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Maximum-entropy technique with logarithmic constraints: Estimation of atomic radial densities

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Abstract. Maximum-entropy (ME) approximations to density functions involving logarithmic constraints are studied. It is proved the existence and uniqueness of the ME approximation constrained by the normalization, the geometric mean and (i) a moment of arbitrary order, or (ii) the logarithmic uncertainty. A numerical analysis of the accuracy of these ME approximations is carried out for the radial electron densities of neutral atoms in both position and momentum spaces.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 31.15.-p Calculations and mathematical techniques in atomic and molecular physics (excluding electron correlation calculations)

1 Introduction

The formulation of the Density Functional Theory in the description of many-fermion systems reveals the important role played by the one-particle densities in position and momentum spaces (to be denoted by $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$ respectively) in the study of many physical properties of such systems [1]. Here we consider the normalization

$$\int \rho(\mathbf{r})\mathrm{d}\mathbf{r} = \int \gamma(\mathbf{p})\mathrm{d}\mathbf{p} = N, \tag{1}$$

N being the number of constituents of the system. In this work, we will restrict ourselves to the description of atomic systems, for which it is sufficient to deal with the radial distributions

$$D(r) \equiv 4\pi r^2 \rho(r) \tag{2}$$

$$I(p) \equiv 4\pi p^2 \gamma(p) \tag{3}$$

where $\rho(r)$ and $\gamma(p)$ are the spherical averages of $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$, respectively.

Due to the difficulties of obtaining information on such distributions both experimentally and theoretically (even for atoms), several techniques have been recently employed in order to obtain tight approximations to these functions from the knowledge of very limited information on them. One of the most powerful approximation techniques employed is the so-called Maximum-Entropy (ME) technique [2], which provides approximations to the density at any point in terms of its first few moments, defined as

$$\mu_n \equiv \int_0^\infty r^n D(r)\mathrm{d}r, \tag{4}$$

$$\nu_n \equiv \int_0^\infty p^n I(p)\mathrm{d}p. \tag{5}$$

Some of these moments are physically meaningful and/or experimentally accessible. In atomic systems, for instance, μ_{-1} is related to the electron-nucleus attraction energy [3], μ_2 to the diamagnetic susceptibility [4], ν_{-1} is twice the height of the peak of the Compton profile [5] and ν_2 and ν_4 are proportional to the kinetic energy [5] and its relativistic correction due to the mass variation [6], respectively. Notice that $\mu_0 = \nu_0 = N$ for N-fermion systems.

The ME method has been successfully applied by the authors to the analysis of many relevant atomic densities, such as the one-particle densities $\rho(r)$ and $\gamma(p)$ [7], the electron-pair density $h(u)$ [8], the Compton profile $J(q)$ [9], form factors [10], reciprocal form factors [11] and total scattering intensities [12], as well as for more complex N-electron systems, such as diatomic molecules [13]. Such ME approximations have been also compared to other ones obtained by employing different techniques (*i.e.* Stieljes-Chebyshev reconstruction, Padé-like approximations) which involve additionally the knowledge of *local*

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quantities (*e.g.* the value of the density and some of its first derivatives at the origin).

In all the above mentioned works, the information used as constraints to construct the ME approximations were only the first moments of the studied distribution. In the present work, we consider a new type of constraints, namely the mean logarithmic position ($\mu_0^{'}$) or momentum ($\nu_0^{'}$) (which exponential is the geometric mean of the variable involved [14]) and the logarithmic uncertainties (Δ_r and Δ_p), *i.e.*

$$\mu_0^{'} \equiv \left(\frac{\mathrm{d}\mu_n}{\mathrm{d}n}\right)_{n=0} = \int_0^\infty (\ln r) D(r)\mathrm{d}r \tag{6}$$

$$\nu_0^{'} \equiv \left(\frac{\mathrm{d}\nu_n}{\mathrm{d}n}\right)_{n=0} = \int_0^\infty (\ln p) I(p)\mathrm{d}p \tag{7}$$

$$\Delta_r \equiv \left[\frac{\mu_0\mu_0^{''} - (\mu_0^{'})^2}{\mu_0^2}\right]^{1/2} \tag{8}$$

$$\Delta_p \equiv \left[\frac{\nu_0\nu_0^{''} - (\nu_0^{'})^2}{\nu_0^2}\right]^{1/2} \tag{9}$$

where $\mu_0^{''} \equiv \left(\mathrm{d}^2\mu_n/\mathrm{d}n^2\right)_{n=0} = \int_0^\infty (\ln r)^2 D(r)\mathrm{d}r$ and $\nu_0^{''} \equiv \left(\mathrm{d}^2\mu_n/\mathrm{d}n^2\right)_{n=0} = \int_0^\infty (\ln p)^2 I(p)\mathrm{d}p$.

In this sense, it is worthy to mention that the quantities $\mu_0^{'}$ and μ_{-2} determine the high-energy behaviour of the phase shifts η_j for the elastic scattering of electrons of small angular momentum j in the electrostatic potential $V(r)$ of a spherically symmetric charge distribution [15,16] as

$$\eta_j \sim Z\alpha\left[1 - \ln 2k - \frac{\langle \ln r\rangle}{4\pi} - \frac{\left(j+\frac{1}{2}\right)^2}{16\pi k^2}\mu_{-2}\right] + O(1/k^3)$$

where Z is the total charge, α the fine-structure constant and k the wave number.

In Section 2, the ME technique is briefly described, and in Section 3 some solutions involving logarithmic constraints are studied and numerically analyzed for atomic systems within a Hartree-Fock framework.

2 Maximum-entropy technique

The ME technique deals with the information entropy functional

$$S_D \equiv -\int_0^\infty D(r)\ln D(r)\mathrm{d}r. \tag{10}$$

In reference [2] it is proved that, given only partial information on a distribution, the least biased density among all those compatible with the known information is the one which maximizes the quantity S_D. So, the *best choice* that one should consider taking into account only the limited information given is precisely the distribution that, subjected to those constraints, maximizes S_D, which will be denoted by $D_{\mathrm{ME}}(r)$. If the given information consists of one or more expectation values, such as

$$\langle f_i(r)\rangle = \int_0^\infty f_i(r)D(r)\mathrm{d}r \quad (i = 0, 1, \ldots, M) \tag{11}$$

the function $D_{\mathrm{ME}}(r)$ is obtained by solving the variational equation

$$\delta\left[-\int_0^\infty D(r)\ln D(r)\mathrm{d}r + \sum_{i=0}^{M}\lambda_i\left(\langle f_i(r)\rangle - \int_0^\infty f_i(r)D(r)\mathrm{d}r\right)\right] = 0 \tag{12}$$

where $\lambda_0, \lambda_1, \ldots, \lambda_M$ are Lagrange multipliers. The solution to this equation is given by

$$D_{\mathrm{ME}}(r) = \exp\left\{-1 - \sum_{i=0}^{M}\lambda_i f_i(r)\right\} \tag{13}$$

where the Lagrange multipliers have to be obtained by imposing the $M+1$ previous constraints:

$$\int_0^\infty f_i(r)D_{\mathrm{ME}}(r)\mathrm{d}r = \langle f_i(r)\rangle \quad (i = 0, 1, \ldots, M). \tag{14}$$

Existence and uniqueness of the solution to this problem have been extensively studied [17–19] when the considered constraints are integer powers of r, and more precisely when $f_i(r) = r^i$. In this case, the expectation values of equation (11) are the moments μ_i of equation (4). It is known [17–19] that (i) there always exists solution for $M = 1$, and (ii) for $M = 2, 3$, the involved moments must verify a necessary and sufficient condition for the existence of ME solution.

However, such kind of existence conditions for the ME problem associated to other kind of constraints (*e.g.* logarithmic expectation values) are not known, to the best of our knowledge. In the next section we center our attention on two new different problems, the first one concerning the constraints $(N, \langle \ln r\rangle, \langle(\ln r)^2\rangle)$ and the second one associated to $(N, \langle r^\alpha\rangle, \langle \ln r\rangle)$ for any $\alpha > -3$ not necessarily integer. Existence and uniqueness of ME solution is proved in both cases.

3 Maximum-entropy solutions

Let us firstly consider the ME problem associated to the constraints

$$N = \int_0^\infty D(r)\mathrm{d}r, \tag{15}$$

$$\langle \ln r\rangle = \int_0^\infty \ln r D(r)\mathrm{d}r, \tag{16}$$

$$\langle(\ln r)^2\rangle = \int_0^\infty (\ln r)^2 D(r)\mathrm{d}r. \tag{17}$$

Then, let us employ equation (13) in order to obtain the ME distribution, to be denoted by $D^0_{\rm ME}$, as

$$D^0_{\rm ME}(r) = \exp\left\{-1-\lambda_1-\lambda_2\ln r-\lambda_3(\ln r)^2\right\}. \quad (18)$$

It is easy to evaluate the quantities

$$L_k \equiv \int_0^\infty (\ln r)^k D^0_{\rm ME}(r){\rm d}r$$

for $k=0,1,2$. In doing so, we firstly calculate the moments $\sigma_k \equiv \int_0^\infty r^k D^0_{\rm ME}(r){\rm d}r$ of $D^0_{\rm ME}(r)$, giving rise to the expression

$$\sigma_k = \sqrt{\frac{\pi}{\lambda_3}}\exp\left\{-1-\lambda_1+\frac{(k-\lambda_2+1)^2}{4\lambda_3}\right\}. \quad (19)$$

Secondly, we observe that $L_0=\sigma_0$, $L_1=({\rm d}\sigma_k/{\rm d}k)_{k=0}$ and $L_2=\left({\rm d}^2\sigma_k/{\rm d}k^2\right)_{k=0}$, and imposing the constraints in the form $L_0=N$, $L_1=\langle\ln r\rangle$ and $L_2=\langle(\ln r)^2\rangle$, the following system of equations on $\{\lambda_1,\lambda_2,\lambda_3\}$ appears:

$$N = \sqrt{\frac{\pi}{\lambda_3}}\exp\left\{-1-\lambda_1+\frac{(1-\lambda_2)^2}{4\lambda_3}\right\}, \quad (20)$$

$$\frac{\langle\ln r\rangle}{N} = \frac{1-\lambda_2}{2\lambda_3}, \quad (21)$$

$$\Delta_r^2 = \frac{1}{2\lambda_3}\cdot \quad (22)$$

The solution to this system provides the desired analytical expressions for the Lagrange multipliers:

$$\mathrm{e}^{-1-\lambda_1} = \frac{N}{\sqrt{2\pi}\Delta_r}\exp\left\{-\frac{\langle\ln r\rangle^2}{2N^2\Delta_r^2}\right\}, \quad (23)$$

$$\lambda_2 = 1-\frac{\langle\ln r\rangle}{N\Delta_r^2}, \quad (24)$$

$$\lambda_3 = \frac{1}{2\Delta_r^2}\,. \quad (25)$$

Consequently, the density $D^0_{\rm ME}$ of equation (18) in which the values of the Lagrange multipliers are those given by equations (23–25) is the ME one under the constraints $(N,\langle\ln r\rangle,\langle(\ln r)^2\rangle)$.

Let us now consider the problem associated to the constraints $(N,\langle r^\alpha\rangle,\langle\ln r\rangle)$ with $\alpha>-3$. Using equation (18), the ME density obtained in this case (to be denoted by $D^\alpha_{\rm ME}(r)$) is given by the expression

$$D^\alpha_{\rm ME}(r) = \exp\left\{-1-\lambda_1-\lambda_2 r^\alpha-\lambda_3\ln r\right\} \quad (26)$$

or equivalently,

$$D^\alpha_{\rm ME}(r) = Ar^m\exp\{-\lambda r^\alpha\}. \quad (27)$$

The moment $\sigma_k \equiv \int_0^\infty r^k D^\alpha_{\rm ME}(r){\rm d}r$ of order k of such distribution is given by

$$\sigma_k = \frac{A\Gamma\left(\dfrac{m+k+1}{\alpha}\right)}{|\alpha|\lambda^{\frac{m+k+1}{\alpha}}} \quad (28)$$

where $\{A,m,\lambda\}$ have to be determined from the relations

$$\sigma_0 = N \quad (29)$$

$$\sigma_\alpha = \langle r^\alpha\rangle \quad (30)$$

$$\left(\frac{\rm d}{{\rm d}k}\sigma_k\right)_{k=0} = \langle\ln r\rangle \quad (31)$$

giving rise to the equations

$$N = \frac{A\Gamma\left(\dfrac{m+1}{\alpha}\right)}{|\alpha|\lambda^{\frac{m+1}{\alpha}}} \quad (32)$$

$$\frac{\langle r^\alpha\rangle}{N} = \frac{m+1}{\alpha\lambda} \quad (33)$$

$$\frac{\langle\ln r\rangle}{N} = \frac{1}{\alpha}\left[\Psi\left(\frac{m+1}{\alpha}\right)-\ln\lambda\right] \quad (34)$$

with $(m+1)\alpha>0$ and where the Psi function $\Psi(x)$ is the logarithmic derivative of $\Gamma(x)$.

The calculation of the Lagrange multipliers cannot be performed analytically, essentially due to the appearance of the function $\Psi(x)$. However, we prove the existence and uniqueness of solution to this problem. In doing so, let us insert in equation (34) the expression for λ provided by equation (33), giving rise to

$$\Psi\left(\frac{m+1}{\alpha}\right)-\ln\frac{m+1}{\alpha} = \alpha\frac{\langle\ln r\rangle}{N}-\ln\frac{\langle r^\alpha\rangle}{N} \quad (35)$$

with $(m+1)/\alpha>0$. The function $g(x)\equiv\Psi(x)-\ln x$ is continuous for any $x>0$, and increases monotonically from $-\infty$ to 0 when x goes from 0 to ∞. Hence, equation (35) has one and only one solution if the right handside is nonpositive, which is always true due to the log-convexity of the quantities $\langle r^\alpha\rangle/N$. Then, we prove that there exists, for any $\alpha>-3$, one and only one value of the Lagrange multiplier m for which the ME density fulfills the given constraints.

Let us notice that all the expressions appearing in this work are independent of the characteristics of the radial distribution $D(r)$. So, similar relationships for the radial momentum density $I(p)$ are obtained by only replacing the quantities $\langle r^\alpha\rangle$ and $\langle(\ln r)^k\rangle$ by $\langle p^\alpha\rangle$ and $\langle(\ln p)^k\rangle$.

The main structural characteristic of the ME solutions $D^\alpha_{\rm ME}$ and $I^\alpha_{\rm ME}$ here obtained is unimodality when $\alpha\leq 0$, *i.e.* they increase from zero to the maximum value, located at some position $r_{\rm max}$ (or $p_{\rm max}$) to decrease again towards zero as r (or p) goes to infinity. Such position is given by

$$r_{\rm max} = \left[\frac{m\langle r^\alpha\rangle}{(m+1)\alpha N}\right]^{1/\alpha} \quad (36)$$

for $D^\alpha_{\rm ME}(r)$ with $\alpha<0$, and by

$$r_{\rm max} = \exp\left\{\frac{\langle\ln r\rangle}{N}-\Delta_r^2\right\} \quad (37)$$

for $D^0_{\rm ME}(r)$, and similarly for $p_{\rm max}$.

However, the ME distributions when $\alpha>0$ are (i) unimodal when $m>0$, with $r_{\rm max}$ (or $p_{\rm max}$) given by equation (36), and (ii) monotonically decreasing when $m\leq 0$.

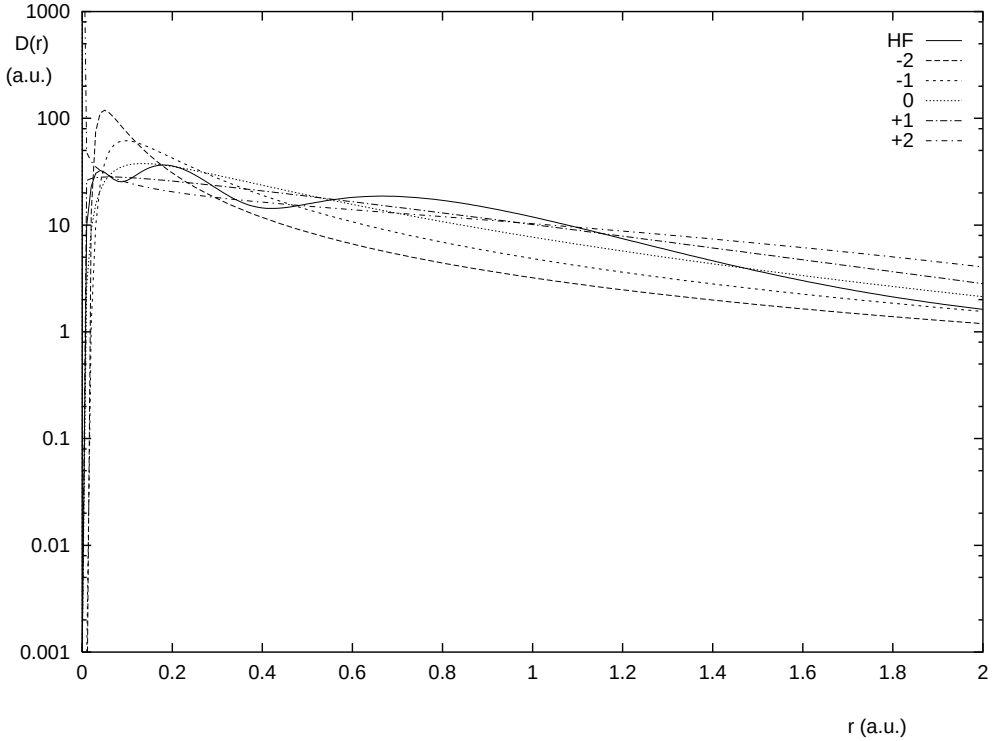

Fig. 1. ME approximations $D^{\alpha}_{\rm ME}(r)$ for $\alpha = 0, \pm 1, \pm 2$ and Hartree-Fock (HF) radial density in position space $D(r)$ for the cobalt atom ($N = 27$). Atomic units are used.

4 Numerical analysis

To have an idea of the accuracy of the above approximations, let us compare them with the corresponding radial distributions of electrons (in position and momentum spaces) for the case of N-electron atomic systems. In doing so, we employ the Hartree-Fock (HF) wavefunctions of reference [20] to compute the distributions as well as the associated radial and logarithmic expectation values used to construct the ME approximations.

In Figure 1, the ME approximations $D^{\alpha}_{\rm ME}(r)$ for $\alpha = -2, 1, 0, 1, 2$ are compared to the HF radial density $D(r)$ for the Co atom ($N = 27$). It is observed the accuracy of all these approximations (even for the cases divergent at the origin) having in mind the very limited information involved, *i.e.* the normalization and two expectation values. Specially accurate are the densities corresponding to the cases $\alpha = 0, 1$, which appart from N and $\langle \ln r \rangle$, depend on $\langle (\ln r)^2 \rangle$ and $\langle r \rangle$, respectively.

In Figure 2, the ME approximations $I^{\alpha}_{\rm ME}(p)$ for $\alpha = -2, 1, 0, 1, 2$ are compared to the HF radial momentum density $I(p)$ for the F atom ($N = 9$). Similar comments to those in Figure 1 can be done here.

It is also interesting to analyze the value of the parameter m associated to the ME solution given by equation (27) in both position and momentum spaces. In doing so, let us observe Figures 3 and 4 corresponding to $D^{\alpha}_{\rm ME}(r)$ and $I^{\alpha}_{\rm ME}(p)$, respectively, for all atoms with $1 \leq N \leq 54$. It is observed that, in both cases, (i) the value of m depends very weakly on the number of electrons N, being almost constant for $N \geq 3$ in the cases $\alpha < 0$ in position space and $\alpha > 0$ in momentum space, (ii) the main deviations from such a constant behavior correspond to $N = 1, 2$, (iii) shell structure is strongly displayed, and (iv) the values m_α for $\alpha = \pm 2, \pm 1$ verify, for any $1 \leq N \leq 54$, the relation $m_{-1} \leq m_{-2} \leq -1 \leq m_2 \leq m_1$. Moreover, $m_\alpha \leq 2$ for any $\alpha = \pm 2, \pm 1$ in both position and momentum spaces, with only one exception: the value $m_1 = 2.11$ for the Hydrogen atom ($N = 1$) in momentum space.

Finally, let us compare the values of the entropies S^{α}_{D} and S^{α}_{I} associated to the ME approximations $D^{\alpha}_{\rm ME}(r)$ and $I^{\alpha}_{\rm ME}(p)$ (for $\alpha = -2, -1, 0, 1, 2$) with those of the HF radial densities $D(r)$ and $I(p)$ in neutral atoms with $1 \leq N \leq 54$. They are shown in Figures 5 and 6, respectively, where normalization to 1 instead of N has been considered. It is observed that the more accurate approximation to the radial density corresponds to: (i) in position space, $\alpha = 0$ for $N = 3$, $11{-}14$, $19{-}23$, $31{-}32$, $37{-}43$, $49{-}52$ and $\alpha = 1$ for the rest of the sample here considered; (ii) in momentum space, always $\alpha = 0$ with the only two exceptions $N = 3, 12$ for which $\alpha = 1$ provides a lower entropy. So, for any $1 \leq N \leq 54$ in both position and momentum spaces, the best ME approximation belongs to $\alpha = 0$ or $\alpha = 1$.

Additionally, Figures 5 and 6 reveal a similar dependence on N for the entropies of the HF density and the approximations here considered. In Figure 5 it is also observed a strong relation between the values of those entropies and the atomic shell structure.

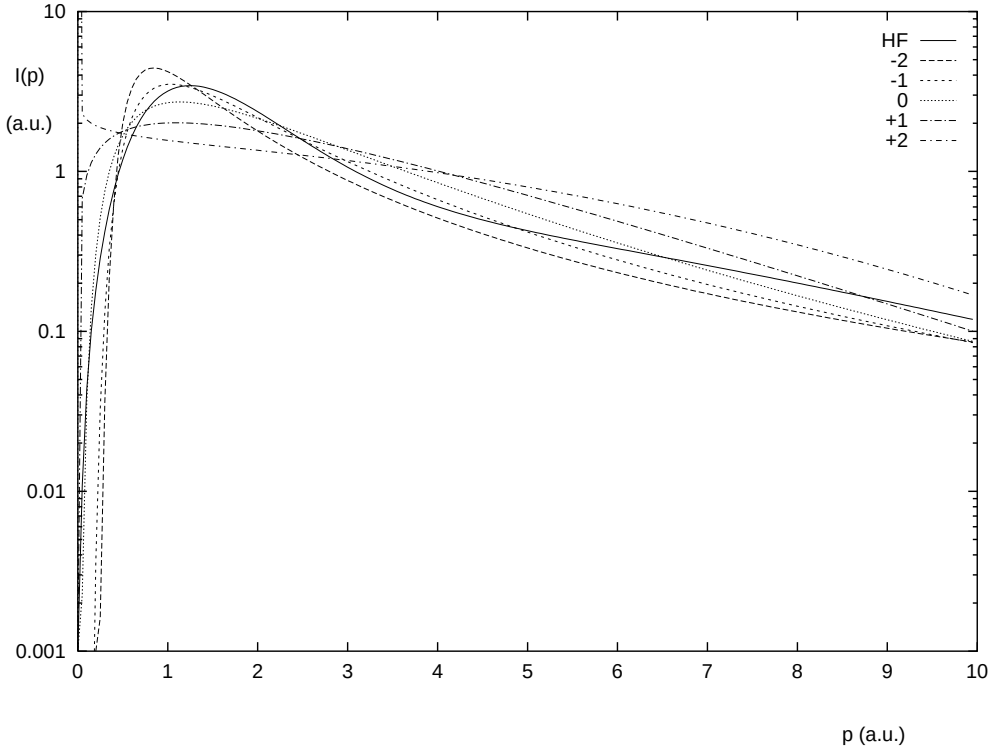

Fig. 2. ME approximations $I^{\alpha}_{\rm ME}(p)$ for $\alpha = 0, \pm 1, \pm 2$ and Hartree-Fock (HF) radial density in momentum space $I(p)$ for the fluor atom ($N = 9$). Atomic units are used.

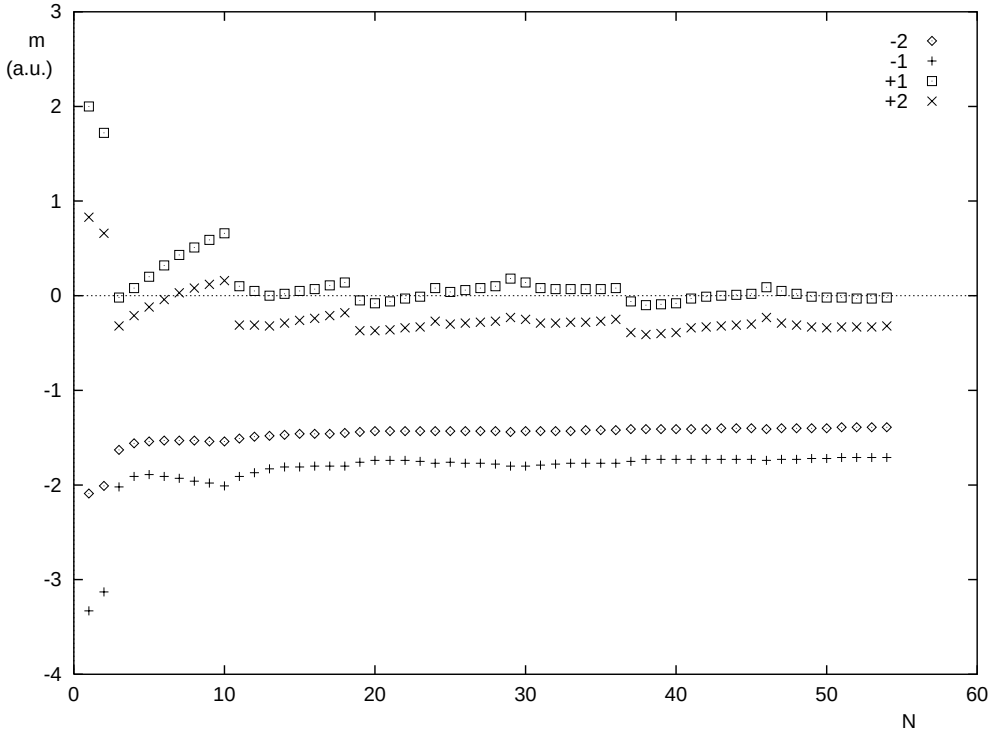

Fig. 3. Value of the Lagrange multiplier m (see Eq. (27)) of the ME approximations $D^{\alpha}_{\rm ME}(r)$ for $\alpha = \pm 1, \pm 2$ in the atomic systems with $1 \leq N \leq 54$. Atomic units are used.

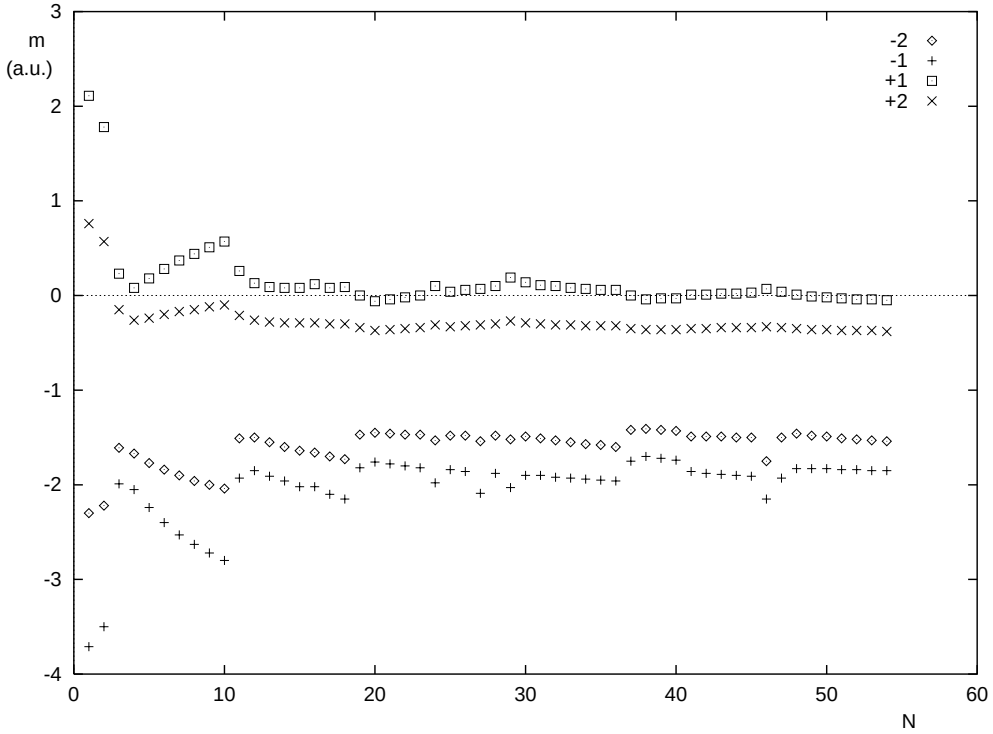

Fig. 4. Value of the Lagrange multiplier m (see Eq. (27)) of the ME approximations $I^{\alpha}_{\mathrm{ME}}(p)$ for $\alpha = \pm 1, \pm 2$ in the atomic systems with $1 \leq N \leq 54$. Atomic units are used.

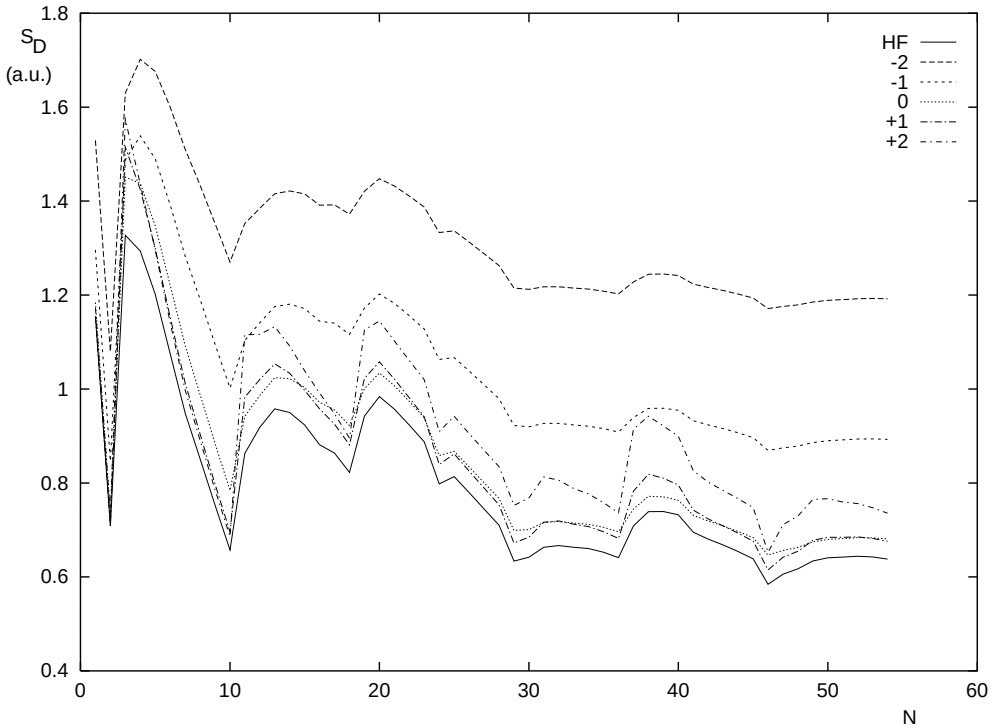

Fig. 5. Comparison among the entropies of the normalized-to-unity ME approximations $D^{\alpha}_{\mathrm{ME}}(r)$ ($\alpha = 0, \pm 1, \pm 2$) and the Hartree-Fock (HF) radial density $D(r)$ for atomic systems with $1 \leq N \leq 54$. Atomic units are used.

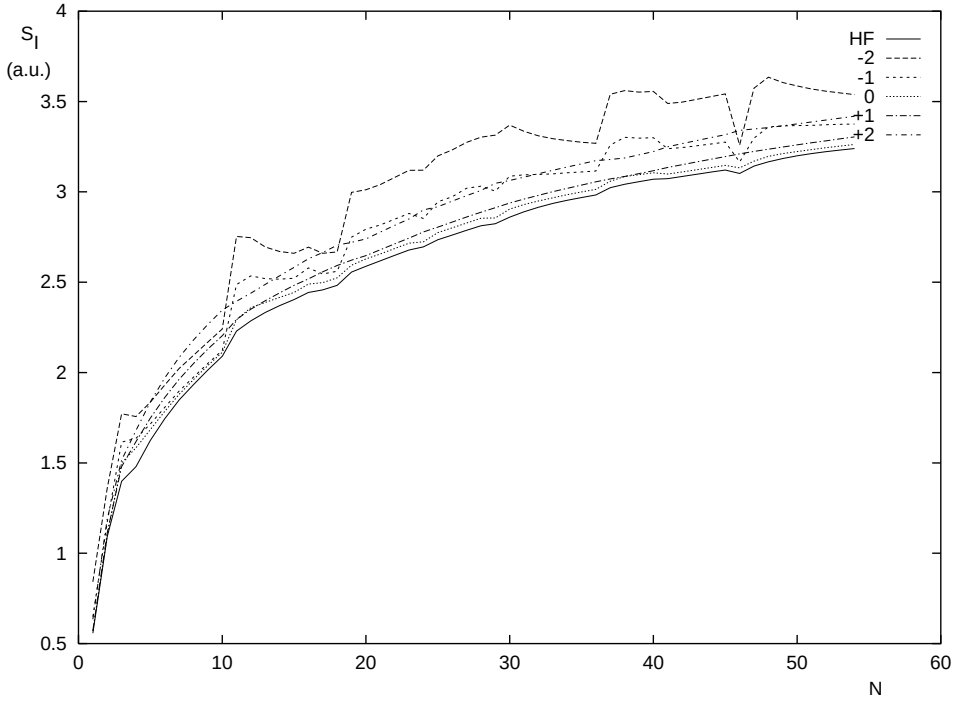

Fig. 6. Comparison among the entropies of the normalized-to-unity ME approximations $I^{\alpha}_{\rm ME}(p)$ ($\alpha = 0, \pm 1, \pm 2$) and the Hartree-Fock (HF) radial density $I(p)$ for atomic systems with $1 \leq N \leq 54$. Atomic units are used.

5 Conclusions

There always exists a unique solution to the problem of finding the Maximum-Entropy distribution constrained by the normalization, the geometric mean and (i) the logarithmic uncertainty, or (ii) a radial expectation value of arbitrary order. In the first case, the ME solution is analytically determined, while in the second case the calculation of only one of the Lagrange multipliers has to be done numerically.

A numerical study of the ME solutions to the radial distributions of neutral atoms from hydrogen to xenon, in both position and momentum spaces, shows up that the more accurate approximations are those constrained by the logarithmic uncertainty or by the radial expectation value of order one ($\langle r \rangle$ in position space, $\langle p \rangle$ in momentum space). In view of the simplicity and the accuracy of the approximations involving logarithmic constraints (specially compared to the ones obtained only in terms of radial expectation values), the experimental determination of such logarithmic averages appears to be very interesting. Moreover, from the point of view of the ME technique, the results we show here reveal that, on improving the ME approximations, it is better to consider logarithmic constraints than increasing the number of the radial ones.

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