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## Relative Fisher information for Morse potential and isotropic quantum oscillators

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E-mail: [yamano@amy.hi-ho.ne.jp](mailto:yamano@amy.hi-ho.ne.jp)**Keywords:** relative Fisher information, isotropic quantum harmonic potential, Morse potential, associated Laguerre polynomials, associated Legendre polynomials**Abstract**

The relative Fisher information associated with quantum-mechanical states for two prototypical models is presented; the radial density functions that characterize the Morse oscillator and the  $d$ -dimensional isotropic quantum oscillators are analyzed in terms of this relative information by specifying the ground state as the reference. We find that the information increases as the eigenvalue (i.e., the degree of the associated Laguerre polynomials) increases for the Morse density function, but for the isotropic quantum harmonic models, it decreases with the dimension and increases almost linearly with the increasing quantum numbers. We present also the explicit expression for the information associated with the angular density as a function of the orbital quantum number and the magnetic quantum number for the three-dimensional isotropic quantum oscillator.

**1. Introduction**

The measure for quantifying a spread of the single-particle density associated with a quantum wave function in position and momentum spaces has traditionally been the Shannon information entropy. However, the calculations of entropy integrals of the orthogonal polynomials such as the Laguerre, the Gegenbauer polynomials and the spherical harmonics functions that appear in the wave functions have been obstacles for obtaining the exact expression of the information theoretical content for systems described by quantum mechanics. These remain open problems to date [1, 2]. On the other hand, subsequently, the Fisher information [3, 4] has attracted interests from a number of researchers as an alternative measure of localization of the single-particle density in the analysis of atomic systems (e.g. [5, 6]). The Fisher information measure represents a measure of localization of density in that it contains a gradient of the functional; the higher value indicates more concentration of the density. It also gives an information on the nodal structure of the associated wave functions [6].

For most cases in physical potentials, it is hard to obtain analytical solutions for the corresponding Schrödinger equations. However, quantum mechanical systems under the harmonic potential, the Morse potential, and the Coulomb potential are one of several cases that allow us to treat them analytically and those wave functions contain the associated Laguerre polynomials in common. Extensive studies on some analytical determinations of integrals of the associated Laguerre polynomials already exist in the literature (e.g. [1, 2, 7]). In this paper, we concentrate our task on the calculations of information content arising from the radial part of the complete wave functions. This is verified because the radial wave function is required to be normalized to unity, meaning the density of radial direction. Since the radial wave functions in the above-mentioned potentials are largely controlled by the properties of the associated Laguerre polynomials, it is natural to think that the information content of the system owes a great deal to their properties. In a previous work, we considered the relative Fisher information of the hydrogen-like atoms by setting the  $1s$  orbital as a reference state [8]. The relative Fisher information is one of similarity or distance measures [9], but it is so far underrepresented in utility compared to the Fisher information (see e.g. [10] for the definition and [11, 12] for some roles in physical

situations and [13, 14] for atomic systems). In this study, we consider this information measure in the position space only, because the corresponding momentum wave function that can be obtained from the Fourier transform of the position-space wave function takes the same form due to a duality property; by the replacement of the parameter  $k \leftrightarrow 1/k$ , which controls the strength of the harmonic potential of the form  $k^2 r^2/2$ .

This paper is organized in the following: In the next section, we introduce the relative Fisher information and define notations. In section 3, we calculate it for systems governed by the Morse potential by setting the ground state as the reference and investigate the behavior. Then, we provide the exact expression of the information measure for the radial density of the isotropic quantum oscillator in D-dimension. The behavior as functions of the dimension and quantum numbers are investigated in section 4.1. In section 4.2, as a function of the quantum numbers, the analytical form of the information measure associated with the angular density for a three-dimensional quantum harmonic potential system are presented. Summary and conclusion are given in the last section.

## 2. Relative Fisher information as a measure of similarity

The relative Fisher information between two density functions specified by parameter sets  $\{\mu\}$  and  $\{\nu\}$  in coordinate  $\xi$  is defined as

$$\int_0^\infty \rho_{\{\mu\}}(\xi) \left| \frac{d}{d\xi} \ln \left( \frac{\rho_{\{\mu\}}(\xi)}{\rho_{\{\nu\}}(\xi)} \right) \right|^2 d\xi. \quad (1)$$

The labels  $\{\mu\}$  and  $\{\nu\}$  may represent any set of quantum numbers and we refer  $\rho_{\{\nu\}}(\xi)$  to a reference state; as we employ it below, we set the ground state density as the reference state for two classes of quantum mechanical models. The information contained in the densities of arbitrary excited states is examined, by which we can measure how the family of excited states are similar to the ground state density. We hereafter write the definition equation (1) as  $d_F[\{\mu\}:\{\nu\}]$  in the present paper.

## 3. Relative Fisher information for Morse potential systems

The Schrödinger equation for a particle with a mass  $\mathcal{M}$  under the Morse potential [15] is provided as (e.g. [16]),

$$-\frac{\hbar^2}{2\mathcal{M}}\psi''(x) + C(1 - e^{-bx})^2\psi(x) = E\psi(x), \quad (2)$$

where  $E$  is energy eigenvalues, and  $C$  and  $b$  are constants that control the shape of the potential. It reduces to the following differential equation by changing variables as  $y = bx$  and by scaling the energy as  $\epsilon = E/C$  with  $\lambda = \sqrt{2\mathcal{M}C}/\hbar$ :

$$\psi''(y) + \lambda^2\{\epsilon - (1 - e^{-y^2})\}\psi(y) = 0. \quad (3)$$

The normalized eigensolutions specified by  $\lambda$  are provided by Morse himself [15] and by the subsequent numerous studies (e.g., [16]):

$$\psi_{\lambda,n}(\xi) = N_{\lambda,n} \xi^{\lambda-n-\frac{1}{2}} e^{-\frac{\xi}{2}} L_n^{(2\lambda-2n-1)}(\xi), \quad N_{\lambda,n} = \sqrt{\frac{\Gamma(n+1)(2\lambda-2n-1)}{\Gamma(2\lambda-n)}} \quad (4)$$

where the variable  $\xi$  is introduced by  $\xi = 2\lambda e^{-y}$  ( $0 \leq \xi < \infty$ ) and  $L_n^{(\alpha)}(\xi)$  is the associated (general) Laguerre polynomials of degree  $n$  and order  $\alpha$ , which is defined by the Rodrigues' formula:

$$L_n^{(\alpha)}(\xi) = \frac{e^{\xi}\xi^{-\alpha}}{n!} \frac{d^n}{d\xi^n} (e^{-\xi}\xi^{n+\alpha}), \quad (\alpha > -1). \quad (5)$$

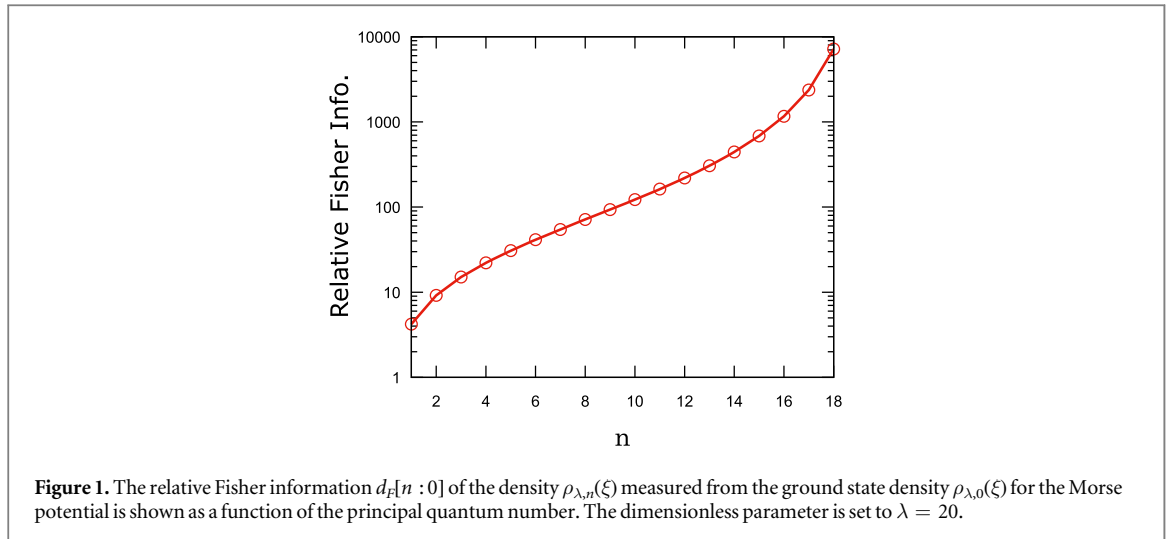
This polynomial satisfies an orthogonality relation [17]:

$$\int_0^\infty \xi^\alpha e^{-\xi} L_n^{(\alpha)}(\xi) L_m^{(\alpha)}(\xi) d\xi = \begin{cases} \frac{\Gamma(\alpha+n+1)}{n!} & (m=n) \\ 0 & (m \neq n) \end{cases}. \quad (6)$$

By the standard interpretation of wave functions, the family of the associated density functions is the square of the modulus of the wave function  $\psi_{\lambda,n}(\xi)$  and thus it is given as

$$\rho_{\lambda,n}(\xi) = |\psi_{\lambda,n}(\xi)|^2 = N_{\lambda,n}^2 \xi^{2\lambda-2n-1} e^{-\xi} [L_n^{(2\lambda-2n-1)}(\xi)]^2. \quad (7)$$

By the definition equation (1), the relative Fisher information measured from the ground state density  $\rho_{\lambda,0}(\xi) = (2\lambda-1)\xi^{2\lambda-1}e^{-\xi}/\Gamma(2\lambda)$ :



**Figure 1.** The relative Fisher information  $d_F[n : 0]$  of the density  $\rho_{\lambda,n}(\xi)$  measured from the ground state density  $\rho_{\lambda,0}(\xi)$  for the Morse potential is shown as a function of the principal quantum number. The dimensionless parameter is set to  $\lambda = 20$ .

$$\begin{aligned}
 d_F[n : 0] &= \int_0^\infty \rho_{\lambda,n}(\xi) \left| \frac{d}{d\xi} \ln \left( \frac{\rho_{\lambda,n}(\xi)}{\rho_{\lambda,0}(\xi)} \right) \right|^2 d\xi \\
 &= \int_0^\infty \rho_{\lambda,n}(\xi) \left( \frac{\rho'_{\lambda,n}(\xi)}{\rho_{\lambda,n}(\xi)} - \frac{\rho'_{\lambda,0}(\xi)}{\rho_{\lambda,0}(\xi)} \right)^2 d\xi,
 \end{aligned} \tag{8}$$

has a definite value, where the prime  $'$  denotes  $d/d\xi$ . By the substitution of equation (7) and by means of the property  $L_0^{(\alpha)}(\xi) = 1$  for any  $\alpha$ , we can write the above quantity as

$$\frac{\rho'_{\lambda,n}(\xi)}{\rho_{\lambda,n}(\xi)} - \frac{\rho'_{\lambda,0}(\xi)}{\rho_{\lambda,0}(\xi)} = 2 \left( \frac{[L_n^{(2\lambda-2n-1)}(\xi)]'}{L_n^{(2\lambda-2n-1)}(\xi)} - \frac{n}{\xi} \right). \tag{9}$$

Thus, we have the following expression

$$d_F[n : 0] = 4N_{\lambda,n}^2 (J_1 + J_2 + J_3), \tag{10}$$

where  $J_1, J_2$  and  $J_3$  are integrals defined respectively as

$$\begin{aligned}
 J_1 &= n^2 \int_0^\infty \xi^{2\lambda-2n-3} e^{-\xi} [L_n^{(2\lambda-2n-1)}(\xi)]^2 d\xi, \\
 J_2 &= \int_0^\infty \xi^{2\lambda-2n-1} e^{-\xi} [L_{n-1}^{(2\lambda-2n)}(\xi)]^2 d\xi, \\
 J_3 &= 2n \int_0^\infty \xi^{2\lambda-2n-2} e^{-\xi} L_n^{(2\lambda-2n-1)}(\xi) L_{n-1}^{(2\lambda-2n)}(\xi) d\xi.
 \end{aligned} \tag{11}$$

In the expression of the integral  $J_2$ , a property of the associated Laguerre polynomials  $[L_n^{(\alpha)}(\xi)]' = -L_{n-1}^{(\alpha+1)}(\xi)$  has invoked. We note that the above three integrals become ill-defined or divergent if the exponent of  $\xi$  in the integrand is negative. Therefore, the condition  $\lambda - n > 3/2$  coming from the integral  $J_1$  is needed to determine the information value. This condition includes the ones coming from the other two integrals. Although some relevant formulas to compute the integral of the product of two Laguerre polynomials with different degrees and different orders for weight functions may produce an analytical expression (e.g. [18–20]), we here have determined the integrals numerically and calculated the values of the information distance  $d_F[n : 0]$  when we set  $\lambda = 20$  (therefore, up to  $n = 18$ ). Figure 1 shows that this measure grows rapidly with increasing  $n$  as a result of increasing degree of oscillation in wave functions; the number of the peaks of the wave function  $\psi_{\lambda,n}(\xi)$  is  $n + 1$ . More specifically, it increases at a much faster rate for lower excited states and for larger ones as  $n$  approaches the value of  $\lambda$ , whilst for the intermediate states, the growth can be regarded as exponential. This behavior contrasts with the one of the Shannon information entropy for the quantum harmonic oscillators and hydrogen atoms in three dimensions reported in [7], where the entropy values exhibit rapid increases for small  $n$  but reach saturated values in higher excited states. We also note that the energy eigenvalues of the states for this model are a quadratic function of  $n$  [15, 16];  $E_n/\hbar\omega_0 = -(n + 1/2)^2/\lambda^2 + n + 1/2$  with a constant  $\omega_0 = \sqrt{2Cb^2/m}$ . Therefore, we do not have a positive reason for attributing the behavior in figure 1 to the dependence of energy levels on  $n$ .

## 4. Relative Fisher information for D-dimensional isotropic quantum oscillator

The quantum harmonic oscillator in several dimensions has attracted much attention as a prototypical physical model of atomic systems. In this section, we focus on the relative Fisher information of these systems analytically and evaluate it numerically how we can quantify the information of excited states against the ground state. For a given principal quantum number  $n (= 0, 1, 2, \dots)$  and the strength of the harmonic potential  $k$ , the exact wave function in position space of the D-dimensional quantum harmonic oscillator under the central potential  $k^2 r^2/2$  is of the following form [1, 21]:

$$\psi_{n,l,\{\mu\}}(r, \Omega_D) = R_{n,l}(r) Y_{l,\{\mu\}}(\Omega_D) = N_{n,l} r^l e^{-\frac{k}{2} r^2} L_n^{(l+\frac{D}{2}-1)}(kr^2) Y_{l,\{\mu\}}(\Omega_D) \quad (12)$$

where  $Y_{l,\{\mu\}}(\Omega_D)$  is the hyperspherical harmonics function for the angular variables  $\Omega_D$  in the spherical polar coordinates. A set of magnetic quantum numbers  $\{\mu\}$  denotes integers that do not exceed the orbital quantum number  $l (= 0, 1, 2, \dots)$ . The normalization constant  $N_{n,l}$  which depends on both  $k$  and  $D$  is given by

$$N_{n,l} = \sqrt{\frac{2n! k^{l+\frac{D}{2}}}{\Gamma(n+l+\frac{D}{2})}}. \quad (13)$$

### 4.1. Relative Fisher information of the radial density function

We first consider the radial density function:

$$\rho_{n,l}^{(rad)}(\vec{r}) := r^{D-1} R_{n,l}^2(r) = N_{n,l}^2 r^{2l+D-1} e^{-kr^2} \left[ L_n^{(l+\frac{D}{2}-1)}(kr^2) \right]^2, \quad (14)$$

which satisfies the normalization; i.e.,  $\int_0^\infty \rho_{n,l}^{(rad)}(\vec{r}) dr = 1$ . This indicates that the radial wave function  $R_{n,l}(r)$  vanishes at infinity, which means that it is square integrable and it must be zero at the origin. Transforming the variable from  $r$  to  $\xi$  by  $\xi = kr^2$ , we treat the following radial density function  $\rho_{n,l}^{(rad)}(\xi)$  associated with the radial part of the complete wave function:

$$\rho_{n,l}^{(rad)}(\xi) = \frac{N_{n,l}^2}{k^{l+\frac{D}{2}}} \xi^{l+\frac{D}{2}-1} e^{-\xi} \left[ L_n^{(l+\frac{D}{2}-1)}(\xi) \right]^2. \quad (15)$$

Substituting this into the definition equation (1), the relative Fisher information  $d_F[(n, l): (0, 0)]$  measured from the ground state radial density  $\rho_{0,0}^{(rad)}(\xi) = 2k\xi^{\frac{D-1}{2}} e^{-\xi}/\Gamma(\frac{D}{2})$  is thus given as

$$\begin{aligned} d_F[(n, l): (0, 0)] &= \int_0^\infty r^{D-1} R_{n,l}^2(r) \left| \frac{d}{dr} \ln \left( \frac{R_{n,l}^2(r)}{R_{0,0}^2(r)} \right) \right|^2 dr \\ &= 8k^{1-\frac{D}{2}} \int_0^\infty \xi^{\frac{D}{2}} R_{n,l}^2(\xi) \left( \frac{R'_{n,l}(\xi)}{R_{n,l}(\xi)} - \frac{R'_{0,0}(\xi)}{R_{0,0}(\xi)} \right)^2 d\xi. \end{aligned} \quad (16)$$

Noting that the difference of the logarithmic derivative of the radial wave function gives

$$\frac{R'_{n,l}(\xi)}{R_{n,l}(\xi)} - \frac{R'_{0,0}(\xi)}{R_{0,0}(\xi)} = \frac{l}{2\xi} + \frac{\left[ L_n^{(l+\frac{D}{2}-1)}(\xi) \right]'}{L_n^{(l+\frac{D}{2}-1)}(\xi)}, \quad (17)$$

we can rewrite equation (16) as

$$d_F[(n, l): (0, 0)] = B_{n,l}(I_1 + I_2 + I_3), \quad (18)$$

where  $I_1, I_2$  and  $I_3$  are integrals defined respectively by

$$\begin{aligned} I_1 &= \frac{l^2}{4} \int_0^\infty \xi^{l+\frac{D}{2}-2} e^{-\xi} \left[ L_n^{(l+\frac{D}{2}-1)}(\xi) \right]^2 d\xi, \\ I_2 &= -l \int_0^\infty \xi^{l+\frac{D}{2}-1} e^{-\xi} L_n^{(l+\frac{D}{2}-1)}(\xi) L_{n-1}^{(l+\frac{D}{2})}(\xi) d\xi, \\ I_3 &= \int_0^\infty \xi^{l+\frac{D}{2}} e^{-\xi} \left[ L_{n-1}^{(l+\frac{D}{2})}(\xi) \right]^2 d\xi. \end{aligned} \quad (19)$$

The coefficient  $B_{n,l}$  denotes

$$B_{n,l} = \frac{16kn!}{\Gamma\left(n + l + \frac{D}{2}\right)}. \tag{20}$$

To calculate the integral  $I_1$ , one way is to recall the normalization integral provided in the Morse’s original paper (equation (12) in [15]):

$$\int_0^\infty \xi^{\beta-1} e^{-\xi} \mathcal{L}_{n+\beta}^{(\beta)}(\xi) \mathcal{L}_{m+\beta}^{(\beta)}(\xi) d\xi = \begin{cases} [\Gamma(\beta + n + 1)]^2 \sum_{s=0}^n \frac{\Gamma(\beta+s)}{\Gamma(s+1)} & (m = n) \\ 0 & (m \neq n), \end{cases} \tag{21}$$

where  $\mathcal{L}_{n+\beta}^{(\beta)}(\xi)$  denotes another definition of the associated Laguerre polynomials

$$\mathcal{L}_{n+\beta}^{(\beta)}(\xi) = \frac{d^\beta}{d\xi^\beta} \left[ e^\xi \frac{d^{n+\beta}}{d\xi^{n+\beta}} (e^{-\xi} \xi^{n+\beta}) \right], \tag{22}$$

which is traditionally used in quantum mechanics and the relation to the present definition  $L_n^{(\beta)}(\xi)$  by the Rodrigues’ formula is given as

$$\mathcal{L}_{n+\beta}^{(\beta)}(\xi) = (-1)^\beta \Gamma(n + \beta + 1) L_n^{(\beta)}(\xi). \tag{23}$$

We note here that the gamma function in the denominator of the right-hand side of the above orthogonal relation equation (21) is written as  $\Gamma(s - 1)$  in equation (12) of [15]. However, it should be  $\Gamma(s + 1)$  because  $s$  starts from zero. Substituting equation (23) by setting the order  $\beta = l + D/2 - 1$  into equation (21), we have an analytical expression,

$$I_1 = \frac{l^2}{4} \sum_{s=0}^n \frac{\Gamma\left(l + \frac{D}{2} - 1 + s\right)}{\Gamma(s + 1)}. \tag{24}$$

Another way for the calculation of  $I_1$  is to perform the integration by parts of  $I_2$  by means of the property  $L_{n-1}^{(\alpha+1)}(\xi) = -\frac{d}{d\xi} L_n^{(\alpha)}(\xi)$  (Note that the integral  $I_2$  itself vanishes as we describe below). This leads to a relation:

$$4\left(l + \frac{D}{2} - 1\right) \frac{I_1}{l^2} = \int_0^\infty \xi^{l+\frac{D}{2}-1} e^{-\xi} [L_n^{(l+\frac{D}{2}-1)}(\xi)]^2 d\xi. \tag{25}$$

The integral on the right-hand side can further be calculated by the orthogonality relation as  $\Gamma\left(l + \frac{D}{2} - 1\right)/n!$ . Thus one has the following expression

$$I_1 = \frac{l^2}{4n!} \frac{\Gamma\left(l + \frac{D}{2} + n\right)}{l + \frac{D}{2} - 1}. \tag{26}$$

One can readily confirm that the former expression equation (24) is equivalent to this.

Regarding the integral  $I_2$ , one readily confirms that it is a special case (with  $s = 1, \sigma = 1$  and  $\beta = \alpha$ ) of a known integral formula for the product of two Laguerre polynomials (e.g. [19, 20]):

$$\int_0^\infty \xi^\beta e^{-\sigma\xi} L_n^{(\alpha)}(\sigma\xi) L_{n-s}^{(\beta)}(\sigma\xi) = (-1)^s \frac{\Gamma(\beta + 1)}{\sigma^{\beta+1}} \binom{\beta + n - s}{n - s} \binom{\beta - \alpha}{s}, \tag{27}$$

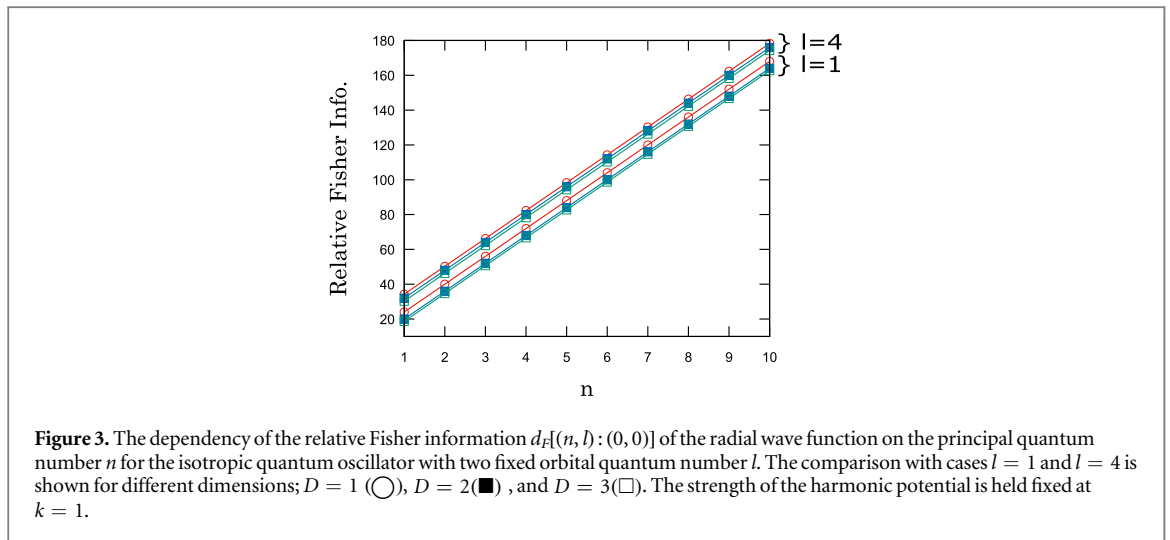
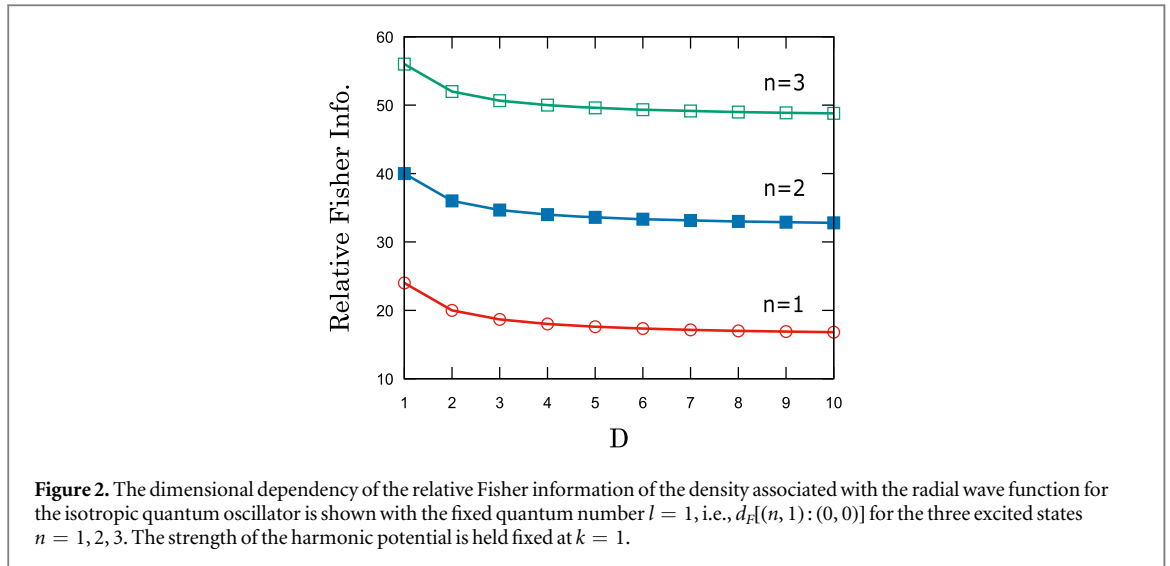
$(\beta > -1; \sigma > 0; n - l \geq 0),$

where, as usual,  $\binom{a}{b}$  in the right-hand side denotes the binomial coefficient. Using this concludes  $I_2 = 0$  by identifying  $\beta = l + D/2 - 1$ . Note also that another special case of the above relation with  $s = 0, \sigma = 1$  and  $\beta = \alpha$  precisely corresponds to the familiar orthogonality relation equation (6). On the other hand, the direct application of the orthogonality relation equation (6) readily reduces the integral  $I_3$  to the following expression,

$$I_3 = \frac{\Gamma\left(l + \frac{D}{2} + n\right)}{(n - 1)!}. \tag{28}$$

By equation (18), collecting these integrals constitutes the analytical form of the Fisher information relative to the ground state ( $n = 0, l = 0$ ) for the D-dimensional harmonic oscillators. In the following, we present numerically calculated behavior of the value of  $d_F[n, D]: (0, 0)$ .

Figure 2 gives the dependency of  $d_F[n, D]: (0, 0)$  on the dimension up to 10 for the first three principal quantum numbers when the quantum orbital number is held fixed ( $l = 1$ ). It decreases monotonically as the dimension increases and approaches a constant value depending on  $n$ . The excited states have higher information values than the lower ones for the same dimension.



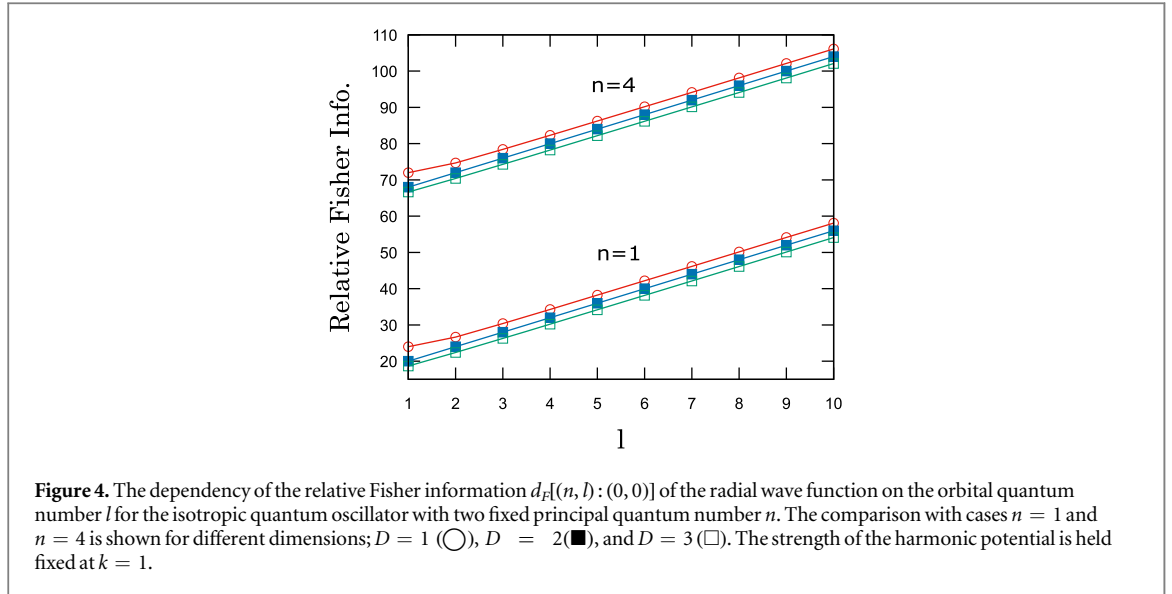
In figure 3, we show the dependency of the measure  $d_F[(n, l) : (0, 0)]$  on the principal quantum number  $n$  for two excited states  $l = 1$  and  $l = 4$  in three different dimensions. As  $n$  changes up to  $n = 10$ , we observe that the values of the measure grow linearly in all three dimensions and it gets higher as the orbital quantum number increases. The information values with the same  $l$  have a tendency to be small as the dimension increases and the intervals between the straight lines for different dimensions are more uniform for  $l = 4$  than for  $l = 1$ .

On the other hand, figure 4 shows how the measure  $d_F[(n, l) : (0, 0)]$  depends on the orbital quantum number  $l$  in two excited states ( $n = 1$  and  $n = 4$ ) for three dimensions respectively when  $l$  varies up to  $l = 10$ . We observe that it grows almost linearly except for lower excited states ( $l = 1$  and  $l = 2$ ) for three dimensions and it gets higher as the principal quantum number  $n$  increases. For the identical  $n$ , the values tend to be small as the dimension increases.

#### 4.2. Relative Fisher information of angular density for $D = 3$

This section focuses on a specialization to the angular part of the wave function for the three-dimensional quantum harmonic oscillator. As a by-product, we derive also the integral formula of the weighted product of the two associated Legendre polynomials with a little ingenuity, which is different from the previously known calculation.

In the preceding studies ([6, 7]), the explicit expression of the Fisher information for the full density function (both the radial and the angular parts are taken into consideration) of the hydrogen-like systems (i.e., Coulomb potential) in a three-dimensional case was reported. According to the results, it is independent of the orbital quantum number  $l$  and it rapidly decreases with increasing the principal quantum number  $n$ , reflecting delocalized electronic densities in excited states. Our concern here is to have an explicit form of the relative Fisher information of the density functions  $\eta_{lm}(\theta)$  associated with the angular part wave function  $\Theta_{lm}(\theta)$ ; that is,



**Figure 4.** The dependency of the relative Fisher information  $d_F[(n, l) : (0, 0)]$  of the radial wave function on the orbital quantum number  $l$  for the isotropic quantum oscillator with two fixed principal quantum number  $n$ . The comparison with cases  $n = 1$  and  $n = 4$  is shown for different dimensions;  $D = 1$  (○),  $D = 2$  (■), and  $D = 3$  (□). The strength of the harmonic potential is held fixed at  $k = 1$ .

$\eta_{lm}(\theta) = \Theta_{lm}^2(\theta)$  in the complete wave function  $\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi)$ , where the azimuthal part is  $\Phi_m(\phi) = e^{im\phi}/\sqrt{2\pi}$  ( $0 \leq \phi \leq 2\pi$ ,  $|m| \leq l$ ). The normalization for it is assured (e.g. [22]):

$$\int_0^\pi \Theta_{lm}^2(\theta) \sin \theta d\theta = 1, \tag{29}$$

with

$$\Theta_{lm}(\theta) = A_{lm} P_l^{|m|}(\cos \theta), \quad A_{lm} = \sqrt{\frac{(2l+1)(l-|m|)!}{2(l+|m|)!}}, \tag{30}$$

where  $P_l^{|m|}(z)$  are the associated Legendre polynomials defined by

$$P_l^{|m|}(z) = (1-z^2)^{\frac{|m|}{2}} \frac{d^{|m|}}{dz^{|m|}} P_l(z), \quad (|m| \leq l), \quad P_l(z) = \frac{1}{2^l l!} \frac{d^l}{dz^l} (z^2-1)^l. \tag{31}$$

The relative Fisher information between any pairs of quantum numbers  $(l, m)$  and  $(l', m')$  is by definition given as

$$d_F[(l, m) : (l', m')] = \int_0^\pi \eta_{lm}(\theta) \left[ \frac{d}{d\theta} \ln \left( \frac{\eta_{lm}(\theta)}{\eta_{l'm'}(\theta)} \right) \right]^2 \sin \theta d\theta. \tag{32}$$

To get the exact expression of the above for the arbitrary reference angular density specified by  $(l', m')$  involves challenging integrations. We here set it by the ground state  $\Theta_{00}(\theta) = 1/\sqrt{2}$ , that is, uniform over the polar angle  $\theta$ . Hence, it reduces to the calculation of the Fisher information  $F(\eta_{lm}(\theta))$  of the density  $\eta_{lm}(\theta)$ :

$$\begin{aligned} d_F[(l, m) : (0, 0)] &= \int_0^\pi \frac{1}{\eta_{lm}(\theta)} \left( \frac{d\eta_{lm}(\theta)}{d\theta} \right)^2 \sin \theta d\theta \\ &= F(\eta_{lm}(\theta)) \\ &= 4 \int_0^\pi \left( \frac{\Theta_{lm}(\theta)}{d\theta} \right)^2 \sin \theta d\theta. \end{aligned} \tag{33}$$

Since the relation  $\frac{dP_l^{|m|}(\cos \theta)}{d\theta} = -\sqrt{1-z^2} \frac{dP_l^{|m|}(z)}{dz}$  holds with  $z = \cos \theta$  and making use of the recurrence relation derived from the definition equation (31):

$$\left[ (1-z^2) \frac{d}{dz} + |m|z \right] P_l^{|m|}(z) = \sqrt{1-z^2} P_l^{|m|+1}(z), \tag{34}$$

we can rewrite equation (33) as

$$\begin{aligned} d_F[(l, m) : (0, 0)] &= 4A_{lm}^2 \int_{-1}^{+1} (1-z^2) \left( \frac{P_l^{|m|}(z)}{dz} \right)^2 dz \\ &= 4A_{lm}^2 (K_1 + K_2 + K_3), \end{aligned} \tag{35}$$

where the integrals  $K_1, K_2$  and  $K_3$  are defined respectively by

$$\begin{aligned} K_1 &= \int_{-1}^{+1} [P_l^{l+1}(z)]^2 dz, \\ K_2 &= -2|m| \int_{-1}^{+1} \frac{z}{\sqrt{1-z^2}} P_l^{l+1}(z) P_l^{l+1}(z) dz, \\ K_3 &= m^2 \int_{-1}^{+1} \frac{z^2}{1-z^2} [P_l^{l+1}(z)]^2 dz. \end{aligned} \tag{36}$$

The first and third integrals of the above can be computed respectively by means of the following useful orthogonality relations that one encounters frequently in many applications:

$$\begin{aligned} \int_{-1}^{+1} P_l^{l+1}(z) P_{l'}^{l'+1}(z) dz &= \frac{2}{2l+1} \frac{(l+|m|)!}{(l-|m|)!} \delta_{l,l'}, \\ \int_{-1}^{+1} \frac{P_l^{l+1}(z) P_{l'}^{l'+1}(z)}{1-z^2} dz &= \frac{(l+|m|)!}{|m|(l-|m|)!} \delta_{m,m'}. \end{aligned} \tag{37}$$

Therefore, we have the expressions respectively:

$$\begin{aligned} K_1 &= \frac{2}{2l+1} \frac{(l+|m|+1)!}{(l-|m|-1)!}, \\ K_3 &= m^2 \int_{-1}^{+1} \left( \frac{1}{1-z^2} - 1 \right) [P_l^{l+1}(z)]^2 dz = \frac{|m|(l+|m|)!}{(l-|m|)!} \frac{2(l-|m|)+1}{2l+1}. \end{aligned} \tag{38}$$

We now turn to the integration of the first line of equation (35), which we label it as  $K$ . Recall that  $P_l^{l+1}(z)$  is the solution of the associated Legendre differential equation:

$$\frac{d}{dz} \left[ (1-z^2) \frac{dP_l^{l+1}(z)}{dz} \right] + \left[ l(l+1) - \frac{m^2}{1-z^2} \right] P_l^{l+1}(z) = 0. \tag{39}$$

Multiplying both sides by  $P_{l'}^{l'+1}(z)$  and integrating it over the interval  $[-1, 1]$  gives

$$\begin{aligned} m^2 \int_{-1}^{+1} \frac{P_l^{l+1}(z) P_{l'}^{l'+1}(z)}{1-z^2} dz &= \int_{-1}^{+1} \frac{d}{dz} \left[ (1-z^2) \frac{dP_l^{l+1}(z)}{dz} \right] P_{l'}^{l'+1}(z) dz \\ &+ l(l+1) \int_{-1}^{+1} P_l^{l+1}(z) P_{l'}^{l'+1}(z) dz. \end{aligned} \tag{40}$$

The integral of the first term of the right-hand side reduces by the integration by parts to

$$- \int_{-1}^{+1} (1-z^2) \frac{dP_l^{l+1}(z)}{dz} \frac{dP_{l'}^{l'+1}(z)}{dz} dz, \tag{41}$$

and the second term can be calculated by means of the first orthogonality relation in equation (37). Making a similar equation by replacing  $l$  with  $l'$  in equation (40) and adding both sides, we have

$$\begin{aligned} m^2 \int_{-1}^{+1} \frac{P_l^{l+1}(z) P_{l'}^{l'+1}(z)}{1-z^2} dz &= - \int_{-1}^{+1} (1-z^2) \frac{dP_l^{l+1}(z)}{dz} \frac{dP_{l'}^{l'+1}(z)}{dz} dz \\ &+ \frac{1}{2} [l(l+1) + l'(l'+1)] \frac{2}{2l+1} \frac{(l+|m|)!}{(l-|m|)!} \delta_{ll'}. \end{aligned} \tag{42}$$

We thus have the expression

$$\begin{aligned} K &= \int_{-1}^{+1} (1-z^2) \left( \frac{dP_l^{l+1}(z)}{dz} \right)^2 dz = -m^2 \int_{-1}^{+1} \frac{[P_l^{l+1}(z)]^2}{1-z^2} dz + \frac{2l(l+1)}{2l+1} \frac{(l+|m|)!}{(l-|m|)!} \\ &= \frac{(l+|m|)!}{(l-|m|)!} \left\{ \frac{2l(l+1)}{2l+1} - |m| \right\}, \end{aligned} \tag{43}$$

where the second orthogonality relation in equation (37) has been used.

Remark: as a by-product, we obtain a formula for the integral below, which is not listed in the table of integrals, e.g., [17]:

$$\int_{-1}^{+1} \frac{z}{\sqrt{1-z^2}} P_l^{l+1}(z) P_l^{l+1}(z) dz \tag{44}$$

by equating with the relation  $(K_1 + K_3 - K)/2|m|$  from equation (36). From equation (43), one arrives at the expression for the relative Fisher information

$$d_F[(l, m) : (0, 0)] = 4A_{lm}^2 K = 2[2l(l+1) - |m|(2l+1)], \quad (|m| \leq l), \quad (45)$$

which is clearly a function of the two quantum numbers  $l$  and  $m$ . We note that a similar calculation for the spherical harmonics is performed in [7] to determine the analytical form of the Fisher information of hydrogen atoms, but the result is independent of the quantum number  $l$ .

## 5. Summary and concluding remarks

In addition to the traditional information theoretical measures such as the Shannon entropy and the Fisher information, which has been extensively focused in the literature, we demonstrated that to quantify a distance of the excited states from a specific reference state the relative Fisher information is a useful measure. We have determined the analytical expressions that arise from the radial density in position space for the two prototypical quantum mechanical potentials. The reference state is set to be the ground state, by which we measure how much the densities of excited states are similar to it. In the quantum harmonic potential case, we found that the information decreases with the dimension. This behavior contrasts markedly with the one of the Shannon entropy that was calculated numerically in [1]; i.e., the entropy grows linearly with dimension. The theoretical reason of our finding is not immediately obvious in terms of the mere comparisons of the shapes of the radial density functions. The followings are relevant: (a) the positions of  $n + 1$  peaks in the radial density functions depart largely from the origin ( $\xi = 0$ ) as the dimension increases for the same principal quantum number, (b) the magnitudes of the peaks depend on whether the dimension is even or odd, (c) the relative Fisher information involves the gradient of the radial density functions at the whole range of the position. To be convinced by the result, one will require the evaluation of the asymptotic limits of  $d_F[(n, l) : (0, 0)]$  (i.e., the value of equation (18) when  $D \rightarrow \infty$ ).

Because of the nodal structure of the wave functions, the calculations of the logarithmic measures such as the Shannon entropy for the Laguerre polynomials face non-definiteness. However, as shown also in the previous work for the electron density of the hydrogen-like atoms [8], the relative Fisher information always has definite values. In this sense, this work provides an additional insight into the role of the relative Fisher information to analyze information content of some typical quantum mechanical systems as well as atomic systems. The behavior of the relative Fisher information when evaluated on time-dependent solutions of the Schrödinger equation for some quantum systems may exhibit a distinct property. Since the time evolution of the product of the Fisher information in coordinate and momentum spaces under the Schrödinger equation converges with zero as time goes to infinity (e.g., [23]), this inquiry would be interesting as a future work.

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