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# Connection between the spectrum and the moments of the ground-state density in *N*-dimensional space

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**Abstract**
We show that a series of recurrent inequalities derived in $N = 3$ have the same formal expressions in any dimension $N \geqslant 2$. They are derived from the multipole sum rules, and provide us with upper bounds for the moments of the ground-state density depending only on the lowest multipole excitation energy. These bounds are transformed into approximate recurrent relations by means of an empirical correction factor. The $1/r$ potential and the harmonic oscillator play a key role in establishing this factor, which is exact for these two potentials by construction. For a large class of potentials, we show that this factor tends to 1 as $N \rightarrow \infty$. In such cases, at the large-$N$ limit, the lowest state for each multipole excitation exhausts the sum rule. It thus acquires the characteristics of the one-phonon excitation typical of the harmonic oscillator.

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The extension of physical problems to higher-dimensional space is of current interest [1–10]. It has the virtue of underlining general mathematical features [11–17], group theory [18–20] and supersymmetry [21–23]. Work on quantum gravity theories in extra dimensions has also been reported [24–29]. Application to quantum mechanics goes back at least to the 1980s [30, 31].

The purpose of this paper is to point out an interesting feature of the Schrödinger equation in the large-*N* limit. It concerns a series of recurrent relations first derived in $N = 3$ [32, 33]. We shall show that they have the same formal expression in any dimensional space $N \geqslant 2$. Starting from multipole sum rules, we obtain a recurrent series of strict upper bounds for the moment of the ground state depending on the energy differences between the ground state and each of the lowest multipole excitation energy. This part generalizes the original Bertlmann–Martin inequality [34] linking the ground-state mean-square radius to the lowest dipole excitation energy in $N = 3$.

These recurrent relations can be transformed into recurrent approximate relations by introducing multiplicative correction factors. These last are not known *a priori*, and we may wonder what is gained in such a purely formal writing. In $N = 3$, however, it turns out that an

empirical form has been proposed byBertlmann and Martin [34]. It is exact for the harmonic oscillator and the Coulomb potential by construction. It is quite efficient for a large class of potentials, and may be use successfully in iterative procedures [32, 33].

Considering the $N$-dimensional Schrödinger equation, the only two potentials admitting analytical solutions for $N \geqslant 2$ are the harmonic oscillator and the $1/r$ potentials. This situation provides us with a chance to investigate the approximate recurrent relations as a function of $N$. The harmonic oscillator case being trivial, we shall first recall the $1/r$ potential solutions in the $N$-dimensional space. It will fix the framework, notations and units.

## 1. Schrödinger equation for the $1/r$ potential in $N$-dimensional space

The Coulomb potential in $N$-dimensional space is of special interest [35, 36]. Here we shall merely speak of the $1/r$ potential, where

$$r = \left[ \sum_{i=1}^{N} x_i^2 \right]^{1/2}. \tag{1}$$

In $N = 3$, this is nothing but the Coulomb potential. In other dimensions it can represent a many-body force, as advocated by Khare and Bhaduri [37] for the one-dimensional three-body problem:

$$1/r \propto \left[ \sum_{i \neq j} (x_i - x_j)^2 \right]^{-1/2}, \tag{2}$$

when expressed in the centre-of-mass system.

The solutions of the Schrödinger equation for the $1/r$ potential in $N$-dimensional space are known [35]. They are recalled here for the sake of being self-contained and for fixing the notations. Use is made of polar coordinates. Units are $\hbar = 2m = 1$. The variable separation leads to

$$\Psi(\vec{r})_{n,[L]} = \psi(r)_{n,L} Y_{[L]}(\Omega). \tag{3}$$

The $Y_{[L]}(\Omega)$ are eigenfunctions of the angular part of the Laplacian $\triangle_\Omega$. Here $[L]$ denotes the ensemble of quantum numbers required to specify the angular part of the eigenfunction. Since we shall consider potentials depending only on the radial coordinate, the bound states will be labelled by $\{n, L\}$: $n$ is the number of nodes of the radial wavefunction, $L$ is the grand orbital quantum number, which reduces to the orbital momentum in $N = 3$ and to the azimuthal quantum number in $N = 2$. The lowest Regge trajectory states have $n = 0$.

The radial equation reads

$$\left[ -\frac{\partial^2}{\partial r^2} - \frac{(N-1)}{r} \frac{\partial}{\partial r} + \frac{L(L+N-2)}{r^2} + V(r) \right] \psi(r)_{n,L} = E_{n,L} \psi(r)_{n,L}. \tag{4}$$

Here, $V(r) = -\lambda/r$. Bound states exist for $\lambda > 0$.

The ansatz $\psi_{n,L}(r) = r^L e^{-\alpha_{n,L} r} f_{n,L}(r)$ together with the variable change $z = 2\alpha_{n,L} r$ leads to the Laplace equation

$$\left[ z \frac{\partial^2}{\partial z^2} + [2L + N - 1 - z] \frac{\partial}{\partial z} - \left[ L + \frac{N-1}{2} - \frac{\lambda}{2\alpha_{n,L}} \right] \right] f_{n,L}(z) = 0. \tag{5}$$

It is solved by means of confluent hypergeometric functions. The quantum mechanically acceptable solution leads to (up to normalization factors)

$$\psi_{n,L}(r) = r^L \, e^{-\alpha_{n,L}r} \mathcal{L}_n^{(2L+N-2)}(2\alpha_{n,L}r) \tag{6}$$

with

$$\alpha_{n,L} = \frac{\lambda}{2L + 2n + N - 1}. \tag{7}$$

Here, $\mathcal{L}_n^{(2L+N-2)}$ denotes Laguerre polynomials. The energy discrete spectrum is given by

$$E_{n,L} = -\alpha_{n,L}^2. \tag{8}$$

## 2. The recurrent relations

The idea of connecting the moments of the ground-state density to the lowest multipole excitation energy originates in the Bertlmann–Martin inequality [34]. This last is obtained by taking an underestimate of the dipole sum rule. Its generalization uses the same procedure applied to each multipole sum rule. We sketch the derivation in $N$-dimensional space as follows.

Consider the Hamiltonian $H(r) = p^2 + V(r)$, $V(r)$ local, and the operator

$$Q_L = r^L Y_{[L,0]} \tag{9}$$

(all angular quantum numbers $= 0$ except the grand orbital $L$). We have

$$\triangle_\Omega Y_{[L,0]} = L(L + N - 2)Y_{[L,0]}, \qquad \triangle Q_L = 0. \tag{10}$$

The double commutator of $H$ and $Q_L$ reads

$$[[H, Q_L], Q_L] = -2\vec{\nabla} Q_L \cdot \vec{\nabla} Q_L. \tag{11}$$

Its ground-state average provides us with the following multipole sum rules:

$$\sum_{n=0}^{\infty}[E_{n,L} - E_{0,0}]|\langle n, L|Q_L|0, 0\rangle|^2 = L(2L + N - 2)\langle r^{2L-2}\rangle. \tag{12}$$

(To simplify notation $\langle A \rangle$ denotes the ground-state average of $A$.)

The sums are clearly underestimated by setting $E_{n,L} = E_{0,L}$. Thus, by factorizing $E_{0,L} - E_{0,0}$ and using closure, we get an ensemble recurrent inequalities

$$\langle r^{2L}\rangle \leqslant \frac{L(2L + N - 2)}{E_{0,L} - E_{0,0}}\langle r^{2L-2}\rangle. \tag{13}$$

Note that relations (13) turn to equalities when the lowest excited state for each multipole exhausts its sum rule, which occurs for the harmonic oscillator.

These recurrent inequalities establish strict bounds on the ground-state moments, independently on the potential, within the class of local potentials depending only on $r$. Furthermore, whereas the number of valid bounds is unlimited for the case of potentials admitting an infinite number of bound states, such as power-law potentials, for short-range potentials it is restricted to the actual bound states. We recall briefly that short-range potentials are so defined that they possess a finite number of bounds states, and a bound $(n, L)$ state does not exist for coupling constant below a critical value. This critical value depends on $L, n$ and $N$.

The usefulness of relations (13) is essentially link to their degree of saturation. In other words, they are efficient if, for each multipole, the lowest state exhaust a sizeable amount of the sum rule (12). Inequalities (13) can be transformed into approximate recurrence relations by

applying a multiplicative correction factor. *A priori*, this factor is dependent on the potential, and nothing is gained. However, as stated in the introduction, it has been shown, in $N = 3$, that a simple empirical expression is very efficient for a wide class of potentials [32, 33]. It has been constructed in a way to be exact for the Coulomb potential and the harmonic oscillator. It can be used as the first step of an iterative procedure. Consequently, it is very natural to check whether this form is valid in any $N \geqslant 2$.

The approximate expressions read

$$\langle r^{2L} \rangle \approx \frac{L(2L + N - 2)}{E_{0,L} - E_{0,0}} \langle r^{2L-2} \rangle \left[ 1 - \frac{L}{N + 2L - 1} C(L, N) \right], \tag{14}$$

with

$$C(L, N) = \left[ \frac{E_{L,0} + E_{0,0} - 2E_{0,L}}{E_{L,0} - E_{0,0}} \right]^2. \tag{15}$$

In order to test (14) and (15) for the $1/r$ potential in $N \geqslant 2$ dimensions, we note that the ground state moments are given by

$$\langle r^k \rangle = \frac{1}{(2\alpha_{0,0})^k} \frac{\Gamma(N + k)}{\Gamma(N)}. \tag{16}$$

By using this expression together with the energy eigenvalues (8), the recurrent relations (14) are found to be indeed equalities. Actually, it is a trivial matter to check that equation (15) yields $C(L, N) = 1$ and $0 \ \forall N, L$ for the $1/r$ potential, and the harmonic oscillator, respectively. This result is independent of the coupling constant $\lambda \ (\lambda > 0)$. Consequently, for these two potentials, equation (14) is a series of exact recurrent relations. Moreover, as $N \to \infty$, $1 - \frac{L}{N+2L-1} C(L, N) \to 1$. It means that for the $1/r$ potential in the large-$N$ limit, the lowest multipole excited state exhausts the sum rule, a characteristic property of the harmonic oscillator.

The question is to know whether the same situation occurs as in $N = 3$, i.e. if relations (14) are useful for a large class of potentials. It clearly amounts to the behaviour of $C(L, N)$ as a function of $N$, which is linked to the variation of $E_{n,L}$ with $N$. In the Schrödinger equation (4), consider $N$ as a continuous parameter. The Feynman–Hellmann theorem [39, 40] implies

$$\frac{\partial E_{n,L}}{\partial N} = \langle \Psi_{n,L}(N, r) | \frac{\partial H(N)}{\partial N} | \Psi_{n,L}(N, r) \rangle. \tag{17}$$

It leads to

$$\frac{\partial E_{n,L}}{\partial N} = \langle \Psi_{n,L}(N, r) | - \frac{1}{r} \frac{\mathrm{d}}{\mathrm{d}r} + \frac{L}{r^2} | \Psi_{n,L}(N, r) \rangle = \frac{N + 2L - 2}{2} \langle r^{-2} \rangle_{n,L}. \tag{18}$$

At first glance, this relation does not bring any simplification, since it depends on $\langle r^{-2} \rangle_{n,L}$. However, we note that for fixed $N$, we have

$$\frac{\partial E_{n,L}}{\partial L} = (N + 2L - 2) \langle r^{-2} \rangle_{n,L}. \tag{19}$$

In other words, the variation of $C(L, N)$ with $N$ can be inferred from its variation with $L$ in $N = 3$. From previous works, we know that in $C(L, 3)$ reaches a limit as $L$ increases [32, 33]. Moreover, let us consider the reduced wavefunction

$$u_{n,L}(r) = r^{(N-1)/2} \Psi_{n,L}(r). \tag{20}$$

It is solution of

$$\left[ -\frac{\mathrm{d}}{\mathrm{d}r^2} + \frac{L(L + N - 2)}{r^2} + \frac{N^2 - 4N + 3}{4r^2} + V(r) \right] u_{n.L}(r) = E_{n,L} u_{n,L}(r). \tag{21}$$

**Table 1.** For power-law potentials, the ratios $R_1$ and $R_{1c}$ are displayed as a function of $\nu$. They are the ratio between the upper bound (13) and the approximate expression (14) to the exact value of $\langle r^2 \rangle$, respectively.

| $\nu$ | $N = 3$ | | $N = 5$ | |
|---|---|---|---|---|
| | $R_1$ | $R_{1c}$ | $R_1$ | $R_{1c}$ |
| $-1.5$ | 0.50 | 0.70 | 0.59 | 0.78 |
| $-1.0$ | 0.75 | 1.00 | 0.83 | 1.00 |
| $-0.5$ | 0.88 | 0.97 | 0.93 | 1.00 |
| 0.5 | 0.98 | 1.00 | 0.99 | 1.00 |
| 1.0 | 0.99 | 1.00 | 1.00 | 1.00 |
| 2.0 | 1.00 | 1.00 | 1.00 | 1.00 |

We remark that $N$ is acting as a centrifugal barrier pushing the solutions towards larger $r$ as $N$ increases. Thus, the moment

$$\langle r^{-2} \rangle_{n,L} = \int_0^\infty u_{n,L}^2(r) \frac{\mathrm{d}r}{r^2} \tag{22}$$

is expected to decrease with $N$, quite generally.

Consequently, we conclude that $\frac{1}{(N+2l-1)} C(L, N)$ is decreasing with increasing $N$ for the large class of potentials studied previously in $N = 3$ [32, 33].

For illustrative purpose, we have tested these properties on $C(1, N)$, by solving the Schrödinger equation numerically for a few power-law potentials. They are defined by

$$V(r) = \mathrm{sign}(\nu) \lambda r^\nu, \qquad \nu > -2. \tag{23}$$

First, we have verified for $\nu = -1.5$ and $\nu = 1$ that $C(1, N)$ is slowly decreasing as $N$ increases from 3 to 7. Secondly, for $N = 3$ and 5, we display in table 1 the variation of $R_1$, the ratio between the upper bound (13) and the exact value, as well as $R_{1c}$, the ratio between the approximate value (14) and the exact value as a function of $\nu$. Note that $R_1$ is also roughly indicating the fraction of the sum rule which is taken by the lowest dipole excited state.

These results underline a nice property of the solution of the Schrödinger equation for local potential in the large-$N$ limit. Because of this tendency of (13) to saturate the bounds as $N$ increases, the system behaves like an harmonic oscillator: the multipole excitations take the characteristic of the one-phonon excitations. Furthermore, the precise determination of the correction factors becomes less acute.

Relations (14) and (15) can be used in two ways. If the ground-state solution is known analytically, part of the spectrum ($E_{L,0} L \neq 0$) can be estimated in a simple way. If the $E_{L,0}$ eigenvalues are measured, the method yields the ground-state moments and constitutes a first step towards the determination of the ground-sate wavefunction and the potential. In the latter, the accuracy depends on the number of measured levels. Examples in $N = 3$ give an overview of what can be achieved [32, 33, 38] (see in particular the application to the $^{208}$Pb muonic atom [38]).

At a more general level, relations (14) emphasize that the energies of the $(0, L)$ states are the most efficient ones to search for the shape of a potential when the spectrum is known.

## 3. Conclusions

A series of recurrent relations have been derived in $N$-dimensional space from the multipole sum rules. They connect the moments of the ground-state density to the lowest multipole

excitation energy. Their formal expression is the same as those previously derived in $N = 3$. They provide us with upper bounds to the moments of the ground-state density for any potential having bound states.

These bounds are transformed into approximate recurrent relations by introducing a correction factor. In $N = 3$, this last has been established on empirical grounds and constructed in a way to yield the exact values for the $1/r$ and the harmonic oscillator potentials. It constitutes a useful approximation in many cases [32, 33], with the exception of the weakly bound states of short range potentials. We have shown that the correction factor can be constructed in the same way $\forall N \geqslant 2$. Its importance diminishes as $1/N$, at least for a wide class of potentials. The case of short range potentials admitting a limited number of bound states deserves further studies, but it lies outside the scope of the present work.

In the limit $N \to \infty$, an interesting consequence of the decrease of the correction factor with $N$ is that the lowest excited state has a tendency to exhaust the sum rule, for each multipole excitation. In this respect, the situation is analogous to the one-phonon excitation of the harmonic oscillator. It underlines a new interesting property of the solutions of the Schrödinger equation in the large-$N$ limit for local potentials.

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