Exact correspondence relationship for the expectation values of r^{-k} for hydrogenlike states

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An exact correspondence relationship between the classical and quantum-mechanical expectation values of r^{-k} for arbitrary hydrogenic states with quantum numbers n and l is established. The quantum-mechanical result for arbitrary powers of k is explicitly expressed in terms of relatively simple orthogonal polynomials which are intimately related to the Legendre polynomials and which consist of only the minimum of $n-l$ or $k+1$ terms. The correspondence between the sets of polynomials, and the complete formal analogy of the classical and quantum results, are found to originate in the fact that the correspondence limit of the Pasternack-Kramers recursion relation for the $\langle r^{-k}\rangle$ is the three-term recursion for the Legendre polynomials.

I. INTRODUCTION

The derivation of a general expression for the expectation values of r^{-k} for an arbitrary hydrogenlike state characterized by quantum numbers n and l and for arbitrary k has been pursued throughout the history of quantum mechanics. Perhaps the earliest such work was that of Waller [1], who was mainly interested in the polarization potential ($k=4$), in connection with the second-order Stark effect of two-electron atoms. A derivation of $\langle r^{-k}\rangle$ by Van Vleck [2] was corrected and replaced by a simpler approach by Pasternack [3]. The main result of Pasternack is a recursion relation for the $\langle r^{-k}\rangle$ that is computationally very convenient. Since it was found independently by Kramers [4], it is known as the Pasternack-Kramers recursion relation. Bockasten [5] used these relations to compute explicit expressions for the range $-5\leq k\leq 8$ that have been very valuable for many applications like the magnetic susceptibility of atoms in the independent-particle model ($k=-2$) or the mean lifetimes of hydrogenlike states [6–8] ($k=3$ or 4). Furthermore, polarization models of excited states of helium [9] and optical potential analyses of Rydberg states of helium [10] call for values of k up to 8 as do relativistic and other second-order corrections of multipole polarizabilities of hydrogenic ions [11]. Similar applications are provided by a whole class of retarded or long-range potentials [12,13] such as the interaction of an atom with a wall ($k=3$) or the Casimir-Polder interaction between two neutral atoms at *very* large distances ($k=7$) (as opposed to the usual van der Waals interaction with $k=6$). More examples for the appearance of positive powers of r up to 6 are given by a variational approach to quadrupole polarizabilities of ions [14], and variational estimates of such expectation values for atoms have been developed [15]. However, recent refinements in the measurement of Rydberg states of helium [16] have lead Drake and Swainson [17] to extend the tabulation to values of $-13\leq k\leq 16$. The results are given in terms of a series expansion in powers of n with the l-dependent coefficients determined by a set of recursions derived from the Pasternack-Kramers recursion. Finally, semiclassical expectation values of r^{-k} have been used to describe spectroscopic term energies of many-electron atoms [18], and recently Curtis [19] also succeeded in establishing a mnemonic connection of the quantum result for $\langle r^{-k}\rangle$ with the classical result, whereby the angular momentum quantum number l is replaced by certain functions of l given in terms of the above-mentioned coefficients from the work of Drake and Swainson. (Purely classical expectation values are of interest in the study of, for example, relativistic corrections of the kinetic energy or gravitational corrections in perturbed Kepler problems [20].) The above-mentioned examples for the use of expectation values of r^{-k} are, of course, far from being physically or historically complete, and are recalled only to give the reader an impression of the very broad and important range of applications.

It would seem, however, that despite the many fruitful efforts, a simple exact correspondence between the classical and quantum results for the $\langle r^{-k}\rangle$ still calls for a more rigorous foundation. The purpose of this work is therefore to establish an analytical connection between these results in terms of certain generalizations of Legendre polynomials. In this way the formally complete analogy between the classical and quantum-mechanical results becomes transparent, allowing one to study the transition from the quantum to the classical domain in full detail, whereas common applications of the correspondence principle, on the other hand, yield only asymptotic results, usually in terms of an asymptotic series in inverse powers of the relevant quantum numbers [7,8]. In Sec. II A we first recapitulate the classical result and discuss an ambiguity inherent to any use of the correspondence principle. The quantum-mechanical result is recalled in Sec. II B, and generalized Legendre polynomials that yield explicit expressions for the $\langle r^{-k}\rangle$ are derived in Sec. II C. Some more general remarks in Sec. III conclude the derivation.

II. AN EXACT CORRESPONDENCE RELATION

A. The classical and semiclassical results

The interest in classical expectation values of r^{-k} is, of course, much older than quantum-mechanical and semiclassical applications suggest. Probably the earliest general work was done by Laplace to determine the shape of the earth [21]. His method of computing these expectation values in polar coordinates can easily be adapted to the problem of two particles of charge $-e$ (an electron) and Ze (a nucleus), respectively, moving in a Keplerian orbit. Applications of this method to obtain a semiclassical formula for the expectation values of r^{-k} have been studied in detail by Curtis [18], and a fairly historical account on the connection to the old quantum theory is given in that work. To establish a reference for later comparison, we briefly recapitulate the derivation of the classical expectation values. The geometry of the elliptic orbit of the two particles of reduced mass μ can be determined by the semimajor axis

$$a=\frac{Ze^2}{2|E|} \tag{1}$$

and the eccentricity

$$\epsilon=\left[1-\frac{2|E|L^2}{\mu Z^2e^4}\right]^{1/2}, \tag{2}$$

where E is the energy and L the total angular momentum of the electron with respect to the nucleus. The polar equation of the orbit,

$$1+\epsilon\cos\varphi=\frac{a(1-\epsilon^2)}{r}, \tag{3}$$

where r is the separation between the two charges and φ is the polar angle measured with one of the charges at the origin, allows one to express the average value of r^{-k-2} over a period of motion

$$T=2\pi\left[\frac{\mu a^3}{Ze^2}\right]^{1/2}, \tag{4}$$

using $dt=(\mu r^2/L)d\varphi$, as

$$\begin{aligned}\langle r^{-k-2}\rangle_{\text{cl}}&=\frac{2\pi\mu}{TLa(1-\epsilon^2)}\frac{1}{\pi}\int_0^\pi d\varphi(1+\epsilon\cos\varphi)^k\\&=a^{-k-2}(1-\epsilon^2)^{-(k+1)/2}\\&\quad\times P_k\left[\frac{1}{(1-\epsilon^2)^{1/2}}\right].\end{aligned} \tag{5}$$

Here we have added the index cl to indicate a classical average. P_k is a Legendre polynomial, and since $P_{-k-1}(x)=P_k(x)$, the formula can be used for all k, positive as well as negative. The angular integral involved in Eq. (5) is an integral representation of the Legendre polynomials known as Laplace's first integral and the similar representation with k replaced by $-k-1$ in the integrand as Laplace's second integral [22]. So far this simply reproduces the formula given by Curtis (in terms of the semimajor axis and the semiminor axis, rather than ϵ) [18].

The derivation of a semiclassical result, however, encounters a difficulty that is inherent to any method based on the correspondence principle: the replacements of classical quantities by quantum-mechanical expressions, by virtue of which one usually converts a classical formula into a semiclassical result depending on quantum numbers, are by no means unique. This intrinsic ambiguity has been discussed by Marxer and Spruch [7,8] in connection with a semiclassical derivation of mean lifetimes of excited hydrogenlike states and of Landau states in a uniform magnetic field based on the correspondence principle and a treatment of the rate of loss of angular momentum. For example, in the case of hydrogenlike states, mentioned in the Introduction, various semiclassical replacements for the angular momentum lead to different possible semiclassical formulas for the mean lifetimes of states specified by their appropriate quantum numbers n and l. The point is that the correspondence principle rigorously justifies only the leading order of a semiclassical expression in inverse powers of the quantum numbers. (Generically, such an expression will, at best, represent an asymptotic series. In other words, if one considers, for mathematical purposes only, Planck's constant as a small parameter, then an expansion of a quantum-mechanical result in terms of this parameter around zero will have a vanishing radius of convergence.) Anything beyond the leading order is a matter of choice and convenience. To be specific, consider again the mean lifetime of a hydrogenlike state, where the use of the well-known Langer modification of the angular momentum quantum number $l\to l+\frac{1}{2}$ (the modification $\frac{1}{2}$ can be interpreted more rigorously as a Maslov index) does not give quite as good a result (more than 50% off) for low-lying states [6] as another substitution for l, equally well justified by the correspondence principle, which yields results accurate to at least 6% even for the lowest possible states [7]. (For large quantum numbers, both results are equally good and accurate.) The choice then is dictated by the desire to obtain a convenient formula for the mean lifetime that holds reasonably well for as many states as possible, even though the correspondence principle by itself justifies only a statement for highly excited states.

In the present problem, the same ambiguity arises. To obtain a semiclassical result for the expectation values of r^{-k}, one possible choice is to substitute the quantum-mechanical values for the energy (the modified Bohr radius is denoted by a_0 and $\hbar$ is Planck's constant divided by 2π)

$$E_{n,l}=-\frac{Z^2}{2n^2}\frac{e^2}{a_0} \tag{6}$$

and the angular momentum

$$L^2=l(l+1)\hbar^2 \tag{7}$$

of a state with quantum numbers n and l in Eq. (5). Incidentally, we note that the eccentricity thereby becomes

$$\epsilon=\left[1-\frac{l(l+1)}{n^2}\right]^{1/2}, \tag{8}$$

which even in the case of maximal l, $l=n-1$, commonly referred to as a circular orbit, does not vanish. An alternative procedure would be to express $\langle r^{-k}\rangle_{\rm cl}$ in terms of the energy E and the angular momentum L and to use the semiclassical substitution $L\to(l+\frac{1}{2})\hbar$ throughout. Obviously, one would obtain a different expression for the eccentricity and thus for $\langle r^{-k}\rangle$. The semimajor axis poses no difficulty here, since the use of Eq. (6) in Eq. (1) yields

$$a=\left[\frac{a_0}{Z}\right]n^2 \tag{9}$$

without any higher-order terms in $1/n$. Since the above discussion of mean lifetimes, for example, shows that the correspondence principle does not uniquely favor any specific semiclassical substitution, we choose to keep only the leading order of the semiclassical expressions for $(1-\epsilon^2)^{1/2}$ that result from the mentioned various possibilities, that is,

$$(1-\epsilon^2)^{1/2}=\frac{l}{n}. \tag{10}$$

To leading order, the semiclassical result for $\langle r^{-k}\rangle$, denoted by the index sc, then reads

$$\langle r^{-k-2}\rangle_{\rm sc}=\left[\frac{Z}{a_0}\right]^{k+2}\frac{1}{n^{k+3}l^{k+1}}P_k\left[\frac{n}{l}\right]. \tag{11}$$

B. The quantum-mechanical result

The quantum-mechanical expectation values of r^{-k}, carrying the index QM to distinguish it from the classical averages, are given for all k by the Pasternack-Kramers recursion relation [3–5]

$$\langle r^{-k-2}\rangle_{\rm QM}=\frac{4}{(2l+1)^2-k^2}\times\left[\left[\frac{2k-1}{k}\right]\frac{Z}{a_0}\langle r^{-k-1}\rangle_{\rm QM}-\left[\frac{k-1}{k}\right]\frac{Z^2}{n^2a_0^2}\langle r^{-k}\rangle_{\rm QM}\right], \tag{12}$$

which holds for $k\le 0$, together with the inversion formula

$$\langle r^{k}\rangle_{\rm QM}=\frac{(2l+k+2)!}{(2l-k-1)!}\left[\frac{na_0}{2Z}\right]^{2k+3}\langle r^{-k-3}\rangle_{\rm QM}. \tag{13}$$

From this relation, an explicit formula for low n can be easily computed [5]. To point out the well-known close analogy between the classical and the quantum results, mentioned already by, among others, Curtis [18,19], it may suffice to consider, for example,

$$\langle r^{-6}\rangle_{\rm QM}=\left[\frac{Z}{a_0}\right]^6\frac{35n^4-n^2[30l(l+1)-25]+3(l-1)l(l+1)(l+2)}{8n^7(l-\frac{3}{2})(l-1)(l-\frac{1}{2})l(l+\frac{1}{2})(l+1)(l+\frac{3}{2})(l+2)(l+\frac{5}{2})}, \tag{14}$$

valid for $l>1$. Comparison with the semiclassical result of Eq. (11),

$$\langle r^{-6}\rangle_{\rm sc}=\left[\frac{Z}{a_0}\right]^6\frac{35n^4-30n^2l^2+3l^4}{8n^7l^9}, \tag{15}$$

shows clearly how the coefficients of the Legendre polynomials appear in the quantum-mechanical expression; one simply neglects terms of order $1/n$ and $1/l$. However, this observation has thus far not given rise to a closed and simple analytical correspondence.

C. Generalized Legendre polynomials

Instead of replacing l in the semiclassical formula for $\langle r^{-k}\rangle$ by the angular momentum operators, as suggested by Curtis [19], we here pursue a somewhat complementary approach. We so modify the Legendre polynomials in Eq. (11) that the classical and quantum results are expressed in the same way and the analogies mentioned above thereby become obvious. The advantage of Curtis's procedure is that it allows one to retain the usual Legendre polynomials. However, this is achieved at the expense of introducing substitutions for the angular momentum quantum number that depend on the power k. At variance, the approach presented here uses the same simple angular momentum quantum number, namely, l itself, in any event. To begin, we derive the recursion relation that is obeyed by the semiclassical expectation values. To this end, we simply insert the three-term recursion relation for the Legendre polynomials, which we write in the form

$$P_k(x)=\frac{2k-1}{k}xP_{k-1}(x)-\frac{k-1}{k}P_{k-2}(x),\quad k\ge 1, \qquad P_0(x)=1, \tag{16}$$

into the semiclassical result from Eq. (11). This immediately yields the recursion relation

$$\langle r^{-k-2}\rangle_{\rm sc}=\frac{1}{l^2}\left[\left[\frac{2k-1}{k}\right]\frac{Z}{a_0}\langle r^{-k-1}\rangle_{\rm sc}-\left[\frac{k-1}{k}\right]\frac{Z^2}{n^2a_0^2}\langle r^{-k}\rangle_{\rm sc}\right]. \tag{17}$$

Apart from the overall factor $1/l^2$ this is obviously the same as the Pasternack-Kramers recursion relation given by Eq. (12). Put differently, since for high quantum number l we have

$$\frac{4}{(2l+1)^2-k^2}\to\frac{1}{l^2}\ , \tag{18}$$

we recognize that the correspondence limit of the Pasternack-Kramers recursion can be interpreted as the three-term recursion for the Legendre polynomials.

This result strongly suggests [23] the existence of orthogonal generalized Legendre polynomials, to be denoted by $\mathcal{P}_k$, such that the quantum-mechanical result for $\langle r^{-k}\rangle$ agrees formally with the semiclassical result in Eq. (11). Let us thus assume that there exist orthogonal polynomials $\mathcal{P}_{k,l}$ such that

$$\langle r^{-k-2}\rangle_{\rm QM}=\left[\frac{Z}{a_0}\right]^{k+2}\frac{1}{n^{k+3}l^{k+1}}\mathcal{P}_{k,l}\left[\frac{n}{l}\right]\ . \tag{19}$$

Of course, these polynomials will depend parametrically on l, and we have introduced a corresponding index for the sake of clarity in the above formula. However, to simplify the notation, we will suppress that index in the following. A polynomial $\mathcal{P}_k$ (and correspondingly any collection of coefficients with index k) thus is meant to belong to a set of orthogonal polynomials $\{\mathcal{P}_{k,l}\}|_l$ with l held fixed. In this notation, then, the set $\{\mathcal{P}_k\}$ is a different set of orthogonal polynomials for every fixed l. Furthermore, due to their orthogonality, the $\mathcal{P}_k$ will satisfy a three-term recursion relation of the form

$$\alpha_k\mathcal{P}_k(x)=(\beta_k+\gamma_k x)\mathcal{P}_{k-1}(x)-\delta_k\mathcal{P}_{k-2}(x),\ k\ge 1\ , \tag{20}$$

with α_k, β_k, γ_k, and δ_k independent of x. Due to a theorem ascribed to Favard [24], this kind of recursion guarantees the orthogonality of the polynomials $\mathcal{P}_k$. If we now demand that the Pasternack-Kramers recursion relation follows from recursion Eq. (20) for the $\mathcal{P}_k$ in the same way as the classical recursion Eq. (17) followed from the recursion for the Legendre polynomials (with x assumed not yet determined), we are led to the condition

$$\frac{\beta_k+\gamma_k x}{2k-1}n^{k+2}l^k=\frac{n^2\delta_k}{k-1}n^{k+1}l^{k-1}=\frac{4}{[(2l+1)^2-k^2]}\frac{\alpha_k}{k}n^{k+3}l^{k+1}\ , \tag{21}$$

which has to be true for all $k\ge 1$. Fortunately, the solution of this condition is obvious and reads

$$\begin{aligned}&\alpha_k=k,\quad \beta_k=0\ ,\\ &\gamma_k=(2k-1)d_k,\quad \delta_k=(k-1)d_k\ ,\\ &x=\frac{n}{l}\ ,\end{aligned} \tag{22}$$

where we have introduced

$$d_k=\frac{4l^2}{(2l+1)^2-k^2}\ . \tag{23}$$

[Note, that if we keep the argument of $\mathcal{P}_{k,l}$ undetermined in Eq. (19), condition (21) yields what we have anticipated in Eq. (19).] The generalized Legendre polynomials $\mathcal{P}_k$ can thus be defined by the three-term recursion relation

$$\mathcal{P}_k(x)=\frac{2k-1}{k}d_k x\mathcal{P}_{k-1}(x)-\frac{k-1}{k}d_k\mathcal{P}_{k-2}(x),\quad k\ge 1\ . \tag{24}$$

The initial value for this recursion can be readily derived from $\langle r^{-1}\rangle_{\rm QM}$; thus, for example, from the virial theorem we immediately obtain

$$\langle r^{-1}\rangle_{\rm QM}=\frac{Z}{a_0 n^2}\ , \tag{25}$$

from which we infer, using Eq. (13) for $k=-1$ and Eq. (19) for $k=0$, that

$$\mathcal{P}_0(x)=\frac{2l}{2l+1}=\frac{l}{l+\frac{1}{2}}\ . \tag{26}$$

(It is interesting to observe that $\mathcal{P}_0$ differs from unity only by the ratio of l and $l+\frac{1}{2}$, which is a standard semiclassical replacement for l. It is here that the Langer modification—or better the topological Maslov index—makes its appearance.) Since for fixed k we have

$$\lim_{l\to\infty}d_k=1 \tag{27}$$

and

$$\lim_{l\to\infty}\mathcal{P}_0(x)=1\ , \tag{28}$$

the recursion Eq. (24) becomes exactly the recursion for the Legendre polynomials, Eq. (16), in the correspondence limit. It is therefore clear that the correspondence limit of the $\mathcal{P}_k$ are the Legendre polynomials:

$$\lim_{l\to\infty}\mathcal{P}_k(x)=P_k(x)\ . \tag{29}$$

(Note the correct meaning of this equation; in letting l tend to infinity we consider a sequence of $\mathcal{P}_{k,l}$ for fixed k; this sequence then runs through every different set of orthogonal polynomials characterized by a fixed l). Of course, we can derive a simple recursion for the coefficients of the power-series representation for the $\mathcal{P}_k$ by assuming the ansatz

$$\mathcal{P}_k(x)=\sum_{\nu=0}^{k}a_{k,\nu}x^\nu\ , \tag{30}$$

from which we obtain

$$\begin{aligned}&a_{k+1,\nu}=\frac{2k+1}{k+1}d_{k+1}a_{k,\nu-1}-\frac{k}{k+1}d_{k+1}a_{k-1,\nu}\ ,\\ &a_{0,0}=\frac{2l}{2l+1},a_{k,-1}=a_{k,\nu>k}=0\ ;\\ &\qquad k\ge 0,\quad \nu=0,\ldots,k+1\ .\end{aligned} \tag{31}$$

Since the $\langle r^{-k}\rangle$ are given by the $\mathcal{P}_k$ with argument $x=n/l$, these coefficients give, after multiplication by l^k, the l-dependent coefficients of the power series in n in the quantum result for $\langle r^{-k}\rangle$. A solution of this recursion therefore leads to a result analogous to the representation of $\langle r^{-k}\rangle$ given by Drake and Swainson [17] and we will not pursue this matter further here. For later reference, however, let us record the coefficient of the leading power in x in $\mathcal{P}_k$:

$$a_{k,k}=a_{0,0}\prod_{i=0}^{k-1}\frac{2i+1}{i+1}d_{i+1}$$
$$=\frac{(2k-1)!}{k!}\frac{2l^{2k+1}}{\left[l+\frac{1-k}{2}\right]\left[l+\frac{-k}{2}\right]\cdots\left[l+\frac{k}{2}\right]\left[l+\frac{1+k}{2}\right]} . \qquad (32)$$

It now becomes rather transparent how the typical denominators of the quantum results, as seen, for example, in Eq. (14) and in the tabulation of Bockasten [5], emerge from the modified normalization of the polynomials due to the d_k.

Instead of explicitly solving the recursion Eq. (31), we infer the explicit form of the $\mathcal{P}_k$ from certain properties of generalized hypergeometric series and from an argument of analogy with the classical result. To start with, we recall that the representation of the Legendre polynomials in terms of hypergeometric series is

$$P_k(x)={}_2F_1\left[-k,k+1;1;\frac{1-x}{2}\right] . \qquad (33)$$

The close analogy of the recursions for the P_k and the $\mathcal{P}_k$ suggests that the latter may be written as a generalized hypergeometric series of the form

$$_{p+2}F_q(-k,k+1,a_1,\ldots,a_p;c_1,\ldots,c_q;z) , \qquad (34)$$

with one of the entries a linear function of x. Most of the ambiguity in this form can be ruled out by using a theorem due to Al-Salam [25], who proved that any generalized hypergeometric series of the form

$$_{p+2}F_q(-k,k+\gamma,a_1,\ldots,a_p;c_1,\ldots,c_q;x) , \qquad (35)$$

where all the parameters are independent of x, are either Jacobi or Bessel polynomials. The correspondence limit stated in Eq. (29) thus eliminates the possibility of z in the form (34) being a function of x. The only choice left to ensure a representation of $\mathcal{P}_k(x)$ according to the scheme given in (34) is therefore that the argument x appears in the set of parameters, that is, that the $\mathcal{P}_k(x)$ are of the form

$$_{p+3}F_q(-k,k+1,\alpha x+\beta,a_1,\ldots,a_p;c_1,\ldots,c_q;1) , \qquad (36)$$

Another theorem of Al-Salam [25] finally narrows down the degrees of freedom in the pattern given by (36). In order that a generalized hypergeometric series of the kind given by (36) satisfies a three-term recursion relation, and thus in order that it may possibly represent orthogonal polynomials, it is necessary that $p=0$ and $q=2$. We conclude that the $\mathcal{P}_k(x)$ are of the form

$$_3F_2(-k,k+1,\alpha x+\beta;c_1,c_2;1) . \qquad (37)$$

The remaining parameters could, of course, be determined directly from the recursion relation Eq. (24). However, Pasternack [26] has already studied series of this kind, namely the polynomials

$$F_k^m(z)={}_3F_2\left[-k,k+1,\frac{1+m+z}{2};1,m+1;1\right] , \qquad (38)$$

and found that they satisfy the recursion

$$k(k+m)F_k^m(z)=-(2k-1)zF_{k-1}^m(z)+(k-1)(k-1-m)F_{k-2}^m(z) . \qquad (39)$$

A comparison with the recursion Eq. (24) then shows that the $\mathcal{P}_k(x)$ satisfy Eq. (39) if we choose $m=2l+1$ and $z=2lx$. Finally, the correct normalization can be inferred from Eq. (32) and, using $F_k^m(z)=(-1)^kF_k^m(-z)$, we end up with the explicit representation

$$\mathcal{P}_{k,l}(x)=\frac{(2l)^{k+1}(2l-k)!}{(2l+1)!}\times{}_3F_2(-k,k+1,l+1-lx;1,2l+2;1) , \qquad (40)$$

where, for clarity, we have reintroduced the index l on the left-hand side. This, in connection with Eq. (19), then gives a simple and most convenient explicit representation of the expectation values $\langle r^{-k-2}\rangle$. Note that these expectation values are evaluated with $x=n/l$; the third entry in the generalized hypergeometric series in Eq. (40) then becomes $l+1-n=-n_r$, that is, the negative of the radial quantum number n_r. Therefore, although the $\mathcal{P}_k$ are generally polynomials of order k, for the evaluation of expectation values the series in Eq. (40) actually terminates after the minimum of $n-l$ or $k+1$ terms. Thus, for example, for $l=n-1$ the $\langle r^{-k-2}\rangle$ are given by just one term. The usual restrictions on the angular momentum quantum number l are reflected in the factor $(2l-k)!$ in Eq. (40); the quantum-mechanical expectation values of r^{-k} diverge for $l<(k/2)-1$. Furthermore, since for $x=n/l$ the fact that the generalized hypergeometric series in Eq. (40) terminates at all does not depend on k, the formula for $\langle r^{-k-2}\rangle$ given by Eqs. (19) and (40) can be analytically continued and the result is good for arbitrary (complex) values of k [except at the poles caused by $(2l-k)!$]. The generalization of the equality $P_k(x)=P_{-k-1}(x)$ can also be derived from Eq. (40). Since the $_3F_2$ series is still invariant under the transformation $k\rightarrow -k-1$, we easily find

$$\mathcal{P}_{-k-1,l}(x)=\frac{(2l+k+1)!}{(2l)^{2k+1}(2l-k)!}\mathcal{P}_{k,l}(x) , \qquad (41)$$

in agreement with the quantum-mechanical inversion formula stated in Eq. (13). Finally, the correspondence limit shows up in Eq. (40) via the limiting relations

$$\lim_{l \to \infty} \frac{(2l)^{k+1}(2l-k)!}{(2l+1)!} = 1 \tag{42}$$

and

$$\lim_{l \to \infty} {}_3F_2(-k,k+1,l+1-lx;1,2l+2;1) = {}_2F_1\left[-k,k+1;1;\frac{1-x}{2}\right], \tag{43}$$

confirming the result stated in Eq. (29).

III. CONCLUDING REMARKS

We wish to stress the fact that the analytical results obtained here and by others are contained, essentially, in the later work of Pasternack [26]. However, Pasternack's work was primarily a purely mathematical investigation of various properties of certain series, apparently without any reference to the fact that they represent interesting sets of orthogonal polynomials. Furthermore, we have pointed out an independent alternative and simpler derivation, and have clarified the close relation to the classical result, which does not seem to have been fully appreciated before. For example, we have interpreted the recursion relation of the Legendre polynomials as the correspondence limit of the Pasternack-Kramers recursion relation and have traced back the typical denominators appearing in tabulations of quantum-mechanical results to the modified normalization of generalized Legendre polynomials. Furthermore, the semiclassical and quantum-mechanical expectation values of r^{-k} can be expressed in terms of these polynomials without introducing modifications of the angular momentum quantum number, which, in any event, are not rigorously justified by the correspondence principle. Another point we want to emphasize here is that it is apparently possible to generalize classical results that correspond to matrix elements in the quantum-mechanical domain in such a way that the results are in formal analogy and that important properties, such as the orthogonality of the involved polynomials in the present case, are preserved. Such a situation then allows one to study the correspondence limit in its full analytical beauty and not only in terms of asymptotic results, as may be obtained from, say, the Wentzel-Kramers-Brillouin method. In the present work this has been achieved for diagonal matrix elements only, whereas many quantities of great interest, for example, mean lifetimes, linewidths, or transition rates in general, are given in terms of off-diagonal matrix elements. It will therefore be interesting to see whether such relationships can be extended to the off-diagonal case, thus furnishing a semiclassical interpretation of off-diagonal matrix elements, and the mentioned derivations of the lifetimes of excited hydrogenlike states [7] or of Landau states in a uniform magnetic field [8] from the classical radiation reaction force give two examples that such an interpretation is possible. This point is being investigated.

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