Maximum-Entropy Analysis of Momentum Densities in Diatomic Molecules

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ABSTRACT

The one-particle density in momentum space $\gamma(p)$ is studied for diatomic molecules by using the maximum-entropy technique. The knowledge of one or more momentum expectation values $\langle p^n \rangle$ provides approximations on the density $\gamma(p)$ for any value of the momentum, which are convergent when increasing the number of known moments. Other unknown expectation values are estimated in terms of the constructed maximum-entropy densities. A numerical study of the quality of the approximations is carried out by means of experimental and theoretical data for the momentum expectation values involved. Experimental errors are also taken into account to have an idea of the sensibility of the results to the information from which they are obtained. © 1997 John Wiley & Sons, Inc.

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Introduction

The study of atomic and molecular systems in terms of their electron densities has been a subject of considerable interest and the focus of much research because it provides a good description of the electronic structure of such systems.

The charge density, $\rho(\mathbf{r})$, defined as

$$\rho(\mathbf{r}) = N\int \Psi^*(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N) \times \Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)\, d\mathbf{r}_2 \ldots d\mathbf{r}_N \quad (1)$$

(where Ψ is the wave function of the N-electron system and sumation over spins is implicit), is a quantity which can be indirectly deduced from elastic X-ray and electron scattering experiments [1] and is the basic variable in the study of many physical properties of atoms and molecules from a density functional theory perspective [2].

Historically, most of quantum chemistry has been carried out from the position space point of view, leading to concepts in traditional chemistry based upon this particular approach: bond lengths and angles, atomic radii, electronegativity, etc. Some authors have claimed that although the Hohenberg–Kohn theorem establishes that the energy of a nondegenerate ground state is a functional of the associated charge density, it does not provide an explicit functional and therefore the charge density does not always give us all the information about the system of interest [3].

The complementary quantity to $\rho(\mathbf{r})$ in momentum space, i.e., the electron momentum density $\gamma(\mathbf{p})$, is defined as

$$\gamma(\mathbf{p}) = N\int \phi^*(\mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N) \times \phi(\mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N)\, d\mathbf{p}_2 \ldots d\mathbf{p}_N, \quad (2)$$

where $\phi(\mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N)$ is the momentum space wave function obtained by $3N$-dimensional Fourier–Dirac transform of the position wave function as

$$\phi(\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N) = (2\pi)^{-3N/2}\int \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \times \exp\left\{ i\sum_{j=1}^{N} \mathbf{p}_j \cdot \mathbf{r}_j \right\} d\mathbf{r}_1 \ldots d\mathbf{r}_N. \quad (3)$$

This momentum density is also directly related to the Compton profiles which are obtained experimentally [4] and is a natural and potential source of additional information.

However, while the coordinate space density has been studied extensively, the momentum density still remains difficult to visualize and interpret as compared to its position counterpart $\rho(\mathbf{r})$. On the other hand, the relationship between both densities in the conjugate spaces is far from direct.

Relevant physical magnitudes are the moments of $\gamma(\mathbf{p})$,

$$\mu_k = \frac{\langle p^{k-2} \rangle}{4\pi} = \frac{1}{4\pi}\int p^{k-2}\gamma(\mathbf{p})\, d\mathbf{p} = \frac{1}{4\pi}\int_0^\infty p^{k-2} I(p)\, dp = \int_0^\infty p^k \gamma(p)\, dp, \quad (4)$$

defined in terms of the momentum density, the spherically averaged momentum density $\gamma(p)$, or the radial momentum density $I(p)$ given by

$$I(p) = 4\pi p^2 \gamma(p) = p^2 \int \gamma(\mathbf{p})\, d\Omega_p. \quad (5)$$

The normalization $\langle p^0 \rangle = N$ is used throughout.

There has been considerable interest in recent years in one-electron momentum distributions of molecules to implement the information on electron localization obtained from the charge distributions [5]. A few investigations on the symmetry and extremal properties [6] and studies on the anisotropy [7] of the momentum density in molecules have also been done.

Relations between magnitudes in position and momentum space are of great importance because they allow one to translate information between the conjugate spaces [8]. Moments of the momentum density have been related to charge density power integrals and interelectronic repulsion in diatomic molecules [9]. On the other hand, some general and rigorous inequalities involving radial expectation values in coordinate and momentum spaces have been obtained [10]. Koga and Morita also investigated the origin and nature of interatomic interactions in terms of the momentum density [11] and constructed inference momentum densities from energy constraints [12].

The obtention of approximate (model-independent) momentum densities has also been an important task owing to the above considerations. Information theory has revealed as a powerful approach to obtain unknown probability distributions when only partial information is given [13]. The maximum entropy (ME) principle states that when only limited knowledge about a probability density is available we should choose, among the densities compatible with the constraints, the one that has the maximum entropy. This is so because the entropy concentration theorem [14] shows that the great majority of the allowed distributions concentrate around the one of maximum entropy.

In this article, we use this inference principle to obtain approximate molecular momentum densities from growing information based on momentum expectation values. Previously, information theory has been used to construct approximate radial momentum densities $I(p)$ and isotropic Compton profiles $J(q)$ of atoms and molecules, when only normalization and an additional constraint is used [15, 16]. The resultant inferential analytical densities were qualitatively acceptable. More sophisticated analyses, including bounds and ME approximations for atomic systems, have been recently done [17, 18].

Our aim was to obtain the necessary conditions that the moments of the momentum density of some diatomic molecules must satisfy in order to have ME momentum density and to obtain and compare successive approximations to this magnitude. To check the goodness of these approximations, a numerical study with near-Hartree–Fock (NHF) and configuration interaction (CI) momentum densities was done. Additionally, the effects of the experimental errors of the moments on the results were also considered.

Maximum-Entropy Technique

The ME method, based on information theory, provides, among all the admissible momentum densities, the least biased function compatible with the information that we actually have. Considering the momentum density as an statistical probability density, the ME density is calculated by maximizing the information entropy functional

$$S[\gamma] \equiv -\int_0^\infty \gamma(p) \ln \gamma(p)\, dp \tag{6}$$

under the constraints given by the knowledge of its first few $M+1$ moments μ_k $(k = 0, 1, \ldots, M)$ as defined in Eq. (4).

Functional variation of $S[\gamma]$ subject to the moment constraints leads to the unique ME solution

$$\gamma_{12\ldots M}^{\mathrm{ME}} = \exp\left\{-\sum_{n=0}^{M} \lambda_n p^n\right\}, \tag{7}$$

where λ_0 is related to the normalization and the remaining Lagrange multipliers $\lambda_1, \ldots, \lambda_n$ must be numerically calculated from the extremely nonlinear system of equations:

$$\int_0^\infty p^n \gamma_{12\ldots M}^{\mathrm{ME}}(p)\, dp = \mu_n \qquad (n = 1, \ldots, M), \tag{8}$$

where the subscript $12\ldots M$ gives the list of moments included in the constraints. The information entropy associated to the solution can be readily calculated and it represents a measure of the information content of the given constraints:

$$S\left[\gamma_{12\ldots M}^{\mathrm{ME}}\right] = \sum_{n=0}^{M} \mu_n \lambda_n. \tag{9}$$

Two desirable features of this methodology have been recently obtained in the case of a semiinfinite or Stieltjes moment problem: existence of the ME density given by the $M+1$ assigned moments [19, 20] and entropy-convergence to the unknown density as the number of given moments increases [21].

Necessary and sufficient conditions for the existence of the ME solution, except for the cases $M = 2, 3$, are identical to the Stieltjes conditions for the solution of the reduced moment problem, i.e., the positivity of the Hankel determinants [19, 20] $\Delta_n (n = 0, 1, \ldots, 2k+1)$, where

$$\Delta_{2n} = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \vdots & \vdots & \ddots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n} \end{vmatrix}; \qquad \Delta_{2n+1} = \begin{vmatrix} \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{n+1} & \mu_{n+2} & \cdots & \mu_{2n+1} \end{vmatrix}. \tag{10}$$

Here, one has $2k = M$ or $2k+1 = M$ depending on the parity of the number M of normalized moments.

The simplest case, $M = 1$, can be analytically solved as

$$\gamma_1^{\mathrm{ME}}(p) = \frac{\mu_0^2}{\mu_1} \exp\left\{-\frac{\mu_0}{\mu_1} p\right\}. \tag{11}$$

It provides [11, 12, 15, 16] approximate relations between moment expectation values and other relevant quantities. It is worthy to note that similar relations can be obtained by using $I(p)$ or $J(q)$ as unknown densities in terms of their respective moments, easily related to those of $\gamma(p)$.

In a similar way, one obtains the more general solution subject to the constraints $\{\mu_0, \mu_k\}$:

$$\gamma_k^{\mathrm{ME}}(p) = \frac{k\mu_0}{\Gamma(1/k)}\left(\frac{\mu_0}{k\mu_k}\right)^{1/k} \times \exp\left\{-\frac{\mu_0}{k\mu_k}p^k\right\} \qquad (k > 0). \qquad (12)$$

The above relations can be expressed in terms of the radial expectation values by using Eq. (4). Some interesting examples are

$$\gamma_1^{\mathrm{ME}}(p) = \frac{\langle p^{-2}\rangle^2}{4\pi\langle p^{-1}\rangle}\exp\left\{-\frac{\langle p^{-2}\rangle}{\langle p^{-1}\rangle}p\right\} \qquad (13)$$

$$\gamma_2^{\mathrm{ME}}(p) = \left(\frac{\langle p^{-2}\rangle^3}{8\pi^3 N}\right)^{1/2}\exp\left\{-\frac{\langle p^{-2}\rangle}{2N}p^2\right\}. \qquad (14)$$

From these two ME solutions, approximations to the following expectation values are obtained in terms of $\langle p^{-2}\rangle$, $\langle p^{-1}\rangle$ and N:

$$\langle p^k\rangle_1^{\mathrm{ME}} = \int_0^\infty p^k\gamma_1^{\mathrm{ME}}(p)\,dp = \Gamma(k+3)\frac{\langle p^{-1}\rangle^{k+2}}{\langle p^{-2}\rangle^{k+1}} \qquad (k > -3)$$

$$\langle p^k\rangle_2^{\mathrm{ME}} = \int_0^\infty p^k\gamma_2^{\mathrm{ME}}(p)\,dp = \left[\frac{(2N)^{(k+2)}}{\pi}\right]^{1/2}\frac{\Gamma[(k+3)/2]}{\langle p^{-2}\rangle^{k/2}} \qquad (k > -3).$$

Moreover, taking into account Eq. (4), the information entropy of these approximations are

$$S[\gamma_1^{\mathrm{ME}}] = \mu_0\left(1 - \ln\frac{\mu_0^2}{\mu_1}\right) \qquad (15)$$

$$S[\gamma_2^{\mathrm{ME}}] = \frac{\mu_0}{2}\left(1 - \ln\frac{2\mu_0^3}{\pi\mu_2}\right). \qquad (16)$$

In the case $M = 2$, besides Hankel positivity, a supplementary upper bound on μ_2 must be satisfied in order to have an ME solution [22]. Similarly, Kociszewski [23] and Tagliani [19] found numerically and analytically the supplementary upper bound on μ_3 that allows one to have an ME solution for $M = 3$.

ME approximations for $M \geq 4$ always exists [19], provided that the Hankel constraints are fulfilled [see Eq. (10)]. Numerical computations of this kind of approximations revealed the complexity of the entropy functional. As an illustration, some approximate densities are calculated in the next section. We will focus our attention on the hydrogen (H_2) and nitrogen (N_2) molecules, for which some calculations in momentum space have been done during the last years.

Maximum-Entropy Densities

The hydrogen molecule H_2 is an excellent system for this kind of studies since both accurate theoretical and experimental work is available. Bench-mark calculations of momentum space properties of two-electron systems were based on multiconfigurational self-consistent-field (MCSCF) and configuration interaction (CI) wave functions which can be Fourier−Dirac-transformed without difficulty for most of the usual choices of underlying orbital basis set [24].

Jeziorski and Szalewicz [25] pointed out that wave functions built up from correlated Gaussian geminals can be Fourier−Dirac-transformed in a closed form. Momentum space properties of molecular hydrogen calculated from such a wave function were found to be in close agreement with those calculated from a large-scale configuration interaction wave function [26].

As an example, we reconstructed by ME methods the H_2 momentum distribution from the moments of Jeziorski and Szalewicz as well as from the experimental moments obtained by Lee [27]. Theoretical and experimental moments of molecular hydrogen do not fulfil the Kociszewski conditions; therefore, $\gamma_{123}(p)$ does not exist. Figure 1 shows the successive ME approximations using different moment information, together with the radial momentum distribution. It is apparent that the more information that is considered the more accurate the approximations are. Table I collects the predictions for the unknown expectation values of the different approximations.

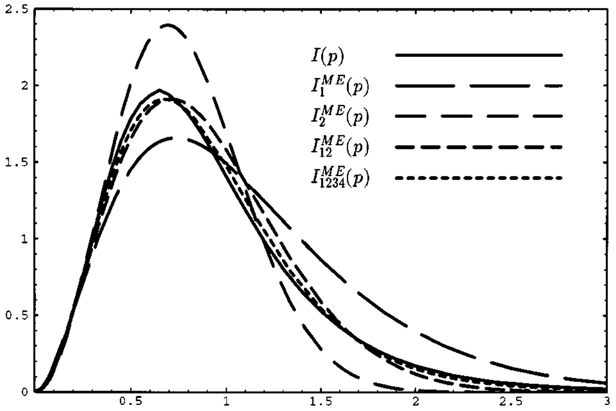

FIGURE 1. NHF [24] radial momentum density $I(p) = 4\pi p^2\gamma(p)$ and ME approximations $I_1^{\mathrm{ME}}(p)$, $I_2^{\mathrm{ME}}(p)$, $I_{12}^{\mathrm{ME}}(p)$, and $I_{1234}^{\mathrm{ME}}(p)$, where $I(p) \equiv 4\pi p^2\gamma(p)$, for the H_2 molecule. The theoretical moments were taken from [25]. Atomic units (au) are used.

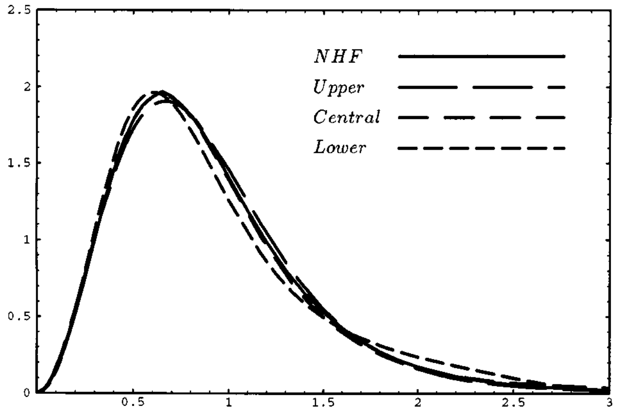

FIGURE 2. NHF [24] radial momentum density $I(p) = 4\pi p^2\gamma(p)$ and ME approximation $I_{1234}^{\mathrm{ME}}(p) \equiv 4\pi p^2\gamma_{1234}^{(\mathrm{ME})}(p)$, calculated for the upper, central, and lower sequences of moments of [27] for the H_2 molecule (see text for further details). Atomic units (au) are used.

Figure 2 shows the 4-moment approximation obtained in terms of the experimental moments calculated from high-energy electron-impact spectroscopy. We have used three moment sequences: the central sequence and the lower and upper sequences by using, in a coherent manner, the error bars in the calculated moments, in order to have a first estimation of the spread of the aproximations.

In Figures 1 and 2, it is observed that there exists a strong agreement between all the approximations constructed, independently of the source (theoretical or experimental) of the moment sequences involved. In this sense, it is worthy to observe that the density at the origin $\gamma(0)$ associated to the lower ($\gamma(0) = 1.009$), central ($\gamma(0) = 1.288$), and upper ($\gamma(0) = 1.524$) ME approximations are, respectively, to be compared with the corresponding values shown in Table I. It is worthy to remark on the similarity among these values and those given in Table I.

TABLE I

Predictions given for the H_2 molecule by the first few ME approximations on the values of the momentum density at the origin, $\gamma(0)$, and some radial expectation values $\langle p^n \rangle$, compared with the Hartree–Fock ones; atomic units (au) are used.

	$\gamma(0)$	$\langle p \rangle$	$\langle p^2 \rangle$	$\langle p^3 \rangle$
γ_{HF}	1.169	1.857	2.351	4.218
γ_1^{ME}	1.797	2.494	3.674	6.765
γ_2^{ME}	1.077	1.565	1.442	1.505
$\gamma_{12}^{\mathrm{ME}}$	1.521	1.781	1.956	2.514
$\gamma_{1234}^{\mathrm{ME}}$	1.421	1.857	2.351	4.240

The momentum distribution of the nitrogen molecule, N_2, in its ground electronic state was also studied by a variety of experimental [28] and theoretical [29] methods. In spite of many efforts, the quality of these calculations are not as accurate as those of helium or molecular hydrogen.

Some momentum space properties of N_2 were computed not only from an NHF wave function but also from a CI wave function [30] that was substantially more accurate than those used in previous calculations of this nature. We reconstructed the N_2 momentum density from the CI expectation values calculated in [30] and from experimental moments obtained by means of electron-impact experiments [31].

Concerning the existence conditions, it is remarkable that, for the N_2 molecule, (i) the CI moments verify the existence condition of Dowson and Wragg [22] (i.e., γ_{12} does exist) while the NHF ones do not (i.e., γ_{123} does exist), (ii) in both cases, the values of the moments are very close to the limit case $\mu_0\,\mu_2 = 2\mu_1^2$, and therefore the above-mentioned approximations γ_{12} and γ_{123} are very similar to γ_1, and (iii) the central and lower sequences of experimental data verify the Dowson and Wragg condition while the upper do not.

Table II shows the predicted values on unknown quantities given by the different ME approximations. It is worthy to observe that

TABLE II

Predictions given for the N_2 molecule by the first few ME approximations on the values of the momentum density at the origin, $\gamma(0)$, and some radial expectation values $\langle p^n \rangle$, compared with the CI ones; atomic units (au) are used.

	$\gamma(0)$	$\langle p \rangle$	$\langle p^2 \rangle$	$\langle p^3 \rangle$
γ_{CI}	1.321	38.294	218.6	2268.2
γ_1^{ME}	2.002	27.982	74.51	248.01
γ_2^{ME}	1.127	21.023	37.19	74.469
γ_{1234}^{ME}	1.526	38.294	218.6	1831.4

$\gamma_{1234}(0) = 1.578$ is closer to the "experimental" values (around 1.6 ± 0.2 [30]) than to the CI one.

Figure 3 shows the ME approximations to $I(p)$ obtained by using the above CI information. Because the CI γ_{12} (and also the NHF γ_{123}) is very similar to γ_1, it is omitted in the figure.

In Figure 4, the 4-moment ME approximation of N_2 is plotted for the upper, central, and lower sequences of experimental values given in [31]. Similar comments on the agreement of solutions to those given in the H_2 case can be done for the N_2 diatomic molecule.

We have also calculated the allowed moment region for the existence of γ_{12}^{ME} and γ_{123}^{ME} approximations (Fig. 5). Results for the 35 light diatomic molecules studied in [9] are quoted in Figure 1. Regions I and II show, respectively, the allowed and forbidden Kociszewski regions for the existence of ME momentum densities, having prescribed the first three normalized moments. The figure, plotted in terms of the relative moments defined as $\overline{\mu}_n = \mu_0^{n-1}\mu_n/\mu_1^n$, also shows the allowed region for γ_{12}^{ME}, which is $1 < \overline{\mu}_2 < 2$.

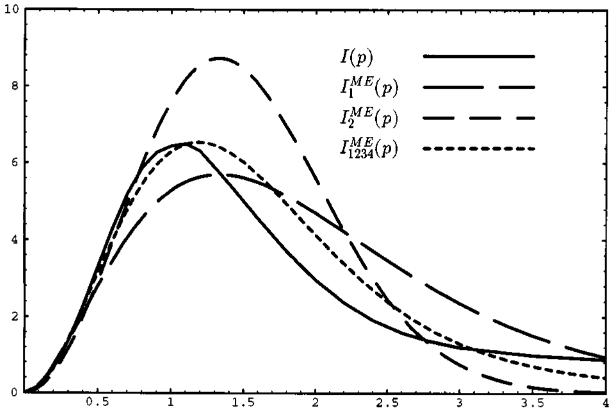

FIGURE 3. CI [30] radial momentum density $I(p) = 4\pi p^2\gamma(p)$ and ME approximations $I_1^{ME}(p)$, $I_2^{ME}(p)$, and $I_{1234}^{ME}(p)$, where $I(p) \equiv 4\pi p^2\gamma(p)$, for the N_2 molecule. The theoretical moments were taken from [30]. Atomic units (au) are used.

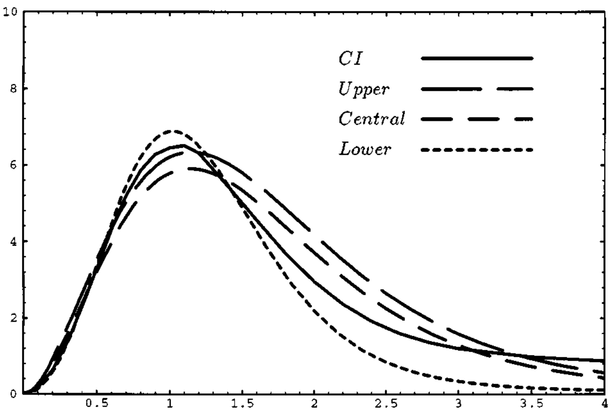

FIGURE 4. CI [30] radial momentum density $I(p) = 4\pi p^2\gamma(p)$ and ME approximation $I_{1234}^{ME}(p) \equiv 4\pi p^2\gamma_{1234}^{(ME)}(p)$, calculated for the upper, central, and lower sequences of moments of [31] for the N_2 molecule (see text for further details). Atomic units (au) are used.

Conclusions

The ME technique has been successfully used to approximate unknown momentum densities of diatomic molecules from the knowledge of a very small set of experimental or theoretical data, i.e., the first few radial expectation values of the density. Those approximations allow one to estimate the values of other unknown and physically relevant properties of the system (e.g., moments and local values of the density). The obtained results are (i) the least biased ones by the information not used, and (ii) convergent to the exact values of the approximated quantities.

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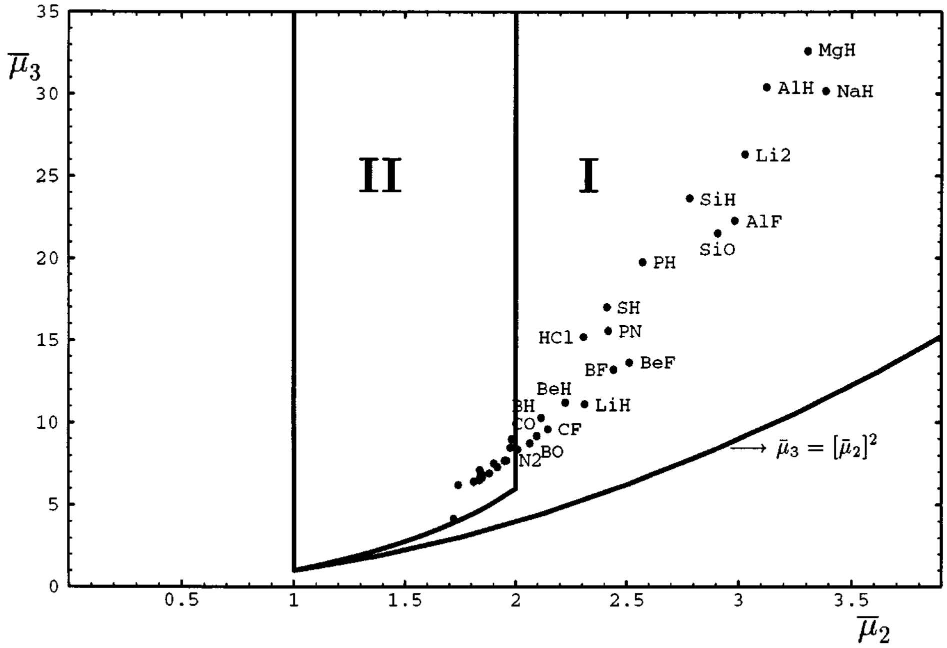

FIGURE 5. Existence conditions for ME distributions having prescribed the first three moments in terms of relative moments $\overline{\mu}_2 = \mu_0 \mu_2/\mu_1^2$ and $\overline{\mu}_3 = \mu_0^2 \mu_3/\mu_1^3$. Regions I and II represent the positivity inequalities for these relative moments. Moreover, region I is allowed and region II is forbidden for the existence of an ME distribution in accordance with the Kociszewski [23] conditions. The moments were taken from [9]. Atomic units (au) are used.

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