Statistical correlations in the Moshinsky atom

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We study the influence of the interparticle and confining potentials on statistical correlation via the correlation coefficient and mutual information in ground and some excited states of the Moshinsky atom in position and momentum space. The magnitude of the correlation between positions and between momenta is equal in the ground state. In excited states, the correlation between the momenta of the particles is greater than between their positions when they interact through an attractive potential whereas for repulsive interparticle potentials the opposite is true. Shannon entropies, and their sums (entropic formulations of the uncertainty principle), are also analyzed, showing that the one-particle entropy sum is dependent on the interparticle potential and thus able to detect the correlation between particles.

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I. INTRODUCTION

Correlation is a key concept in understanding a variety of chemical and physical phenomena. Physically, the idea of correlated objects (particles) stems from the interaction between them. Mathematically, these interactions may be studied by quantifying the extent of the dependence of the variable representing one of the particles, on the variable representing another particle. Quantum mechanics (QM) provides us with a statistical interpretation of nature through distribution functions, thus correlation can be studied from a statistical perspective with tools such as the correlation coefficient [\[1\]](#page-5-0) or mutual information [\[2\]](#page-5-0).

The position and momentum representations are different but complementary spaces where one may formulate QM problems. Thus one can speak about correlation between positions (position space) of the particles or correlation between their momenta (momentum space). A natural question is how characteristics of the system, such as indistinguishability of the particles [\[3\]](#page-5-0), or the potentials present, influence the statistical correlation in the system. What are the physical constraints on the system that impose that the correlation between the momenta of the particles is larger than that of their positions or vice versa? This paper is focused on the effect of potentials on the correlation measures.

We investigate how changing the potential in an analytically solvable model influences the relative values of pair correlations in position and momentum space. For this purpose we calculate correlation measures in position and momentum space as a function of the interaction between particles in the Moshinsky atom and discuss the differences in the ground and some excited states. We also discuss the Shannon entropies that are interpreted as localization measures of the distributions as a function of the interparticle and confining potentials. Shannon entropies at one- and two-particle levels have been discussed in the literature for models, atoms, and molecules, [\[4–](#page-5-0)[22\]](#page-6-0). We also analyze the Shannon entropy sums that are entropic formulations of the uncertainty principle [\[22,23\]](#page-6-0).

Statistical correlation can be quantified in terms of correlation coefficients in position and momentum spaces

$$
\sigma_x = \frac{\langle x_1 x_2 \rangle - \langle x \rangle^2}{\langle x^2 \rangle - \langle x \rangle^2}, \quad -1 \leq \sigma_x \leq 1, \tag{1}
$$

and

$$
\sigma_p = \frac{\langle p_1 p_2 \rangle - \langle p \rangle^2}{\langle p^2 \rangle - \langle p \rangle^2}, \quad -1 \leq \sigma_p \leq 1,
$$
 (2)

where the moments of the one- and two-particle densities are defined as

$$
\langle x_1 x_2 \rangle = \int dx_1 \, dx_2 \, x_1 x_2 \, \Gamma(x_1, x_2), \tag{3}
$$

$$
\langle x \rangle = \int dx \, x \, \rho(x), \quad \langle x^2 \rangle = \int dx \, x^2 \, \rho(x), \tag{4}
$$

$$
\langle p_1 p_2 \rangle = \int dp_1 \, dp_2 \, p_1 p_2 \, \Pi(p_1, p_2), \tag{5}
$$

$$
\langle p \rangle = \int dp \ p \ \pi(p), \quad \langle p^2 \rangle = \int dp \ p^2 \ \pi(p), \qquad (6)
$$

and $\Gamma(x_1, x_2)$ [$\Pi(p_1, p_2)$] and $\rho(x)$ [$\pi(p)$] are the pair and one-particle (marginal) position [momentum] space densities normalized to unity, respectively, and the suppression of the subscripts reflects the indistinguishability between particles. Negative values of the correlation coefficient can be interpreted as *repulsive* correlation while positive values are indicative of *attractive* correlation. That is, negative values occur when variables are correlated in the opposite sense while positive values occur when the variables are correlated in the same sense. The pair densities are defined in terms of the wave functions Ψ , Φ in each representation while the one-particle densities are defined in terms of pair densities as

$$
\Gamma(x_1, x_2) = |\Psi(x_1, x_2)|^2, \quad \rho(x) = \int dx_2 \Gamma(x, x_2), \quad (7)
$$

$$
\Pi(p_1, p_2) = |\Phi(p_1, p_2)|^2, \quad \pi(p) = \int dp_2 \, \Pi(p, p_2). \tag{8}
$$

A more general measure of correlation is obtained from information theory. It is known as mutual information and is

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defined in terms of Shannon entropies and interpreted as a statistical (Kullback-Leibler) distance from a reference which is separable and is formed by the product of the marginals of the pair distribution [\[2\]](#page-5-0). It has been applied to study correlation in quantum systems [\[24–26\]](#page-6-0). Mutual information in position space is defined as

$$
I_x = \int dx_1 dx_2 \, \Gamma(x_1, x_2) \ln \left[\frac{\Gamma(x_1, x_2)}{\rho(x_1)\rho(x_2)} \right] = 2s_\rho - s_\Gamma \geq 0,
$$
\n(9)

where s_{Γ} and s_{ρ} are the pair and one-particle Shannon entropies in position space, respectively,

$$
s_{\Gamma} = -\int dx_1 dx_2 \Gamma(x_1, x_2) \ln \Gamma(x_1, x_2),
$$

\n
$$
s_{\rho} = -\int dx \, \rho(x) \ln \rho(x).
$$
\n(10)

Similarly, mutual information can be defined for the momentum space densities

$$
I_p = \int dp_1 \, dp_2 \, \Pi(p_1, p_2) \ln \left[\frac{\Pi(p_1, p_2)}{\pi(p_1)\pi(p_2)} \right] = 2s_\pi - s_\Pi \geq 0,
$$
\n(11)

and s_{Π} and s_{π} are the pair and one-particle Shannon entropies in momentum space, respectively,

$$
s_{\Pi} = -\int dp_1 dp_2 \, \Pi(p_1, p_2) \ln \Pi(p_1, p_2),
$$

$$
s_{\pi} = -\int dp \, \pi(p) \ln \pi(p).
$$
 (12)

Shannon entropies are measures of uncertainty and hence of the extent of (localization) delocalization, or spread in the distributions. The delocalization of a distribution is an important concept in QM. On comparing two distributions that with a smaller entropic value is the more localized one and which has less uncertainty.

As measures of uncertainty, there are entropic uncertainty relations at the one- $[23]$ and two-particle $[22]$ levels

$$
s_{\rho} + s_{\pi} \geqslant 1 + \ln \pi, \tag{13}
$$

$$
s_{\Gamma} + s_{\Pi} \geqslant 2(1 + \ln \pi). \tag{14}
$$

These entropy sums have been related to and shown to be sensitive to electron correlation [\[26,27\]](#page-6-0).

II. MOSHINSKY ATOM

The Moshinsky atom [\[28,29\]](#page-6-0) is the system whose Hamiltonian corresponds to two particles confined by, and interacting through, harmonic potentials. In atomic units ($m = \hbar = 1$), the Hamiltonian operator is (for a one-dimensional system) [\[30\]](#page-6-0)

$$
\hat{H} = \frac{1}{2} \left[\hat{p}_1^2 + \hat{p}_2^2 + \omega^2 \hat{x}_1^2 + \omega^2 \hat{x}_2^2 + \omega^2 \kappa (\hat{x}_1 - \hat{x}_2)^2 \right], \tag{15}
$$

where subscripts label the particles, ω is the harmonic oscillator confining potential, and *κ* can be identified as the controller of the harmonic frequency of the interparticle interaction.

This system is analytically solvable in relative-center-of-mass coordinates by defining

$$
\hat{R} = \frac{\hat{x}_1 + \hat{x}_2}{\sqrt{2}}, \qquad \hat{r} = \frac{\hat{x}_1 - \hat{x}_2}{\sqrt{2}}, \tag{16}
$$

and

$$
\hat{P} = \frac{\hat{p}_1 + \hat{p}_2}{\sqrt{2}}, \qquad \hat{p} = \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{2}}, \tag{17}
$$

where \hat{R} and \hat{P} are the center-of-mass coordinates and \hat{r} and \hat{p} are relative coordinates. The Hamiltonian can then be rewritten and is separable between center-of-mass and relative Hamiltonians

$$
\hat{H} = \hat{H}_{\text{c.m.}} + \hat{H}_{\text{rel}} = \frac{1}{2}(\hat{P}^2 + \omega^2 \hat{R}^2) + \frac{1}{2}(\hat{p}^2 + \Lambda^2 \hat{r}^2), \quad (18)
$$

with the new interparticle potential $\Lambda = \omega \sqrt{2\kappa + 1}$, where $-\frac{1}{2} < \kappa < \infty$ for the potential to be real valued. $\kappa < 0$ is the repulsive case, $\kappa > 0$ is the attractive case, and $\kappa = 0$ is the noninteracting case.

Solutions are then separable, and are well known wave functions for the harmonic oscillator of the center of mass, and for the relative coordinates, with the respective potential. Position space solutions are [\[31\]](#page-6-0)

$$
\psi_{n_{\text{c.m.}}}(R) = \left(\frac{\omega^{1/2}}{2^{n_{\text{c.m.}}} n_{\text{c.m.}}! \pi^{1/2}}\right)^{1/2} e^{-\omega R^2/2} H_{n_{\text{c.m.}}}(\sqrt{\omega}R),\tag{19}
$$

and

$$
\psi_{n_{\text{rel}}}(r) = \left(\frac{\Lambda^{1/2}}{2^{n_{\text{rel}}} n_{\text{rel}}! \pi^{1/2}}\right)^{1/2} e^{-\Lambda r^2/2} H_{n_{\text{rel}}}(\sqrt{\Lambda}r). \quad (20)
$$

Then

(*P*)

$$
\Psi(x_1, x_2) = \psi_{n_{\text{c.m.}}}(R)\psi_{n_{\text{rel}}}(r). \tag{21}
$$

Expressing the Hamiltonian in the momentum representation yields solutions

$$
\phi_{n_{\text{c.m.}}}(P)
$$
\n
$$
= \left(\frac{1}{2^{n_{\text{c.m.}}} n_{\text{c.m.}}! \omega^{1/2} \pi^{1/2}}\right)^{1/2} e^{-P^2/2\omega} H_{n_{\text{c.m.}}}(P/\sqrt{\omega}),
$$
\n(22)

and

$$
\phi_{n_{\text{rel}}}(p) = \left(\frac{1}{2^{n_{\text{rel}}} n_{\text{rel}}! \Lambda^{1/2} \pi^{1/2}}\right)^{1/2} e^{-p^2/2\Lambda} H_{n_{\text{rel}}}(p/\sqrt{\Lambda}).
$$
\n(23)

Then

$$
\Phi(p_1, p_2) = \phi_{n_{\text{c.m.}}}(P)\phi_{n_{\text{rel}}}(p). \tag{24}
$$

In all cases, $n_{c.m.}$ and n_{rel} are the quantum numbers associated with the center-of-mass and relative coordinates, respectively, and $H_n(x)$ are the *n*th order Hermite polynomials. It must be noted that although solutions are separable with the new coordinates, they are not in terms of the original variables (x_1 and x_2 or p_1 and p_2), and we expect the statistical correlation to arise.

This model has been extensively studied in many areas [\[19,](#page-5-0)[30,32–46\]](#page-6-0). In particular, it has been studied from the perspective of the correlation as measured by the correlation energy [\[47\]](#page-6-0).

III. RESULTS AND DISCUSSION

A. Ground state

1. Localization measures

Analytical expressions for entropies in position and momentum space may be obtained as

$$
s_{\Gamma} = 1 + \ln \pi - \left[\ln \omega + \frac{1}{4} \ln (2\kappa + 1) \right],\tag{25}
$$

$$
s_{\rho} = \frac{1}{2}(1 + \ln \pi) + \frac{1}{2}\left\{-\ln 2 - \ln \omega + \ln \left[\frac{1 + (2\kappa + 1)^{1/2}}{(2\kappa + 1)^{1/2}}\right]\right\}, (26)
$$

$$
s_{\Pi} = 1 + \ln \pi + \left[\ln \omega + \frac{1}{4} \ln (2\kappa + 1) \right],\tag{27}
$$

$$
s_{\pi} = \frac{1}{2}(1 + \ln \pi) + \frac{1}{2}\{-\ln 2 + \ln \omega + \ln [1 + (2\kappa + 1)^{1/2}]\}.
$$
\n(28)

All entropies depend on both potentials and are given in the logarithmic unit of information (nats). In position space, pair, and one-particle entropies are monotonic decreasing functions of the confining*ω* and interparticle *κ* potentials while in momentum space the entropies are monotonic increasing functions of them.

Figure $1(a)$ shows plots of pair entropies as functions of *κ* for three cases of the confining potential $ω = 0.7, 1, 1.2$. s_{Γ} increases as the magnitude of the repulsive interparticle potential $(k < 0)$ is increased, that is, the position space pair distribution delocalizes as the intensity of the interaction increases. In momentum space, s_{Π} decreases, thus the momentum space pair distribution localizes as the potential is increased. The inverse behavior between position and momentum space may be interpreted as a consequence of the uncertainty-type relationships. For attractive potentials $(k > 0)$, the behavior is opposite to that observed for the repulsive potentials. s_{Γ} decreases with the strength of the potential (i.e., a more localized distribution) while s_{Π} increases and the momentum space distribution delocalizes. The same type of behavior is observed for the one-particle entropies, which are not presented for brevity.

The crossover point, where $s_{\Gamma} = s_{\Pi}$, separates regions where $s_{\Gamma} > s_{\Pi}$ (left of this point) and where $s_{\Gamma} < s_{\Pi}$ (right of this point). This point, which is also the same in the one-particle entropies, occurs when

$$
\kappa = \frac{1 - \omega^4}{2\omega^4}.
$$
\n(29)

Summing Eqs. (25) and (27) , one can see that the entropy sum at the two-particle level does not depend on any of the potentials

$$
s_{\Gamma} + s_{\Pi} = 2(1 + \ln \pi), \tag{30}
$$

and is exactly its lower bound. Whereas from Eqs. (26) and (28), one observes that the one-particle entropic sum is

$$
s_{\rho} + s_{\pi} = 1 + \ln \pi - \ln 2 + \ln \left[\frac{1 + (2\kappa + 1)^{1/2}}{(2\kappa + 1)^{1/4}} \right],
$$
 (31)

which only depends on the interparticle potential and not on the confining potential *ω*. Its lower bound is obtained for $\kappa = 0$ and increases for other values of κ . Previous numerical work has related this entropy sum with the effects of electron correlation in real atomic systems with Coulomb potentials [\[27\]](#page-6-0). Equation (31) provides an analytical expression which shows that the entropy sum does depend on the harmonic interparticle potential in this particular model.

FIG. 1. (Color online) Shannon pair entropies s_F (blue dashed line) and s_H (red solid line) for the (a) ground (0,0) and (b) excited (0,1) states as functions of interparticle potential κ for confining potentials $\omega = 0.7, 1, 1.2$. Entropies are given in nats and κ in atomic units.

FIG. 2. (Color online) Correlation coefficient (CC) σ_x (blue dashed line) and σ_p (red solid line) for the ground state of the Moshinsky atom (0*,*0) as functions of the interacting potential *κ* (in atomic units).

2. Correlation measures

Expressions for the correlation coefficient of the ground state in both spaces are

$$
\sigma_x = \frac{(2\kappa + 1)^{1/2} - 1}{(2\kappa + 1)^{1/2} + 1} = -\sigma_p.
$$
 (32)

Thus the correlation coefficient indicates the same magnitude of correlation between positions or momenta of the particles, independent of the particular value of *κ*. However, correlation between positions is different from those between momenta since they are opposite in sign. It must be stressed that the correlation coefficient does not depend on the confining potential *ω*, but only on the interparticle potential *κ*. Plots are given in Fig. 2. For a repulsive potential $(\kappa < 0)$, there are *repulsive* correlations between particle positions ($\sigma_x < 0$) and *attractive* correlations between their momenta ($\sigma_p > 0$). For an attractive potential $(\kappa > 0)$ the inverse situation is true. Note also that σ increases in magnitude as we move away from $\kappa = 0$, the noncorrelated case ($\sigma = 0$).

The relations for mutual information are

$$
I_x = \ln\left[\frac{1 + (2\kappa + 1)^{1/2}}{2(2\kappa + 1)^{1/4}}\right] = I_p.
$$
 (33)

Similar to the correlation coefficient, the magnitude I_x is equal to I_p and does not depend on the confining potential ω , but only on the interparticle potential κ . I_x and I_p are shown in Fig. 3. Also, the magnitude of *I* increases as one moves away from the noncorrelated case $\kappa = 0$. Mutual information is different from the correlation coefficient since it is greater than or equal to zero and thus no physical interpretation can be made based upon its sign.

B. Excited state $(n_{c.m.}, n_{rel}) = (0, 1)$

1. Localization measures

Entropies of the excited states were obtained by numerical integration of Eqs. [\(10\)](#page-1-0) and [\(12\)](#page-1-0). Figure [1\(b\)](#page-2-0) compares s_{Γ} and s_{Π} as functions of κ for three different values of the confining potential $\omega = 0.7, 1, 1.2$ in this excited state. First, the overall trends and interpretation as a function of the interparticle

FIG. 3. (Color online) Mutual information (MI) I_x and I_p for the ground state of the Moshinsky atom (0*,*0) as functions of the interacting potential κ . Note that $I_x = I_p$ for this state. MI is given in nats and *κ* in atomic units.

potential are the same as those in the ground state. Compared to the ground state, the excited-state entropies are larger (more delocalized densities) in both position and momentum space.

It is relevant that the relative localization (i.e., $s_{\Gamma} < s_{\Pi}$ or $s_{\Gamma} > s_{\Pi}$) is controlled by both potentials as in the ground state. We numerically verified that the crossover points are the same as in the ground state. This also occurs for other excited states $(n_{c.m.}, n_{rel}) = (1, 2), (1, 3)$. This suggests that the crossover point (where $s_{\Gamma} = s_{\Pi}$) is a function of the potentials and not dependent on the particular state we are addressing. We also mention that the same trends are observed for the one-particle Shannon entropies, which are not shown for brevity.

The symmetry (with respect to the interchange of the original variables x_1 and x_2 or p_1 and p_2) of the wave function is controlled by n_{rel} , the quantum number associated with the relative coordinates. If n_{rel} is even the wave function is symmetric. If it is odd the wave function is antisymmetric. Hence it is relevant to note that the relative localization between position and momentum distributions seems to be controlled only by potentials. Qualitative changes are not observed for different symmetries. The argument is based on noting that the crossover point is the same for the ground state $[(0,0),$ symmetric wave function], for the excited state discussed in this section [(0*,*1), antisymmetric wave function], and also for the other calculated excited states [(1*,*2), symmetric wave function and (1*,*3), antisymmetric wave function].

The results for entropy sums (numerically obtained) at the one- and two-particle levels are consistent with those of the ground state and are not presented for conciseness. The pair entropy sum is a constant and does not depend on any of the potentials. The one-particle entropy sum does not depend on the confining potential ω , but only on the interparticle potential κ , and thus sensitive to interparticle correlations. Its value increases as one departs from $\kappa = 0$, which is consistent with the ground state. Both one-particle and pair entropy sums are larger in this excited state than in the ground state.

FIG. 4. (Color online) CC σ_x (blue dashed line) and σ_p (red solid line) for an excited state of the Moshinsky atom (0*,*1) as functions of the interacting potential κ (in atomic units).

2. Correlation measures

The correlation coefficients for this state are

$$
\sigma_x = \frac{(2\kappa + 1)^{1/2} - 3}{(2\kappa + 1)^{1/2} + 3},\tag{34}
$$

and

$$
\sigma_p = \frac{1 - 3(2\kappa + 1)^{1/2}}{1 + 3(2\kappa + 1)^{1/2}}.
$$
\n(35)

Both correlation coefficients are equal for $\kappa = 0$. At this point, correlation is nonzero because we are treating an excited state and these functions are not separable in terms of the original variables $(x_1$ and x_2 or p_1 and p_2). The correlation coefficients do not depend on the confining potential only on the interparticle one, consistent with the behavior of the ground state.

Plots of the correlation coefficients are shown in Fig. 4. For a repulsive interparticle potential (*κ <* 0) correlation is greater in position space than in momentum space $(|\sigma_x| >$ $|\sigma_p|$), whereas for an attractive interparticle potential ($\kappa > 0$) correlation is greater in momentum space ($|\sigma_p| > |\sigma_x|$). Hence, the kind of interaction between particles (if it is attractive or repulsive) is the unique parameter that controls the relative magnitude of the correlation between the particles positions or between their momenta (i.e., which one of them is greater).

The interpretation regarding the sign of the correlation coefficient is not as clear as in the ground state. This behavior is summarized in Table I. In momentum space, a small-enough value of the repulsive potential $\left[\kappa \in \left(-\frac{4}{9}, 0\right)\right]$ can provoke that there is a *repulsive* correlation (unlike the ground state) while for attractive potentials $[\kappa \in (0,4)]$ there is a *repulsive* correlation in position space (unlike the ground state). Note that correlation is predicted to be zero in position space for $\kappa = 4$ and in momentum space for $\kappa = -4/9$. This does not mean that there is no correlation, but rather that the correlation coefficient does not detect the correlation at these points. Thus the magnitude of correlation decreases from the left toward these points and increases to the right.

Calculations were performed for different values of the confining potential $\omega = 0.7, 1, 1.2, 2$, with the result that mutual information was not observed to be dependent on

the potential, similar to the ground state. Figure 5 illustrates that $I_x > I_p$ for repulsive interactions ($\kappa < 0$) while $I_p > I_x$ for attractive interactions ($\kappa > 0$). This is consistent with the behavior of the correlation coefficient.

There are two minima where correlation increases (toward the left or right) in both spaces, similar in interpretation to the zeros in the correlation coefficient. These points are $\kappa \approx 3.33$ for position space and $\kappa \approx -0.43$ for momentum space. An analysis of these two regions is shown in Fig. [6](#page-5-0) where the minima can be clearly observed. These points do not coincide with the zeros in the correlation coefficient and are not zero valued. Also, mutual information is nonzero at the points where the correlation coefficient is zero $(k = 4 \text{ in } r \text{ space and})$ $\kappa = -4/9$ in *p* space). At these points, mutual information is able to detect correlation while the correlation coefficient

FIG. 5. (Color online) MI I_x (blue dashed line) and I_p (red solid line) for an excited state of the Moshinsky atom (0*,*1) as functions of the interacting potential κ . MI is given in nats and κ in atomic units.

FIG. 6. (Color online) Analysis of the regions in MI *Ix* (left, blue dashed line) and *Ip* (right, red solid line) for an excited state of the Moshinsky atom $(0,1)$, which contains the points where correlation increases when varying the interparticle potential κ . MI is given in nats and *κ* in atomic units.

does not. We also calculated mutual information for other excited states $(n_{c.m.}, n_{rel}) = (1, 2), (1, 3)$ and the same trends were observed.

It should be emphasized that trends in correlation and the (in)dependence on confining and interparticle potentials seem to be independent of the state of the system and hence independent of the symmetry of the wave function.

It remains to be determined whether these results and concepts apply to systems with other (Coulomb) potentials and how the correlation in each space is affected by the presence of an external field. That is, if upon varying a control parameter of the system, one is able to induce a crossover in the relative magnitudes of the correlation in the respective (*x* and *p*) spaces. Also of interest is how the correlation in each space is related to position-momentum correlation.

IV. CONCLUSION

Shannon entropies are used to examine localization in the pair and one-particle distribution functions of the Moshinsky atom in position and in momentum space for ground and excited states. The behavior of the entropies is examined as functions of the confining ω and interparticle κ potentials.

The crossover point, where the entropies in each space are equal in value, depends on the potentials and is independent of the state and the symmetry of the wave function. The ground-state one-particle Shannon entropy sum is shown to depend explicitly on the interparticle potential and hence is sensitive to particle correlations. Numerical results show that these results also hold for excited states. Correlation measures are examined and found to be independent of the confining potential ω , but dependent on the interparticle one κ . In the ground state, the magnitude of the correlation between positions, and between momenta, is equal. In excited states, the magnitude of correlation is greater between the particles momenta than between their positions if they interact through an attractive potential. When they interact through a repulsive potential, correlations between the positions are greater than between the momenta.

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- [1] W. Kutzelnigg, G. Del Re, and G. Berthier, [Phys. Rev.](http://dx.doi.org/10.1103/PhysRev.172.49) **172**, 49 [\(1968\).](http://dx.doi.org/10.1103/PhysRev.172.49)
- [2] T. M. Cover and J. A. Thomas, *Elements of Information Theory* (John Wiley and Sons, New York, 1991).
- [3] H. G. Laguna and R. P. Sagar, J. Phys. A **44**[, 185302 \(2011\).](http://dx.doi.org/10.1088/1751-8113/44/18/185302)
- [4] V. Majerník and Richterek, J. Phys. A **30**[, L49 \(1997\).](http://dx.doi.org/10.1088/0305-4470/30/4/002)
- [5] V. Majerník, R. Charvot, and E. Majerníková, [J. Phys. A](http://dx.doi.org/10.1088/0305-4470/32/11/013) 32, [2207 \(1999\).](http://dx.doi.org/10.1088/0305-4470/32/11/013)
- [6] V. Majerník and T. Opatrný, J. Phys. A **29**[, 2187 \(1996\).](http://dx.doi.org/10.1088/0305-4470/29/9/029)
- [7] S. R. Gadre, S. B. Sears, S. J. Chakravorty, and R. D. Bendale, Phys. Rev. A **32**[, 2602 \(1985\).](http://dx.doi.org/10.1103/PhysRevA.32.2602)
- [8] R. J. Yañez, W. Van Assche, and J. S. Dehesa, *[Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.50.3065)* 50, [3065 \(1994\).](http://dx.doi.org/10.1103/PhysRevA.50.3065)
- [9] S. R. Gadre and R. D. Bendale, Curr. Sci. (India) **54**, 970 (1985).
- [10] S. R. Gadre and R. D. Bendale, Phys. Rev. A **36**[, 1932 \(1987\).](http://dx.doi.org/10.1103/PhysRevA.36.1932)
- [11] E. Romera and J. S. Dehesa, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.1697374) **120**, 8906 (2004).
- [12] Q. Shi and S. Kais, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.1785773) **121**, 5611 (2004).
- [13] K. D. Sen, J. Chem. Phys. **123**[, 074110 \(2005\).](http://dx.doi.org/10.1063/1.2008212)
- [14] K. D. Sen and J. Katriel, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.2263710) **125**, 074117 [\(2006\).](http://dx.doi.org/10.1063/1.2263710)
- [15] K. Ch. Chatzisavvas, Ch. C. Moustakidis, and C. P. Panos, J. Chem. Phys. **123**[, 174111 \(2005\).](http://dx.doi.org/10.1063/1.2121610)
- [16] Q. Shi and S. Kais, Chem. Phys. **309**[, 127 \(2005\).](http://dx.doi.org/10.1016/j.chemphys.2004.08.020)
- [17] S. B. Liu, J. Chem. Phys. **126**[, 191107 \(2007\).](http://dx.doi.org/10.1063/1.2741244)
- [18] Z. Huang and S. Kais, [Chem. Phys. Lett.](http://dx.doi.org/10.1016/j.cplett.2005.07.045) **413**, 1 (2005).
- [19] C. Amovilli and N. H. March, Phys. Rev. A **69**[, 054302 \(2004\).](http://dx.doi.org/10.1103/PhysRevA.69.054302)
- [20] Ch. C. Moustakidis, K. Ch. Chatzisavvas, and C. P. Panos, [Int.](http://dx.doi.org/10.1142/S0218301305003739) [J. Mod. Phys. E](http://dx.doi.org/10.1142/S0218301305003739) **14**, 1087 (2005).
- [21] K. Ch. Chatzisavvas, S. E. Massen, Ch. C. Moustakidis, and C. P. Panos, [Int. J. Mod. Phys. B](http://dx.doi.org/10.1142/S0217979206034558) **20**, 2189 (2006).
- [22] N. L. Guevara, R. P. Sagar, and R. O. Esquivel, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.1605932) **119**[, 7030 \(2003\).](http://dx.doi.org/10.1063/1.1605932)
- [23] I. Bialynicki-Birula and J. Mycielski, [Commun. Math. Phys.](http://dx.doi.org/10.1007/BF01608825) **44**, [129 \(1975\).](http://dx.doi.org/10.1007/BF01608825)
- [24] R. P. Sagar and N. L. Guevara, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.1953327) **123**, 044108 [\(2005\).](http://dx.doi.org/10.1063/1.1953327)
- [25] R. P. Sagar and N. L. Guevara, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.2180777) **124**, 134101 [\(2006\).](http://dx.doi.org/10.1063/1.2180777)
- [26] R. P. Sagar, H. G. Laguna, and N. L. Guevara, [Mol. Phys.](http://dx.doi.org/10.1080/00268970903153675) **107**, [2071 \(2009\).](http://dx.doi.org/10.1080/00268970903153675)
- [27] N. L. Guevara, R. P. Sagar, and R. O. Esquivel, [Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.67.012507) **67**, [012507 \(2003\).](http://dx.doi.org/10.1103/PhysRevA.67.012507)
- [28] M. Moshinsky, [Am. J. Phys.](http://dx.doi.org/10.1119/1.1974410) **36**, 52 (1968).
- [29] M. Moshinsky, Am. J. Phys. **36**[, 763 \(1968\).](http://dx.doi.org/10.1119/1.1975124)
- [30] J. P. Dahl, [Can. J. Chem.](http://dx.doi.org/10.1139/V09-002) **87**, 784 (2009).
- [31] R. J. Yañez, A. R. Plastino, and J. S. Dehesa, [Eur. Phys. J. D](http://dx.doi.org/10.1140/epjd/e2009-00270-x) 56, [141 \(2010\).](http://dx.doi.org/10.1140/epjd/e2009-00270-x)
- [32] C. Amovilli and N. H. March, Phys. Rev. A **67**[, 022509 \(2003\).](http://dx.doi.org/10.1103/PhysRevA.67.022509)
- [33] A. Holas, I. A. Howard, and N. H. March, [Phys. Lett. A](http://dx.doi.org/10.1016/S0375-9601(03)00408-0) **310**, [451 \(2003\).](http://dx.doi.org/10.1016/S0375-9601(03)00408-0)
-
- [34] N. H. March, I. A. Howard, Á. Nagy, and A. Rubio, *[Phys. Lett.](http://dx.doi.org/10.1016/S0375-9601(01)00479-0)* A **288**[, 101 \(2001\).](http://dx.doi.org/10.1016/S0375-9601(01)00479-0)
- [35] Á. Nagy, [Chem. Phys. Lett.](http://dx.doi.org/10.1016/j.cplett.2006.05.013) **425**, 154 (2006).
- [36] N. H. March, A. Cabo, F. Claro, and G. G. N. Angilella, [Phys.](http://dx.doi.org/10.1103/PhysRevA.77.042504) Rev. A **77**[, 042504 \(2008\).](http://dx.doi.org/10.1103/PhysRevA.77.042504)
- [37] J. Pipek and I. Nagy, Phys. Rev. A **79**[, 052501 \(2009\).](http://dx.doi.org/10.1103/PhysRevA.79.052501)
- [38] C. Amovilli and N. H. March, [Int. J. Quantum Chem.](http://dx.doi.org/10.1002/qua.20369) **102**, 132 [\(2005\).](http://dx.doi.org/10.1002/qua.20369)
- [39] I. Nagy and J. Pipek, Phys. Rev. A **81**[, 014501 \(2010\).](http://dx.doi.org/10.1103/PhysRevA.81.014501)
- [40] I. Nagy and J. Pipek, Phys. Rev. A **83**[, 034502 \(2011\).](http://dx.doi.org/10.1103/PhysRevA.83.034502)
- [41] S. Ragot, J. Chem. Phys. **125**[, 014106 \(2006\).](http://dx.doi.org/10.1063/1.2212935)
- [42] A. Akbari, N. H. March, and A. Rubio, [Phys. Rev. A](http://dx.doi.org/10.1103/PhysRevA.76.032510) **76**, 032510 [\(2007\).](http://dx.doi.org/10.1103/PhysRevA.76.032510)
- [43] S. Ragot and M. B. Ruiz, [J. Chem. Phys.](http://dx.doi.org/10.1063/1.2981526) **129**, 124117 [\(2008\).](http://dx.doi.org/10.1063/1.2981526)
- [44] H. Mera and K. Stokbro, Phys. Rev. B **79**[, 125109 \(2009\).](http://dx.doi.org/10.1103/PhysRevB.79.125109)
- [45] T. A. Niehaus, N. H. March, and S. Suhai, [J. Math. Chem.](http://dx.doi.org/10.1007/s10910-009-9592-7) **47**, [505 \(2010\).](http://dx.doi.org/10.1007/s10910-009-9592-7)
- [46] A. Nagy and E. Romera, [Chem. Phys. Lett.](http://dx.doi.org/10.1016/j.cplett.2010.03.057) **490**, 242 (2010).
- [47] P.-F. Loos, Phys. Rev. A **81**[, 032510 \(2010\).](http://dx.doi.org/10.1103/PhysRevA.81.032510)