Inverse momentum expectation values for hydrogenic systems

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Abstract
By using the Fourier transforms of the general hydrogenic bound state wave functions (as ultraspherical polynomials) one may find expectation values of arbitrary functions of momentum $p$. In this manner the effect of a reciprocity perturbation $b/p$ can be evaluated for all hydrogenic states.

1 Motivation

Many years ago and long before the elementary particle spectrum was thoroughly explored experimentally, Born and Green [1] proposed the principle of reciprocity in an attempt to determine the mass spectrum of fermions and bosons. The principle flowed naturally from observed covariance of equations of motion under the momentum-position substitution rule $(P, R) \rightarrow (-bR, P/b)$, with an appropriate scale $b$, but it went a lot further in postulating that the Hamiltonian was actually invariant under such a transformation. This was all done in a relativistic framework but it soon became apparent that it failed rather miserably to reproduce the mass spectrum, since all states were essentially harmonic overtones of a fundamental frequency; thus the idea was soon consigned to the dustbin of history. Recently there has been a resurgence in investigating the concept, not only for its elegance but
for its group theoretical features which incorporate the concept of a maximum force. Much progress has been made along such lines [2] but it remains true that the relativistic scheme is beset with tachyonic state problems if the spectrum is treated along the lines of Wigner’s approach of induced representations, ensuing from the larger ‘quaplectic’ group.

Even at the classical nonrelativistic level where the idea should leave an imprint, the consequence for the (undamped) harmonic oscillator is that all frequencies are universal, which is patently absurd, and seems to indicate that the reciprocity concept has no future. However with the realization that damping with an appropriately small scale $b$ avoids this absurdity, it is worth following through the idea, at least non-relativistically, for some familiar potentials and in particular for Coulomb-like ones about which so much is known. Now nonrelativistic systems placed in a $1/r$ potential with Hamiltonian

$$H(P, R) = P^2/2m - \alpha/R$$

have been thoroughly studied over many years and the results are found in standard textbooks (see eg [3]) of classical and quantum mechanics. More complicated systems or small modifications, including certain relativistic corrections, can be treated by perturbation theory. If we attempt to make such a system reciprocity-invariant the Hamiltonian (1) is accompanied by extra terms $b^2 R^2/2m - \alpha b/P$. Here $b$ is a tiny scale factor which has hardly any effect on atomic physics but can influence phenomena on cosmic scales [4]. Because $b$ is so small the main effect of the reciprocity change lies in the $b/P$ perturbation, so our aim in this paper is to determine the energy level change on all hydrogenic bound state levels due to it, and not just on the ground state as was recently done in [4]. This is the motivation for this article apart from its intrinsic mathematical interest.

The neatest way to obtain the expectation value of any function of momentum $f(P)$ is to evaluate the Fourier transform $\phi(p)$ of the hydrogenic wave functions $\psi(x)$ and work out

$$\langle f(P) \rangle = \int \frac{d^3 p}{(2\pi)^3} \phi^*(p)f(p)\phi(p)$$

in the usual way. If $f$ were purely a polynomial it would not be necessary to go through this process but simply work directly in coordinate space,

$$\langle f(P) \rangle = \int d^3 x \psi^*(x)f(-i\hbar \nabla)\psi(x),$$

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because the spatial wave functions $\psi$ are very well known. However, for expectation values of the reciprocity term where we are dealing with an inverse momentum, it is safest to take route (2). Nevertheless the momentum-space procedure (2) requires us to evaluate first the Fourier transforms,

$$\phi(p) = \int d^3 x \, e^{-ip\cdot x/\hbar} \psi(x),$$

and this is technically tricky! It was first carried out in a classic paper by Podolsky and Pauling [5] but our treatment is slightly different and done in the next section. It also differs radically from Hylleraas’ differential method [6]. The required expectation value of $1/P$, the meat of the paper, is given in the following section; the answer is nontrivial. Interesting sum rules are worked out next and asymptotic estimates conclude the paper.

## 2 Momentum wave functions

We begin by quoting the bound state wave functions for Hamiltonian (1), as stated in the standard texts [3]:

$$\psi_{n\ell m}(x) \equiv \langle r\theta\phi|n\ell m \rangle = 2^{3/2} \kappa^{3/2} \sqrt{(n-\ell-1)! n(n+\ell)!} e^{-\kappa r} (2\kappa r)^\ell L_{n-\ell-1}^{2\ell+1}(2\kappa r) Y_{\ell m}(\theta, \phi),$$

where the quantum numbers $n, \ell, m$ are integers obeying $n > \ell \geq |m| \geq 0$, with $\kappa \equiv 1/na = m\alpha/\hbar^2$, so $a$ connotes the Bohr radius and $Y_{\ell m}$ are the spherical harmonics, orthonormal over the unit sphere. The associated Laguerre polynomials in (7) obey the orthogonality relations (see [7], §5.5.2)

$$\int_0^\infty e^{-t} t^{\nu} L_n^{\nu}(t) L_{n'}^{\nu}(t) \, dt = \delta_{nn'} \Gamma(n+\nu+1)/\Gamma(n+1).$$

Naturally, the wave functions (3) are orthonormal over space,

$$\int d^3 x \psi_{n\ell m}^*(x) \psi_{n'\ell' m'}(x) = \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'},$$

but this is difficult to demonstrate directly from (4) because of the different radial weight; in that respect the intrinsic $n$-dependence of $\kappa$ becomes significant, as shown by Dunkl [8].
To be able to obtain the momentum-space wave function,

\[ \phi_{n\ell m}(k) \equiv \langle k\theta_k\phi_k|n\ell m \rangle = \int d^3 x \ e^{-ik\cdot x} \psi_{n\ell m}(x), \]

we make use of the expansion of plane waves into spherical ones (see [3], eq (B.105)):

\[ e^{-ik\cdot x} = 4\pi \sum_{\ell,m} (-i)^\ell j_\ell(kr)Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta_k,\phi_k); \quad j_\ell(z) \equiv \sqrt{\frac{\pi}{2z}} J_{\ell+1/2}(z). \]

\[ \]

By this means we arrive at \[ \phi_{n\ell m}(k,\theta_k,\phi_k) \equiv (-i)^\ell \mathcal{P}_{n\ell}(k)Y_{\ell m}(\theta_k,\phi_k) \] and the radial momentum wave function

\[ \mathcal{P}_{n\ell}(k) = 4\pi\kappa^{3/2} \sqrt{\frac{(n-\ell-1)!}{n(n+\ell)!}} \int_0^\infty \sqrt{\frac{\pi}{2kr}} J_{\ell+1/2}(kr)(2\kappa r)^\ell e^{-\kappa r} L_{n-\ell-1}^{2\ell+1}(2\kappa r) r^2 dr. \]

This is a formidable integral in general, except for simple cases like \( \ell = 0 \) or \( \ell = n - 1 \).

To proceed further, we make use of an integral which can be found in the standard texts (see [7], §3.8.3), namely

\[ \int_0^\infty t^{\nu+1} e^{-\beta t} J_\nu(\gamma t) \ dt = \frac{2^{\nu+1}\beta^{-\nu} \Gamma(\nu + 3/2)}{\sqrt{\pi (\beta^2 + \gamma^2)^{\nu+3/2}}}, \]

and the generating function (see [7], §5.5.2)

\[ \sum_{\nu=0}^\infty L_\nu^\alpha(x) z^\nu = (1 - z)^{-\alpha - 1} e^{xz/(x - 1)}. \]

By defining (and later on identifying \( \nu = n - \ell - 1 \geq 0 \))

\[ \mathcal{P}_{\ell}(k, z) \equiv \sum_{\nu=0}^\infty \sqrt{\frac{\nu!}{(\nu + \ell + 1)(\nu + 2\ell + 1)! \kappa^{3}}} \mathcal{P}_{n\ell}(k) z^\nu \]

we see that such an expansion in powers of \( z \) yields the momentum space hydrogenic functions. This new generating function is a doable integral like (8),

\[ \mathcal{P}_{\ell}(k) = \frac{4\pi^{3/2}(2\kappa)\ell}{(1 - z)^{2\ell + 2}\sqrt{2k}} \int_0^\infty r^{\ell+3/2} e^{-\kappa r(1+z)/(1-z)} J_{\ell+1/2}(kr) \ dr \]

\[ = \frac{8\pi\kappa (4k\kappa)^\ell(1 - z^2)(\ell + 1)!}{(\kappa^2(1 + z)^2 + k^2(1 - z)^2)^{\ell+2}}. \]
Since ultraspherical (Gegenbauer) polynomials arise via the generating series (see [7], §5.3.2),
\[(1 - 2xz + z^2)^{-\lambda} = \sum_{\nu=0}^{\infty} C_{\nu}^{\lambda}(x) z^\nu; \quad |z| < 1, \quad \lambda \neq 0,\]  
(12)
we are led to identify \(x = (k^2 - \kappa^2)/(k^2 + \kappa^2)\), and derive
\[
\frac{(k^2 + \kappa^2)^{\ell+2}}{8\pi \kappa (4k\kappa)^{\ell}(\ell + 1)!} \mathcal{P}_\ell(k, z) = (1 - z^2) \sum_{\nu=0}^{\infty} C_{\nu}^{\ell+2}(x) z^\nu = \\
\sum_{\nu=0}^{\infty} [C_{\nu}^{\ell+2}(x) - C_{\nu-2}^{\ell+2}(x)] z^\nu = \sum_{\nu=0}^{\infty} (\nu + \ell + 1) C_{\nu}^{\ell+1}(x) z^\nu/\ell + 1),\]  
(13)
on adopting the convention that polynomials of negative degree are identically zero and using recurrence relations. Putting this together with (10), we arrive at the sought-after result for the Fourier transform, \(\phi_{n\ell m}(k) = (-i)^{\ell} \mathcal{P}_{n\ell}(k) Y_{\ell m}(\theta_k, \phi_k)\), namely
\[
\mathcal{P}_{n\ell}(k) = 16\pi \kappa^{5/2} \left[ \frac{n(n - \ell - 1)!}{(n + \ell)!} \frac{(4k\kappa)^{\ell} \mathcal{P}_\ell(k, z)}{(k^2 + \kappa^2)^{\ell+2} C_{n-\ell-1}^{\ell+1} \left( \frac{k^2 - \kappa^2}{k^2 + \kappa^2} \right)} \right].\]  
(14)
This will form the basis for the forthcoming calculations. [Fock’s stereographic representation [9] is also capable to reproducing (14).]

For the present it only remains to check the normalization of these momentum wavefunctions:
\[
\int_0^{\infty} |\mathcal{P}_{n\ell}(k)|^2 \frac{k^2}{8\pi^3} dk = \frac{32n(n - \ell - 1)!/(\ell)!^2 k^5 \kappa^5}{\pi(n + \ell)!} \times \\
\int_0^{\infty} \frac{(4k\kappa)^{2\ell}}{(k^2 + \kappa^2)^{2\ell+4}} \left[ C_{n-\ell-1}^{\ell+1} \left( \frac{k^2 - \kappa^2}{k^2 + \kappa^2} \right) \right]^2 k^2 dk.\]  
(15)
Changing the integration variable back to \(x = (k^2 - \kappa^2)/(k^2 + \kappa^2)\), the rhs of (15) can be simplified to
\[
\frac{2n(n - \ell - 1)!/(2\ell)!^2}{\pi(n + \ell)!} \int_{-1}^{1} (1 - x^2)^{(\ell+1)/2} [C_{n-\ell-1}^{\ell+1}(x)]^2 (1 - x) \, dx.
\]
Discarding the odd term in $x$ and using orthogonality of the Gegenbauer polynomials (see [7], §5.3.2),

$$\int_{-1}^{1} C_{n}^{\lambda}(x) C_{n}^{\lambda'}(x) (1 - x^2)^{\lambda-1/2} \, dx = \delta_{nn'} \frac{2^{1-2\lambda} \pi \Gamma(n + 2\lambda)}{(\lambda + n)n!(\Gamma(\lambda))^2},$$

we can satisfy ourselves that the rhs of (15) does indeed reduce to unity; so all is well for the next initiative.

3 Momentum expectation values

We are ready to tackle the general case,

$$\langle f(P) \rangle_{n\ell} = \langle n\ell m | f(P) | n\ell m \rangle = \int_{0}^{\infty} |\mathcal{P}_{n\ell}(k)|^2 f(hk) \frac{k^2 \, dk}{8\pi^3}$$

$$= \frac{2n(n - \ell - 1)!(2\ell!)^2}{\pi(n + \ell)!} \int_{-1}^{1} (1 - x^2)^{\ell+1/2} [C_{n-\ell-1}^{\ell+1}(x)]^2 (1 - x) f\left(\frac{\hbar k}{\sqrt{\frac{1 + x}{1 - x}}}\right) \, dx,$$

provided of course that the resulting integration is well-behaved so that $f(P)$ makes sense. As we are going to be dealing with squares of ultraspherical polynomials, let us substitute $k = \kappa \tan \theta$, making $x = -\cos(2\theta)$. It then follows that expression (16) can be recast as

$$\langle f(P) \rangle_{n\ell} = \frac{4n(n - \ell - 1)!(2\ell!)^2}{\pi(n + \ell)!} \int_{0}^{\pi/2} (\sin 2\theta)^{2\ell+2} (1 + \cos 2\theta) [C_{n-\ell-1}^{\ell+1}(\cos 2\theta)]^2$$

$$\times f(\hbar \kappa \tan \theta) \, d\theta.$$  

(17)

In particular, for the inverse momentum we meet the dimensionless integrals

$$\langle \frac{\hbar \kappa}{P} \rangle_{n\ell} = \frac{16n(n - \ell - 1)!(2\ell!)^2}{\pi(n + \ell)!} \int_{0}^{\pi/2} (\sin 2\theta)^{2\ell+1} \cos^4 \theta [C_{n-\ell-1}^{\ell+1}(\cos 2\theta)]^2 \, d\theta$$

or $$\frac{2n(n - \ell - 1)!(2\ell!)^2}{\pi(n + \ell)!} \int_{-1}^{1} (1 - x^2)^{\ell} [(1 + x)C_{n-\ell-1}^{\ell+1}(x)]^2 \, dx.$$  

(18)

We shall now show how to evaluate these for special values of $\ell$ before handling the most general angular momentum state.
3.1 The case $\ell = 0$

To demonstrate the nontrivial nature of the problem we firstly turn to the spherical (S-wave) $\ell = 0$ states. Since $C_{n-1}^1(\cos \theta) = \sin(n\theta)/\sin \theta$ (see [7], §5.3.1), we must deal with

$$\langle \bar{h}\kappa/P \rangle_{n0} = \frac{8}{\pi} \int_0^{\pi/2} \frac{\sin^2(2n\theta)}{\sin \theta} \cos^3 \theta \, d\theta. \quad (19)$$

In order to do this (via a recursion procedure) let us define, for integer $\nu \geq 0$,

$$K_{\nu}(n) \equiv \int_0^{\pi/2} \frac{\sin^2(2n\theta)}{\sin \theta} \cos^{2\nu+1} \theta \, d\theta, \quad (20)$$

and treat the case $\nu = 0$ first. We have

$$K_0(n+1) - K_0(n) = \int_0^{\pi/2} \cot \theta \sin^2(2n+2)\theta - \sin^2 2n\theta \, d\theta = 1/(2n+1). \quad (21)$$

But in the particular case $n = 1$ we have trivially $K_0(1) = 1$. It follows from (21) that (see [7], §1.2)

$$K_0(n) = \sum_{m=1}^n \frac{1}{2m-1} = \sum_{m=1}^{2n} \frac{1}{m} - \frac{1}{2} \sum_{m=1}^n \frac{1}{m} = \psi(2n+1) - \frac{1}{2} \psi(n+1) + \frac{\gamma}{2}. \quad (22)$$

Another contiguity relation is

$$K_1(n) - K_0(n) = -\int_0^{\pi/2} \sin \theta \cos \theta \sin^2 2n\theta \, d\theta = \frac{4n^2}{4n^2 - 1}. \quad (23)$$

Combining this with (22) we obtain the final result for S-wave states,

$$\langle (h\kappa/P) \rangle_{n0} = \langle 1/P \rangle_{n0} = \frac{8an}{\hbar} \left[ \psi(n+1/2) - \frac{2n^2}{4n^2 - 1} + \gamma + \ln 4 \right] \quad \text{or}$$

$$\langle (1/P) \rangle_{n0} = \frac{8an}{\hbar} \left[ \psi(n+1/2) - \frac{2n^2}{4n^2 - 1} + \gamma + \ln 4 \right], \quad (24)$$

since $\hbar = 2\pi\hbar$. For large $n$ this behaves asymptotically as

$$\langle (1/P) \rangle_{n0} \sim (8an/\hbar)[\ln(4n) + \gamma - 1/2 - 1/12n^2] + O(n^{-3}).$$
3.2 The cases $\ell = n - 1, n - 2$

The case $\ell = n - 1$ is a relatively easy problem because the Gegenbauer polynomial collapses to unity and the integral (18) becomes quite trivial. We have

$$\langle \hat{h}_K / \mathcal{P} \rangle_{n-1} = \frac{2^{2n-1}n!(n-1)!}{\pi (2n-1)!} \int_{-1}^{1} (1 - x^2)^{n-1}(1 + x^2) \, dx$$

$$= \frac{\Gamma(n)\Gamma(n+2)}{\Gamma(n+1/2)\Gamma(n+3/2)}$$

or

$$\langle 1 / \mathcal{P} \rangle_{n-1} = \frac{2\pi a}{h} \frac{\Gamma(n+1)\Gamma(n+2)}{\Gamma(n+1/2)\Gamma(n+3/2)}.\quad (25)$$

This time the asymptotic behaviour in $n$ is

$$\langle (1 / \mathcal{P})_{n-1} \rangle \sim (8\pi a/h)[1 + 3/4n + O(1/n^2)].$$

In a similar, but somewhat more complicated, vein we can readily treat the case $\ell = n - 2$ so as to obtain

$$\langle \hat{h}_K / \mathcal{P} \rangle_{n-2} = \frac{(n+2)\Gamma(n-1)\Gamma(n+1)}{\Gamma(n-1/2)\Gamma(n+3/2)} \rightarrow 1 + \frac{9}{4n} + O\left(\frac{1}{n^2}\right).$$

But, to proceed any further down in $\ell$, a more systematic approach is necessary.

3.3 The general case $0 \leq \ell \leq n - 1$

We can no longer avoid handling the awkward weight occurring in (18). (Had we been dealing with even powers of $\mathcal{P}$ the weight would not have been too troublesome, by using recurrence properties of the $C_{2n}^N(x)$.\) Realising that $C_{2n}^N(x)$ is merely an $N$th degree polynomial in $x$, it ought to be possible to rewrite it as a combination of $C_{2n}^M(x)$ polynomials, with appropriately chosen $\mu$ (to make the integral (18) more tractable). And indeed there is a result which serves this purpose (see [10], eqs 4.10.27 and 4.10.28):

$$\Gamma(\lambda)C_{n}^\lambda(x) = \sum_{j=0}^{[n/2]} \frac{(n - 2j + \mu)\Gamma(\lambda - \mu + j)\Gamma(n + \lambda - j)}{j!\Gamma(\lambda - \mu)\Gamma(n + \mu - j + 1)}\Gamma(\mu)C_{n-2j}^{\mu}(x).$$

(27)
In this connection, note that for integer \( j \geq 0 \), \( \lim_{\epsilon \to 0} \Gamma(\epsilon + j)/\Gamma(\epsilon) = \delta_{j0} \), so that (27) reduces to a triviality when \( \lambda = \mu \).

Let us therefore alter the weight of \( \ell \) by 1/2 up and down by expressing

\[
C_{n-\ell-1}^{\ell+1}(x) = \sum_{j=0}^{[(n-\ell-1)/2]} \beta_{j\ell} C_{n-\ell-1-2j}^{\ell+1/2}(x) = \sum_{j=0}^{[(n-\ell-1)/2]} \gamma_{j\ell} C_{n-\ell-1-2j}^{\ell+3/2}(x), \tag{28}
\]

where

\[
\beta_{j\ell} = \frac{(n - 2j - 1/2) \Gamma(\ell + 1/2) \Gamma(j + 1/2) \Gamma(n - j)}{j! \Gamma(\ell + 1) \Gamma(1/2) \Gamma(n - j + 1/2)}, \tag{29}
\]

\[
\gamma_{j\ell} = \frac{(n - 2j + 1/2) \Gamma(\ell + 3/2) \Gamma(j - 1/2) \Gamma(n - j)}{j! \Gamma(\ell + 1) \Gamma(-1/2) \Gamma(n - j + 3/2)}. \tag{30}
\]

Then, using the orthogonality property of the ultraspherical polynomials, we end up with the single summations:

\[
\int_{-1}^{1} (1 - x^2)^{\ell} [C_{n-\ell-1}(x)]^2 \, dx = \sum_{j=0}^{[(n-\ell-1)/2]} \left( \frac{2^{-\ell} \beta_{j\ell}}{\Gamma(\ell + 1/2)} \right)^2 \frac{\pi \Gamma(n + \ell + 2j)}{(n - 2j - 1/2)(n - \ell - 2j - 1)!}.
\]

and

\[
\int_{-1}^{1} (1 - x^2)^{\ell+1} [C_{n-\ell-1}(x)]^2 \, dx = \sum_{j=0}^{[(n-\ell-1)/2]} \left( \frac{2^{1-\ell} \gamma_{j\ell}}{\Gamma(\ell + 3/2)} \right)^2 \frac{\pi \Gamma(n + \ell + 2j + 2)}{(n - 2j + 1/2)(n - \ell - 2j - 1)!}.
\]

Applying these to (18) we obtain

\[
\left\langle \frac{\hbar \kappa}{\mathcal{P}} \right\rangle_{n\ell} = \frac{2n(n - \ell - 1)!}{(n + \ell)!} \left( \frac{\Gamma(\ell + 1)}{\Gamma(\ell + 1/2)} \right)^2 \frac{[n-\ell-1/2]}{\Gamma(n - \ell - 2j)} \sum_{j=0}^{[(n-\ell-1)/2]} \frac{2 \beta^2_{j\ell}}{n - 2j - 1/2} \frac{(n + \ell - 2j)(n + \ell + 1 - 2j) \gamma^2_{j\ell}}{(2\ell + 1)^2(n - 2j + 1/2)}. \tag{31}
\]

Substituting the expressions for \( \beta \) and \( \gamma \) from (29) and (30) respectively, we can finally reduce the answer to

\[
\left\langle \frac{\hbar \kappa}{\mathcal{P}} \right\rangle_{n\ell} = \frac{2n(n - \ell - 1)!}{\pi(n + \ell)!} \left( \frac{\Gamma(j + 1/2) \Gamma(n - j)}{\Gamma(j + 1) \Gamma(n - j + 1/2)} \right)^2 \frac{\Gamma(n + \ell - 2j)}{\Gamma(n - \ell - 2j)} \left( 2n - 4j \right) \left( \frac{(n + \ell - 2j)(n + 1/2 - 2j)(n + \ell + 1 - 2j)}{(2j - 1)^2(2n - 2j + 1)^2} \right). \tag{32}
\]
| \( \ell \) \( \backslash \) \( n \) | 1     | 2     | 3     | 4     | 5     | 6     |
|--------|------|------|------|------|------|------|
| 0      | 32   | 256  | 2144 | 1024 | 89088| 1172224|
| 1      | 128  | 356  | 312  | 3465 | 46945| 895344 |
| 2      | 4096 | 16384| 29688| 21856256|
| 3      | 525  | 16384| 29688| 21856256|
| 4      | 525  | 16384| 29688| 21856256|
| 5      | 2205 | 5405 | 85995| 267392 |

Table 1: Calculated values of \( \langle 2\pi\hbar\kappa/P \rangle_{n\ell} \) for principal quantum number \( n \) running from 1 to 6, as given by (32).

We have not succeeded in simplifying this any further, except for the earlier simple cases. In Table 1, we have provided the first few expectation values of \( 2\pi\hbar\kappa/P \) (for \( n \) and \( \ell \) up to 6) as derived from (32). Remember that \( \kappa = 1/na \), where \( a \) is the Bohr radius.

\section{4 Sum rules and integral representation}

There exists an interesting set of sum rules for \( \langle \hbar\kappa/P \rangle_{n\ell} \) which hail from a particular form of the addition theorem for Gegenbauer polynomials (see [7], §5.3), and which produce a neat integral representation. Start with the particular 4-dimensional case

\[ C_{n-1}^{1}(\cos^2\theta + \sin^2\theta \cos \psi) = \sum_{\ell=0}^{n-1} \frac{(2\ell + 1)(\ell!)^2\Gamma(n-\ell)}{\Gamma(n+\ell+1)} (2\sin\theta)^{2\ell} \times [C_{n-\ell-1}^{\ell+1}(\cos \theta)]^2 P_{\ell}(\cos \psi). \]

On putting \( \cos \theta = x \), we find that the rhs has a close connection with the rhs of eq (18) and so recognize that

\[ \int_{-1}^{1} (1 + x)^2 C_{n-1}^{1}(x^2 + (1 - x^2) \cos \psi) \, dx = \frac{\pi}{2n} \sum_{\ell=0}^{n-1} (2\ell + 1) P_{\ell}(\cos \psi) \langle \hbar\kappa/P \rangle_{n\ell}. \]

(33)
Since \( C_{n-1}^1(y) = U_{n-1}(y) \), we can simplify this result to

\[
\sum_{\ell=0}^{n-1} (2\ell + 1) P_\ell(y) \langle \frac{\hbar \kappa}{P} \rangle_{n\ell} = \frac{2n}{\pi} \int_{-1}^{1} (1 + x^2) U_{n-1}(x^2 + (1 - x^2)y) \, dx.
\]  
(34)

To obtain the sum rules, simply set \( y = 1 \) and \( y = -1 \):

\[
\sum_{\ell=0}^{n-1} (2\ell + 1) \langle \frac{\hbar \kappa}{P} \rangle_{n\ell} = \frac{2n^2}{\pi} \int_{-1}^{1} (1 + x^2) \, dx = \frac{16n^2}{3\pi},
\]  
(35)

\[
\sum_{\ell=0}^{n-1} (2\ell + 1)(-1)^\ell \langle \frac{\hbar \kappa}{P} \rangle_{n\ell} = \frac{2n}{\pi} \int_{-1}^{1} (1 + x^2) U_{n-1}(2x^2 - 1) \, dx.
\]  
(36)

In order to evaluate the rhs of eq (36) first define \( J_n = \int_{-1}^{1} U_{n}(2x^2 - 1) \, dx \). The rhs of (36) can then be rewritten as \( (J_n + 6J_{n-1} + J_{n-2})/4 \), so it only remains to determine \( J_n \). This can be done via an easily established recurrence relation, namely \( J_n + J_{n-1} = 2/(2n + 1) \). Hence we deduce that

\[
2J_n = \psi(n/2 + 5/4) - \psi(n/2 + 3/4) + (-1)^n \pi.
\]

Therefore

\[
\sum_{\ell=0}^{n-1} (2\ell + 1)(-1)^\ell \langle \frac{\hbar \kappa}{P} \rangle_{n\ell} = \frac{n}{\pi} \left[ \psi(n + 3/4) - \psi(n + 3/4) + \frac{4n}{4n^2 - 1} + (-1)^{n-1} \pi \right].
\]  
(37)

Finally, on multiplying (34) by a Legendre polynomial in \( y \) and integrating over \((-1,1)\), we obtain a neat double integral representation for the expectation value. Thus

\[
\langle \frac{\hbar \kappa}{P} \rangle_{n\ell} = \frac{n}{\pi} \int_{-1}^{1} (1 + x^2) \left[ \int_{-1}^{1} P_\ell(y) U_{n-1}(x^2 + (1 - x^2)y) \, dy \right] \, dx.
\]  
(38)

One may verify in particular cases that this produces the same results as the series (32) but, more significantly, it allows us to obtain a series representation of \( \langle \frac{\hbar \kappa}{P} \rangle_{n\ell} \), which is different from (32).

To arrive at this new result, we make use of the fact (see [7], §5.7.2) that

\[
U_{n-1}(z) = \sqrt{\pi} \sum_{j=0}^{n-1} \frac{(-1)^j(n + j)!(1 - z)^j}{j!(n - j - 1)!2^{j+1}\Gamma(j + 3/2)}.
\]
and notice the factorization, $1 - (x^2 + (1-x^2)y) = (1-x^2)(1-y)$. Thus (38) factorizes into two parts. The integral over $x$ is easily done, but the integral over $y$ is a bit harder (requiring Rodrigues’ formula and an integration by parts). Carrying out the necessary manoeuvres we end up with

$$\langle \frac{\hbar \kappa}{P} \rangle_{n^\ell} = \sum_{j=0}^{n-\ell-1} \frac{(-1)^j n (\ell + j + 2)(n + \ell + j)!(\ell + j)!}{(n - \ell - j - 1)!(2\ell + j + 1)!j!\Gamma(\ell + j + 3/2)\Gamma(\ell + j + 5/2)}.$$

This is more compact than the series (32).

## 5 Asymptotic behaviour

There are 3 regimes to consider for large $n$ which we shall look at in turn.

### 5.1 $\ell/n \ll 1$

Returning to eq (18) we may replace $\Gamma(n - \ell)/\Gamma(n + \ell + 1)$ asymptotically by $n^{-2\ell-1}$ and use the approximation (see [7], §5.3.3),

$$C_{n,\ell-1}^{\ell+1}(\cos 2\theta) \sim \frac{n^\ell \cos(2n\theta - \pi(\ell + 1/2))}{2^{\ell+1}(\sin 2\theta)^{\ell+1}}, \quad n \gg 1, \ 0 < \theta < \pi/2.$$

This tells us that

$$\langle \frac{\hbar \kappa}{P} \rangle_{n^\ell} \sim \lim_{\epsilon \to 0^+} \frac{16}{\pi} \int_{\epsilon}^{\pi/2-\epsilon} \frac{\cos^4 \theta \cos^2(2n\theta - \pi(\ell + 1/2))}{\sin 2\theta} d\theta,$$

assuming the integral exists. Hence we obtain the asymptotic difference between two $\ell$ values differing by two:

$$\langle \frac{\hbar \kappa}{P} \rangle_{n^{\ell+1}} - \langle \frac{\hbar \kappa}{P} \rangle_{n^{\ell-1}} \sim \lim_{\epsilon \to 0^+} \frac{16}{\pi} \int_{\epsilon}^{\pi/2-\epsilon} \frac{d\theta}{\sin 2\theta} \frac{\cos^4 \theta}{\sin 2\theta} \times \left[ \cos^2(2n\theta - \pi(\ell + 2)/2) - \cos^2(2n\theta - \pi\ell/2) \right] = 0.$$

But we have already shown in (24) that $\langle \hbar \kappa/P \rangle_{n^\ell} \sim 4\psi(n+1/2)/\pi$ for $\ell = 0$, from which we conclude that

$$\langle \frac{\hbar \kappa}{P} \rangle_{n^\ell} \sim 4\psi(n + 1/2)/\pi \quad (40)$$

for $n \gg 1$ and modest values of $\ell$. This result diverges logarithmically like $(4 \log n)/\pi$ as $n \to \infty$. 

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5.2 \( \ell/n \) near 1

In this case return to the series (32) and put \( n = \ell + 1 + \delta \) where \( \delta/n \ll 1 \). Making use of the asymptotic approximation,

\[
\lim_{z \to \infty} \frac{\Gamma(z + a)}{\Gamma(z + b)} \sim z^{a-b} \left[ 1 + \frac{1}{2z} (a-b)(a+b+1) + O\left(\frac{1}{z^2}\right) \right],
\]

the sum collapses to

\[
\langle \frac{\hbar \kappa}{P} \rangle_{n-1-\delta} \sim \frac{1}{\pi} \sum_{j=0}^{[\delta/2]} (2n)^{-2j} \frac{\Gamma(1+\delta)}{\Gamma(1+\delta-2j)} \left( \frac{\Gamma(j+1/2)}{\Gamma(j+1)} \right)^2 \left[ 2 - \frac{1}{(2j-1)^2} + O\left(\frac{1}{n}\right) \right].
\]

Thus \( j = 0 \) is the dominant term in the expansion; this is multiplied by a subdominant factor of order \( 1/n \) via (32), producing the final estimate,

\[
\langle \frac{\hbar \kappa}{P} \rangle_{n-1-\delta} \sim 1 + \frac{3(2\delta + 1)}{4n} + O\left(\frac{1}{n^2}\right).
\]

This agrees with the results of section 3.2 where the cases \( \delta = 0 \) and 1 were studied.

5.3 \( \ell/n \) is finite

This regime is the trickiest to deal with, interpolating between (40) and (42) as it does. Although we have not succeeded in obtaining the analytical dependence on \( \lambda \equiv \ell/(n-1) \), one may readily establish numerically that the sum (39) tends to a constant in the limit of large \( n \) and increases as \( \lambda \) approaches zero; for instance when \( \lambda = 1/2 \) the value is 1.975; when \( \lambda = 1/4 \), the value is 2.88; when \( \lambda = 1/8 \), the value is 3.77, etc. This dependence would appear to be logarithmic as is indicated by (24).

6 Conclusions

In this paper we have principally concentrated on the evaluation of \( \langle 1/P \rangle \) — a challenging problem — because it has special significance for Born reciprocity, but the methods we have used can no doubt be extended to general functions of momentum via eqs (16) and (17). In fact such calculations have
been carried out in [11] for expectation values of $P^N$ and log $P$ to which the reader is referred. At any rate, the conclusion of our analysis is that the $1/p$ perturbation has an increasingly disruptive effect on the higher $n$ states having the lowest $\ell$ (the dependence is logarithmic in $n$). This hails from the full effective potential [4] which shows a maximum below zero energy, at $E_0 = bL - 2\alpha\sqrt{bL}$, where $L$ signifies the classical angular momentum.

References

[1] M. Born, Rev. Mod. Phys. 21, 463 (1949); H.S. Green, Nature 163, 208 (1949)

[2] S.G. Low, J. Phys. A35, 5711 (2002); P.D. Jarvis and S.O. Morgan, Found. Phys. Lett. 19, 501 (2006); J. Govaerts, P.D. Jarvis, S.O. Morgan and S.G. Low, J.Phys. A40, 12095 (2007)

[3] A. Messiah, ”Quantum Mechanics Vol I”, Wiley & Sons, NY (1961)

[4] R. Delbourgo and D. Lashmar, Found. Phys. 38, 995 (2008)

[5] B. Podoslky and L. Pauling, Phys. Rev. 34, 109 (1929)

[6] F.A. Hylleraas, Zeit. Phys. 74, 216 (1932)

[7] W. Magnus, F. Oberhettinger and R.P. Soni, ”Formulas and Theorems for Special Functions of Mathematical Physics”, Springer-Verlag, NY (1966)

[8] C.F. Dunkl, Anal. and Appl. 1, 177 (1957)

[9] V.I. Fock, Zeit. Phys. 98, 145 (1935)

[10] G. Szegö, ”Orthogonal Polynomials”, Amer. Math. Soc. Coll. Publ., Vol 23 (4th edition), Providence (1975)

[11] W. VanAssche, R.J. Yanez, R. Gonzalez-Ferez and J.S. Dehesa, Phys. Rev. 41, 6600 (200).