the advance of the perihelion. Since the Legendre-polynomial formulation of Eq. (3) has well-defined differential properties,[3] and it is the polynomial representation of the angular momentum that characterizes the classical limit, this formulation provides an overlap wherein classical insights might be transferred to quantum-mechanical calculations. This is particularly applicable to studies of core polarization effects in high n and l Rydberg states of complex atoms, since the use of the core polarization model[2] has already introduced a classical element into the description.

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