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Isomorphism in electron-pair densities of atoms

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Abstract. The spherically averaged electron-pair intracule (relative motion) $h(u)$ and extracule (center-of-mass motion) $d(R)$ densities are a couple of densities which characterize the motion of electron pairs in atomic systems. We study a generalized electron-pair density $g(q; a, b)$ that represents the probability density function for the magnitude of two-electron vector $a\mathbf{r}_j + b\mathbf{r}_k$ of any pair of electrons j and k to be q, where a and b are nonzero real numbers. In particular, $h(u) = g(u;1, -1)$ and $d(R) = g(R;\frac{1}{2},\frac{1}{2})$. It is shown that the scaling property of the Dirac delta function and the inversion symmetry of orbitals in atoms due to the central force field generate several isomorphic relations in the electron-pair density $g(q; a, b)$ with respect to the two parameters a and b. The approximate isomorphism $d(R) \cong 8h(2R)$ known in the literature between the intracule and extracule densities is a special case of the present results.

Key words: Isomorphism – Electron-pair density – Intracule density – Extracule density – Atoms

Introduction

The motion of an electron pair in N-electron atoms ($N \geq 2$) is characterized [1–3] by the spherically averaged intracule (relative motion) density $h(u)$,

$$h(u) \equiv (4\pi u^2)^{-1}\left\langle \sum_{j=1}^{N-1}\sum_{k=j+1}^{N} \delta(u - |\mathbf{r}_j - \mathbf{r}_k|) \right\rangle \tag{1}$$

and by the spherically averaged extracule (center-of-mass motion) density $d(R)$,

$$d(R) \equiv (4\pi R^2)^{-1}\left\langle \sum_{j=1}^{N-1}\sum_{k=j+1}^{N} \delta(R - |\mathbf{r}_j + \mathbf{r}_k|/2) \right\rangle \tag{2}$$

where $\delta(x)$ is the one-dimensional Dirac delta function and the angular brackets $\langle\rangle$ stand for the expectation value over the wave function $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ with $\mathbf{x}_j \equiv (\mathbf{r}_j, \sigma_j)$ being the combined position-spin coordinates of the electron j. The intracule density $h(u)$ represents [1–3] the probability density function for the relative distance $|\mathbf{r}_j - \mathbf{r}_k|$ of any pair of electrons j and k to be u. It has been used in several physical and chemical contexts particularly in relation to the electron correlation problem (see references given in [2, 3, 5–8]). On the other hand, the extracule density $d(R)$ represents [1–3] the probability density function for the center-of-mass radius $|\mathbf{r}_j + \mathbf{r}_k|/2$ of any pair of electrons j and k to be R. The density was used to study the shell structure in some atoms and bonding characteristics in simple molecules (see references in [2, 3, 9–12]).

Recently, the distributions of the intracule $h(u)$ and extracule $d(R)$ densities were examined [6, 7, 10, 11, 13] in a systematic manner for the 102 ground-state neutral atoms from He ($Z = 2$) to Lr ($Z = 103$), where Z denotes atomic number. At the Hartree-Fock limit level, it was found that for all the 102 atoms both the densities $h(u)$ and $d(R)$ are monotonically decreasing functions with a single maximum at $u = 0$ or $R = 0$. Moreover, an approximate but interesting isomorphism

$$d(R) \cong 8h(2R) \tag{3}$$

has been found empirically between the two densities in the above numerical studies. The relative motion and the center-of-mass motion of two particles are completely independent. Nevertheless, the approximate relation at Eq. (3) suggests that the coulombic binding in atomic systems generates nontrivial relations between the relative and center-of-mass motions of electrons.

To explore such relations, we study in the present paper the mathematical structure of a generalized electron-pair density $g(q; a, b)$ defined by

$$g(q; a, b) \equiv (4\pi q^2)^{-1}\left\langle \sum_{j=1}^{N-1}\sum_{k=j+1}^{N} \delta(q - |a\mathbf{r}_j + b\mathbf{r}_k|) \right\rangle \tag{4}$$

where a and b are nonzero real numbers. The density $g(q; a, b)$ represents the probability density function for the magnitude of two-electron vector $a\mathbf{r}_j + b\mathbf{r}_k$ of any pair of

electrons j and k to be q, and two particular cases $g(u;1,-1)$ and $g(R;\frac{1}{2},\frac{1}{2})$ correspond to the intracule $h(u)$ and extracule $d(R)$ densities, respectively. Based on a property of the Dirac delta function, it will be first shown that the density $g(q;\,a,\,b)$ is characterized by the ratio a/b, rather than individual values of a and b, for any wave functions. For atomic systems expressed by multi-determinant wave functions, we further find that the magnitude $|a/b|$ of the ratio is important for the space reflection symmetry of orbitals due to the central force field. The approximate isomorphism given by Eq. (3) is obtained as a special case of the present general results. Hartree atomic units are used throughout.

General scaling relations

For a nonzero real number c, the Dirac delta function $\delta(x)$ satisfies [14] a scaling relation

$$\delta(cx) = \frac{1}{|c|}\,\delta(x) \tag{5}$$

Application of Eq. (5) to Eq. (4) yields a general relation

$$g(q;a,b) = |c|^3 g(|c|q;ac,bc) \tag{6a}$$

where c is any nonzero real number. Two special cases of Eq. (6a) for $c = 1/a$ and $c = 1/b$ are

$$g(q;a,b) = \frac{1}{|a|^3}\,g\left(\frac{q}{|a|};1,\frac{b}{a}\right) = \frac{1}{|b|^3}\,g\left(\frac{q}{|b|};\frac{a}{b},1\right) \tag{6b}$$

for any types of wave functions. The result is valid not only for atoms but also for molecules. Equation (6b) implies that apart from the scale factor $|a|$ (or $|b|$), the ratio b/a (or a/b) determines the shape of the electron-pair density $g(q;\,a,\,b)$ as a function of q; individual values of a and b are not important. Particular cases of Eq. (6b) for the intracule $h(u)$ and extracule $d(R)$ densities read

$$h(u) \equiv g(u;1,-1) = g(u;-1,1) \tag{7a}$$

$$d(R) \equiv g(R;\tfrac{1}{2},\tfrac{1}{2}) = 8g(2R;1,1) \tag{7b}$$

We define moments $\langle q^n\rangle_{(a,b)}$ of the electron-pair density $g(q;\,a,\,b)$ by

$$\langle q^n\rangle_{(a,b)} \equiv 4\pi \int_0^\infty dq\; q^{n+2} g(q;a,b) \tag{8}$$

Combination of Eqs. (6a), (6b), and (8) then yields

$$\begin{aligned}\langle q^n\rangle_{(a,b)} &= |c|^{-n}\langle q^n\rangle_{(ac,bc)} = |a|^n\langle q^n\rangle_{(1,b/a)} \\ &= |b|^n\langle q^n\rangle_{(a/b,1)}\end{aligned} \tag{9}$$

which gives scaling relations

$$\langle u^n\rangle \equiv \langle q^n\rangle_{(1,-1)} = \langle q^n\rangle_{(-1,1)} \tag{10a}$$

$$\langle R^n\rangle \equiv \langle q^n\rangle_{(1/2,1/2)} = 2^{-n}\langle q^n\rangle_{(1,1)} \tag{10b}$$

for the intracule $\langle u^n\rangle$ and extracule $\langle R^n\rangle$ moments.

In polar coordinates, the three-dimensional Dirac delta function $\delta^{(3)}(\mathbf{r})$ satisfies [14]

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \frac{1}{r^2}\,\delta(r-r')\delta(\cos\theta-\cos\theta')\delta(\phi-\phi') \tag{11a}$$

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = (2\pi)^{-3}\int d\mathbf{s}\;\exp[+i(\mathbf{r}-\mathbf{r}')\cdot\mathbf{s}] \tag{11b}$$

Then Eq. (4) can be rewritten as

$$\begin{aligned}g(q;a,b) &= (4\pi)^{-1}\int d\Omega_q \left\langle \sum_{j=1}^{N-1}\sum_{k=j+1}^{N}\delta^{(3)}[\mathbf{q}-(a\mathbf{r}_j+b\mathbf{r}_k)]\right\rangle \\ &= (2\pi^2)^{-1}\int_0^\infty ds\; s^2 j_0(qs)\,X(s;a,b)\end{aligned} \tag{12a}$$

where $\mathbf{q} \equiv (q,\Omega_q)$ with $\Omega_q \equiv (\theta_q,\phi_q)$, $j_l(x)$ is the spherical Bessel function of the first kind, and

$$\begin{aligned}X(s;a,b) &\equiv (4\pi)^{-1}\int d\Omega_s \\ &\times \left\langle \sum_{j=1}^{N-1}\sum_{k=j+1}^{N}\exp(-ia\mathbf{s}\cdot\mathbf{r}_j)\exp(-ib\mathbf{s}\cdot\mathbf{r}_k)\right\rangle\end{aligned} \tag{12b}$$

in which $\mathbf{s} \equiv (s,\Omega_s)$ with $\Omega_s \equiv (\theta_s,\phi_s)$. The characteristic function $X(s;\,a,\,b)$ of $g(q;\,a,\,b)$ satisfies

$$\begin{aligned}X(s;a,b) &= X\left(\frac{s}{|c|};ac,bc\right) = X\left(|a|s;1,\frac{b}{a}\right) \\ &= X\left(|b|s;\,\frac{a}{b},1\right)\end{aligned} \tag{13}$$

Combination of Eqs. (12a) and (13) again results in Eqs. (6a) and (6b).

Decomposition into orbital quadruplets

We consider an N-electron wave function $\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)$ expressed by a linear combination of Slater determinants composed of a set of one-electron spin-orbitals, in which the κ-th spin-orbital is assumed to be a product of orthonormal spatial $\psi_\kappa(\mathbf{r})$ and spin $\eta_\kappa(\sigma)$ functions. Then the characteristic function $X(s;\,a,\,b)$ is rearranged (cf. [15]) as

$$X(s;a,b) = \sum_{\kappa\lambda\mu\nu} C_{\kappa\lambda\mu\nu}\,X_{\mu\nu}^{\kappa\lambda}(s;a,b) \tag{14a}$$

where the coefficient $C_{\kappa\lambda\mu\nu}$ gathers the contributions from the coefficients of two Slater determinants, spin integrals, and the permutation parities of relevant spin-orbitals. Note that $C_{\kappa\lambda\mu\nu}$ is independent of a and b. The orbital component $X_{\mu\nu}^{\kappa\lambda}(s;a,b)$ is defined by

$$X_{\mu\nu}^{\kappa\lambda}(s;a,b) \equiv (4\pi)^{-1}\int d\Omega_s f_{\kappa\lambda}^*(\mathbf{s};a) f_{\mu\nu}(-\mathbf{s};b) \tag{14b}$$

$$\begin{aligned}f_{\kappa\lambda}(\mathbf{s};a) &\equiv \int d\mathbf{r}\exp(+ia\mathbf{s}\cdot\mathbf{r})\psi_\kappa^*(\mathbf{r})\psi_\lambda(\mathbf{r}) \\ &= f_{\lambda\kappa}^*(-\mathbf{s};a) = f_{\lambda\kappa}^*(\mathbf{s};-a)\end{aligned} \tag{14c}$$

and satisfies scaling relations analogous to Eq. (13):

$$X_{\mu\nu}^{\kappa\lambda}(s;a,b) = X_{\mu\nu}^{\kappa\lambda}\left(\frac{s}{|c|};ac,bc\right) = X_{\mu\nu}^{\kappa\lambda}\left(|a|s;1,\frac{b}{a}\right) = X_{\mu\nu}^{\kappa\lambda}\left(|b|s;\frac{a}{b},1\right) \tag{15}$$

Corresponding to Eq. (14a), the electron-pair density $g(q;\, a,\, b)$ is also decomposed into orbital components:

$$g(q;a,b) = \sum_{\kappa\lambda\mu\nu} C_{\kappa\lambda\mu\nu}\; g_{\mu\nu}^{\kappa\lambda}(q;a,b) \tag{16a}$$

$$g_{\mu\nu}^{\kappa\lambda}(q;a,b) = (2\pi^2)^{-1} \int_0^\infty ds\; s^2 j_0(qs)\; X_{\mu\nu}^{\kappa\lambda}(s;a,b) \tag{16b}$$

Equations (15) and (16b) give

$$g_{\mu\nu}^{\kappa\lambda}(q;a,b) = |c|^3 g_{\mu\nu}^{\kappa\lambda}(|c|q;ac,bc) = \frac{1}{|a|^3} g_{\mu\nu}^{\kappa\lambda}\left(\frac{q}{|a|};1,\frac{b}{a}\right) = \frac{1}{|b|^3} g_{\mu\nu}^{\kappa\lambda}\left(\frac{q}{|b|};\frac{a}{b},1\right) \tag{17}$$

which is an orbital version of Eqs. (6a) and (6b). For a particular case of single-determinant Hartree-Fock wave functions, Eqs. (14a) and (16a) read

$$X(s;a,b) = \sum_{\kappa=1}^{N-1} \sum_{\lambda=\kappa+1}^{N} \left[X_{\lambda\lambda}^{\kappa\kappa}(s;a,b) - \delta_s(\kappa,\lambda) X_{\kappa\lambda}^{\kappa\lambda}(s;a,b)\right] \tag{18a}$$

$$g(q;a,b) = \sum_{\kappa=1}^{N-1} \sum_{\lambda=\kappa+1}^{N} \left[g_{\lambda\lambda}^{\kappa\kappa}(q;a,b) - \delta_s(\kappa,\lambda) g_{\kappa\lambda}^{\kappa\lambda}(q;a,b)\right] \tag{18b}$$

where $\delta_s(\kappa,\, \lambda)$is unity if the spin-orbitals κ and λ have the same spin and is zero if they have different spins. In the brackets of Eqs. (18a) and (18b), the first terms are ''direct'' contributions, while the second terms are ''exchange'' contributions.

Isomorphism for atoms

We further restrict our discussion to an atomic system, in which the spatial function $\psi_\kappa(\mathbf{r})$ is given by a product of radial $R_\kappa(r)$ and spherical harmonic $Y_{l_\kappa m_\kappa}(\Omega_r)$ functions:

$$\psi_\kappa(\mathbf{r}) = R_\kappa(r) Y_{l_\kappa m_\kappa}(\Omega_r) \tag{19}$$

For a vector $\mathbf{s} = (s, \theta_s, \phi_s)$, we have $a\mathbf{s} = (as, \theta_s, \phi_s)$ if $a > 0$ while $a\mathbf{s} = (|a|s, \pi - \theta_s, \phi_s + \pi)$ if $a < 0$, and the space reflection symmetry [16] of a spherical harmonic is

$$Y_{lm}(\pi - \theta_s, \phi_s + \pi) = (-1)^l Y_{lm}(\theta_s, \phi_s) \tag{20}$$

Therefore, the plane wave expansion [16]

$$\exp(+i\mathbf{s}\cdot\mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(sr)\; Y_{lm}^*(\Omega_s)\; Y_{lm}(\Omega_r) \tag{21a}$$

is generalized to

$$\exp(+ia\mathbf{s}\cdot\mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [i\mathrm{sgn}(a)]^l j_l(|a|sr) \times Y_{lm}^*(\Omega_s)\; Y_{lm}(\Omega_r) \tag{21b}$$

where $\mathrm{sgn}(x)$ is the signum function [17]. Substituting Eqs. (19) and (21b) into Eq. (14c) and performing the angular integrations in Eq. (14c), we find

$$f_{\kappa\lambda}(\mathbf{s};a) = \sqrt{4\pi} \sum_{l=|l_\kappa - l_\lambda|}^{l_\kappa + l_\lambda} [i\mathrm{sgn}(a)]^l \sqrt{2l+1} \times c^l(\kappa;\lambda) Y_{l,m_\kappa - m_\lambda}^*(\Omega_s)\; W_{l\kappa\lambda}(|a|s) \tag{22a}$$

where

$$W_{l\kappa\lambda}(s) \equiv \int_0^\infty dr\; r^2 j_l(sr)\; R_\kappa^*(r)\; R_\lambda(r) = W_{l\lambda\kappa}^*(s) \tag{22b}$$

and $c^l(\kappa;\lambda) \equiv c^l(l_\kappa m_\kappa; l_\lambda m_\lambda)$ is the Condon-Shortley parameter [18]. Using Eq. (22a), the explicit form of $X_{\mu\nu}^{\kappa\lambda}(s;\, a,\, b)$ [Eq. (14b)] for atomic systems is obtained as

$$X_{\mu\nu}^{\kappa\lambda}(s;a,b) = \sum_{l=\max(|l_\kappa - l_\lambda|, |l_\mu - l_\nu|)}^{\min(l_\kappa + l_\lambda, l_\mu + l_\nu)} [-\mathrm{sgn}(ab)]^l (2l+1) \times c^l(\kappa;\lambda) c^l(\mu;\nu) W_{l\kappa\lambda}^*(|a|s) W_{l\mu\nu}(|b|s) \tag{23}$$

if $l_\kappa + l_\lambda + l_\mu + l_\nu = \text{even}$ and $m_\kappa - m_\lambda = m_\mu - m_\nu$. When these two conditions are not satisfied simultaneously, $X_{\mu\nu}^{\kappa\lambda}(s;\, a,\, b)$ vanishes. The two particular cases of Eq. (23) are

$$X_{\lambda\lambda}^{\kappa\kappa}(s;a,b) = \sum_{l=0}^{\min(2l_\kappa, 2l_\lambda)} (2l+1)\; c^l(\kappa;\kappa) \times c^l(\lambda;\lambda) W_{l\kappa\kappa}^*(|a|s) W_{l\lambda\lambda}(|b|s) \tag{24a}$$

$$X_{\kappa\lambda}^{\kappa\lambda}(s;a,b) = \sum_{l=|l_\kappa - l_\lambda|}^{l_\kappa + l_\lambda} [-\mathrm{sgn}(ab)]^l (2l+1) \times [c^l(\kappa;\lambda)]^2 W_{l\kappa\lambda}^*(|a|s) W_{l\kappa\lambda}(|b|s) \tag{24b}$$

which appear in Eq. (18a) for single-determinant wave functions. Note that the summations in Eqs. (22a), (23), (24a), and (24b) run over every other integers between the specified values.

Since $l_\kappa + l_\lambda + l_\mu + l_\nu = \text{even}$, Eq. (23) means that if $l_\kappa + l_\lambda = \text{even}$, the contribution of $[-\mathrm{sgn}(ab)]^l$ is always unity and hence

$$X_{\mu\nu}^{\kappa\lambda}(s;a,b) = X_{\mu\nu}^{\kappa\lambda}(s;|a|,|b|) \tag{25a}$$

$$g_{\mu\nu}^{\kappa\lambda}(q;a,b) = g_{\mu\nu}^{\kappa\lambda}(q;|a|,|b|) \tag{25b}$$

Namely, only the absolute values of the parameters a and b are important for such orbital components, as in the case of Eq. (24a). Moreover, the scaling relations (Eq. 17) conclude that the magnitude $|a/b|$ of the ratio of the two parameters governs the shape of the orbital component $g_{\mu\nu}^{\kappa\lambda}$ $(q;\, a,\, b)$ of the electron-pair density,

$$g_{\mu\nu}^{\kappa\lambda}(q;a,b) = |c|^3 g_{\mu\nu}^{\kappa\lambda}(|c|q;|ac|,|bc|)$$
$$= \frac{1}{|a|^3} g_{\mu\nu}^{\kappa\lambda}\left(\frac{q}{|a|};1,\left|\frac{b}{a}\right|\right)$$
$$= \frac{1}{|b|^3} g_{\mu\nu}^{\kappa\lambda}\left(\frac{q}{|b|};\left|\frac{a}{b}\right|,1\right) \quad (26)$$

If $l_\kappa + l_\lambda =$ odd, however, we do not have such relations in general.

The total electron-pair density $g(q; a, b)$ is the sum of both contributions from $l_\kappa + l_\lambda$, $l_\mu + l_\nu =$ even and $l_\kappa + l_\lambda$, $l_\mu + l_\nu =$ odd with the coefficients $C_{\kappa\lambda\mu\nu}$, and therefore we cannot derive any general yet rigorous relations like Eq. (26). In the Hartree-Fock approximation (see Eq. 18b), however, all the direct terms $g_{\lambda\lambda}^{\kappa\kappa}(q; a, b)$ as well as exchange terms $g_{\kappa\lambda}^{\kappa\lambda}(q;a,b)$ with $l_\kappa + l_\lambda =$ even obey Eq. (26) precisely, and only the remaining exchange terms with $l_\kappa + l_\lambda =$ odd violate the relation. The approximate isomorphism (Eq. 3) observed numerically [10, 11, 13, 19] between the intracule $h(u)$ and extracule $d(R)$ densities for atoms and ions suggests that the violation of the relation at Eq. (26) due to the exchange terms with $l_\kappa + l_\lambda =$ odd is not large. If we accept these numerical results, we reach an approximate isomorphism,

$$g(q;a,b) \cong g(q;|a|,|b|) = |c|^3 g(|c|q;|ac|,|bc|)$$
$$= \frac{1}{|a|^3} g\left(\frac{q}{|a|};1,\left|\frac{b}{a}\right|\right) = \frac{1}{|b|^3} g\left(\frac{q}{|b|};\left|\frac{a}{b}\right|,1\right) \quad (27)$$

for the electron-pair density $g(q; a, b)$ of atoms obtained from Hartree-Fock wave functions and from configuration-interaction wave functions with a predominant Hartree-Fock configuration. Equation (27) further predicts relations

$$\langle q^n\rangle_{(a,b)} \cong \langle q^n\rangle_{(|a|,|b|)} = |c|^{-n}\langle q^n\rangle_{(|ac|,|bc|)}$$
$$= |a|^n\langle q^n\rangle_{(1,|b/a|)} = |b|^n\langle q^n\rangle_{(|a/b|,1)} \quad (28)$$

for the electron-pair moments $\langle q^n\rangle_{(a,b)}$. Special cases of Eqs. (27) and (28) for $b = \pm a$ are

$$g(q;a,\pm a) \cong \frac{1}{|a|^3} g\left(\frac{q}{|a|};1,1\right) \quad (29)$$

$$\langle q^n\rangle_{(a,\pm a)} \cong |a|^n\langle q^n\rangle_{(1,1)} \quad (30)$$

which lead to $d(R) \cong 2^3 h(2R)$ and $\langle u^n\rangle \cong 2^n\langle R^n\rangle$ for the intracule and extracule properties.

Concluding remarks

We have shown that there exists the general yet rigorous isomorphism, Eqs. (6a) and (6b) for the electron-pair densities and Eq. (9) for the electron-pair moments, due to the scaling property of the Dirac delta function. Equations (6a), (6b), and (9) are valid for any wave functions of atoms and molecules. For atomic systems, the space reflection symmetry of wave functions, embodied by Eq. (20), further generates approximate but simplified isomorphism, Eq. (27) for the density, and Eq. (28) for the moments. The approximate relation between the intracule and extracule densities suggests that the electron correlation problem in atoms can be studied not only by the intracule density but also by the extracule density. Though the details are not given, the isomorphism found in this study also results in various relations in other electron-pair properties such as the radial and cumulative electron-pair densities and the coefficients of the Maclaurin expansion of the electron-pair densities (see [20]). We finally note that the mathematical structure of the electron-pair densities in momentum space is exactly the same as that in position space, and the present isomorphic relations also apply to the momentum-space electron-pair densities. Explicit results are simply obtained by replacing the names of functions and variables in position space with the corresponding appropriate names in momentum space.

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