Fisher and Shannon information from one-matrix. Link to the kinetic energy

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A six-dimentional distribution function F is constructed from the one-matrix of a non-interacting system. For double occupied orbitals and real one-matrix, the Fisher information I_F constructed from the distribution function F is proportional to the non-interacting kinetic energy T_s. A local six-dimensional wave-vector q is defined that establishes a link between the Shannon and Fisher information and the local kinetic energy. Illustrative examples for Coulomb systems are presented.

I. INTRODUCTION

The link between information theory and quantum mechanical kinetic energy was first established by Sears, Parr and Dinur [1] three decades ago. They derived an expression for the kinetic energy

$$T = \frac{1}{8}I_n + \frac{1}{8}\int n(\mathbf{r})\tilde{i}_f(\mathbf{r})d\mathbf{r}, \tag{1}$$

where the first term is proportional to Fisher information [2]

$$I_n = \int \frac{|\nabla n|^2}{n}d\mathbf{r} \tag{2}$$

constructed from the electron density n

$$n(\mathbf{r}) = N \int |\Psi(\mathbf{r}, \sigma_1, \mathbf{r}_2, \sigma_2, ..., \mathbf{r}_N, \sigma_N)|^2 d\sigma_1 d\mathbf{r}_2 d\sigma_2 ... d\mathbf{r}_N d\sigma_N, \tag{3}$$

and in the second term $\tilde{i}_f$ is a Fisher information density

$$\tilde{i}_f(1) = \int \frac{[\nabla_1 f(2, ..., N|1)]^2}{f(2, ..., N|1)}d2...dN \tag{4}$$

associated with the conditional density $f(2, ..., N|1) = |\Psi|^2/n(\mathbf{r})$. Ψ is the wave function. (They normalized the one-particle density to 1. In this paper n is normalized to N as is usually done in density functional theory. That is why we applied a different factor in Eq. (1).) The first term in Eq. (1) is the full Weizsäcker kinetic energy T_W [3].

The relationship between the Fisher information and the kinetic energy has been discussed in several papers [4–8, 10, 11]. Ghiringhelli, Hamilton and Delle Site [13] proposed that the second term in Eq. (1) is proportional to the Shannon information [14].

$$S_n = -\int n(\mathbf{r})\ln n(\mathbf{r})d\mathbf{r}, \tag{5}$$

constructed from the electron density n. Uncertainty-type lower bound to the Shannon information sum [15] to the entropy sum in complementary spaces was formulated by Gadre [16, 17]. The upper and lower bounds for the configuration and momentum space entropies were expressed with the kinetic energy [18].

The relationship between the Fisher and Shannon information has been studied by several authors [11, 12, 19]. Fisher information can be defined using pair density [20] and generalized pair density functions [21], as well, leading to interesting relation to the kinetic energy. Generalized Weizsäcker functionals, that is, Fisher information obtained from two-electron, three-electron distribution functions have recently been studied by Chakraborty and Ayers [22]. They found that higher-order Weizsäcker functionals fail in approximating the total kinetic energy.

In Section 2 we show, that one can construct a six-dimentional distribution function F from the one-matrix of the non-interacting system. In case we have double occupied orbitals and real one-matrix, the Fisher information I_F constructed from the distribution function F is proportional to the non-interacting kinetic energy T_s. In Section 3 a local six-dimensional wave-vector q is defined that establishes a link between the Shannon and Fisher information and the local kinetic energy. Section 4 presents illustrations for Coulomb systems and discussion.

II.   FISHER AND SHANNON INFORMATION FROM IDEMPOTENT ONE-MATRIX

Consider a non-interacting system with the wave function Φ. The one-matrix is defined as

$$\gamma(\mathbf{r}, \mathbf{r}') = N \int \Phi^*(\mathbf{r}', \sigma_1, \mathbf{r}_2, \sigma_2, ..., \mathbf{r}_N, \sigma_N) \Phi(\mathbf{r}, \sigma_1, \mathbf{r}_2, \sigma_2, ..., \mathbf{r}_N, \sigma_N) d\sigma_1 d\mathbf{r}_2 d\sigma_2 ... d\mathbf{r}_N d\sigma_N, \tag{6}$$

where N is the number of electrons. If we have double occupied orbitals ϕ_i, the one-matrix can also be written as

$$\gamma(\mathbf{r}, \mathbf{r}') = 2 \sum_{i=1}^{N/2} \phi_i^*(\mathbf{r}') \phi_i(\mathbf{r}). \tag{7}$$

For orthonormal orbitals we obtain that the one-matrix is idempotent:

$$\int \gamma(\mathbf{r}, \mathbf{r}_2) \gamma(\mathbf{r}_2, \mathbf{r}') d\mathbf{r}_2 = 2\gamma(\mathbf{r}, \mathbf{r}'). \tag{8}$$

Define now a six-dimensional probability density as

$$F(\mathbf{r}, \mathbf{r}') = \frac{1}{2N} |\gamma(\mathbf{r}, \mathbf{r}')|^2. \tag{9}$$

F is normalized to 1 as

$$\int F(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' = \frac{1}{2N} \int \gamma(\mathbf{r}', \mathbf{r}) \gamma(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' = \frac{1}{N} \int \gamma(\mathbf{r}, \mathbf{r}) d\mathbf{r} = 1. \tag{10}$$

Introducing the six-dimensional vector $\mathbf{R} = \mathbf{r}, \mathbf{r}'$ the Shannon and the Fisher information are defined as

$$S_F = \int s_F(\mathbf{R}) d\mathbf{R} \tag{11}$$

and

$$I_F = \int i_F(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' = \int i_F(\mathbf{R}) d\mathbf{R}, \tag{12}$$

where

$$s_F = -F(\mathbf{R}) \ln F(\mathbf{R}) \tag{13}$$

and

$$i_F(\mathbf{R}) = \frac{|\nabla_R F(\mathbf{R})|^2}{F(\mathbf{R})} \tag{14}$$

are the Shannon and the Fisher information densities.

For real one-matrix, the Fisher information I_F is proportional to the non-interacting kinetic energy T_s. Keeping in mind that the non-interacting kinetic energy T_s can be written as

$$T_s = \frac{1}{2} \int \nabla_{r_1} \nabla_{r_2} \gamma(\mathbf{r}_1, \mathbf{r}_2)|_{\mathbf{r}_2 = \mathbf{r}_1} d\mathbf{r}_1 \tag{15}$$

the idempotency condition (7) leads to

$$\begin{aligned} T_s &= \frac{1}{4} \int \nabla_{r_1} \nabla_{r_2} \gamma(\mathbf{r}_1, \mathbf{r}_3) \gamma(\mathbf{r}_3, \mathbf{r}_2)|_{\mathbf{r}_2 = \mathbf{r}_1} d\mathbf{r}_1 d\mathbf{r}_3 \\ &= \frac{1}{4} \int \nabla_{r_1} \gamma(\mathbf{r}_1, \mathbf{r}_3) \nabla_{r_1} \gamma(\mathbf{r}_3, \mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_3 \\ &= \frac{1}{8} \int \left[(\nabla_{r_1} \gamma(\mathbf{r}_1, \mathbf{r}_3))^2 + (\nabla_{r_3} \gamma(\mathbf{r}_1, \mathbf{r}_3))^2 \right] d\mathbf{r}_1 d\mathbf{r}_3. \end{aligned} \tag{16}$$

Using the six-dimensional vector $\mathbf{R}$ the non-interacting kinetic energy T_s takes the form

$$T_s = \int \tau_s(\mathbf{R})d\mathbf{R}, \tag{17}$$

where

$$\tau_s(\mathbf{R}) = \frac{1}{8}\left[\nabla_R\gamma(\mathbf{R})\right]^2 \tag{18}$$

is the local kinetic energy. Comparing Eqs. (9), (12),(17) and (18) we are led to the relation between the Fisher information I_F and the non-interacting kinetic energy T_s:

$$I_F = \frac{16}{N}T_s \tag{19}$$

and the corresponding local quantities:

$$i_F = \frac{16}{N}\tau_s. \tag{20}$$

On the other hand, it is known that the moments of the density F ($\langle R^a \rangle = \int R^a F(\mathbf{R})d\mathbf{R}$) are related with the Fisher information as [23]

$$I_F \geq (\beta + D - 1)^2 \frac{\langle r^{\beta-1}\rangle^2}{\langle r^{2\beta}\rangle}, \quad \beta \geq \max\{-D+1, -1\} \tag{21}$$

where D is the dimension of the system. So if we take $D = 6$ and $\beta = 1$ we can write

$$I_F \geq \frac{6^2}{\langle R^2 \rangle}. \tag{22}$$

Now, using equations (3) and (19) we obtain a bound between the non-interacting kinetic energy and the magnetic susceptibility

$$T_s \geq \frac{3^2}{2^3}\frac{N^2}{\langle r^2 \rangle} \tag{23}$$

with $\langle r^2 \rangle = \int r^2 n(\mathbf{r})d\mathbf{r}$. Writing the total non-interacting kinetic energy (Eq.(15)) as $T_s = \langle p^2 \rangle/2$ the uncertainty relation

$$\langle p^2 \rangle \langle r^2 \rangle \geq \frac{9N^2}{4} \tag{24}$$

can be obtained. This inequality was derived earlier by Gadre and Chakravorty [24]. We emphasize here that the idempotent non-interacting one-matrix was used in all inequalities. We can, however, use the fact that the total kinetic energy is related with the non-interacting kinetic energy by $T \geq T_s$ [9], where the total interacting kinetic energy T is given by a relation as Eq.(15) with the difference that the exact interacting one-matrix is applied instead of the idempotent non-interacting one-matrix. Therefore from inequality (23) one can readily obtain an equality for the total interacting kinetic energy T. However, it would be less sharper than (24).

Now, the relationship between the newly defined Shannon information S_F and the usual Shannon information S_n coming from the electron density is explored. Introduce the function f with the definition

$$\gamma(\mathbf{r}, \mathbf{r}') = n^{1/2}(\mathbf{r})n^{1/2}(\mathbf{r}')f(\mathbf{r}, \mathbf{r}'). \tag{25}$$

It can readily seen that $f(\mathbf{r}, \mathbf{r}) = 1$. From the idempotency (Eq. (8)) follows that

$$\int n(\mathbf{r}_2)f^2(\mathbf{r}, \mathbf{r}_2)d\mathbf{r}_2 = 2 \tag{26}$$

for any $\mathbf{r}_1$. Substituting Eq. (25) into Eq. (9) and Eq. (11) we obtain

$$S_F = \frac{2}{N}S_n + 2\ln N - \frac{1}{2N}\int f^2(\mathbf{R})\ln f^2(\mathbf{R})d\mathbf{R}. \tag{27}$$

For a one-level, two-electron system $f(\mathbf{r}, \mathbf{r}') = 1$ and this relation reduces to Eq. (45). This case is studied in Section 4.

III.   THE LOCAL WAVE-VECTOR, LINK BETWEEN THE SHANNON AND FISHER INFORMATION

Following Nagy, Romera and Liu [11, 12] the local wave-vector is defined as

$$\mathbf{q}(\mathbf{R}) = -\frac{\nabla_R F(\mathbf{R})}{F(\mathbf{R})}. \tag{28}$$

It can also be written as

$$\mathbf{q}(\mathbf{R}) = -\nabla_R(\ln F). \tag{29}$$

Eqs. (13),(14),(28) and (29) lead to the relations

$$\mathbf{q} = \nabla_R \left(\frac{s_F}{F}\right) \tag{30}$$

and

$$q^2 = \frac{i_F}{F}. \tag{31}$$

That is, the local wave-vector $\mathbf{q}$ provides a link between the Shannon and Fisher information: the local wave-vector is the gradient of the Shannon information per particle and the square of the local wave-vector is the Fisher information per particle. From Eqs. (20) and (31) follows the relationship between the local kinetic energy and local Fisher information:

$$\tau_s = \frac{N}{16} F q^2, \tag{32}$$

while, the non-interacting kinetic energy takes the form

$$T_s = \frac{N}{16} \int F q^2 d\mathbf{R}, \tag{33}$$

that is, the non-interacting kinetic energy is proportional to the average of the square of the wave vector.

IV.   RESULTS FOR COULOMB SYSTEMS

We illustrate the results above by Coulomb systems. Consider first the case when the γ has the form

$$\gamma = A \exp\left[-a(r_1 + r_2)\right] \tag{34}$$

and consequently F can be written

$$F = \frac{A^2}{2N} \exp\left[-2a(r_1 + r_2)\right]. \tag{35}$$

Expressions (34) and (35) are valid for the asymptotic region ($r_1 \to \infty$ and $r_2 \to \infty$) for any system in Coulomb external potential ($v(r) = -Z/r$) . Eq. (35) gives the asymptotic behaviour of the distribution function F with $a = \sqrt{2I}$, where I is the first ionization potential.

The Shannon and the Fisher information densities then take the form

$$s_F = -F[2 \ln A - \ln (2N) - 2a(r_1 + r_2)] \tag{36}$$

and

$$i_F = a^2 F = \frac{16}{N} \tau_s, \tag{37}$$

respectively.

$$\frac{s_F}{F} = -\ln \tau_s + \ln N a^2 - \ln 2 \tag{38}$$

The square of the local wave vector is

$$q^2 = 8a^2 = \frac{i_F}{F} = \frac{16}{N} \frac{\tau_s}{F}. \tag{39}$$

Consider, now, a zero-order approximation to the one-matrix for the He isoelectronic series [25] :

$$\gamma = \frac{Z - \alpha}{\pi} \exp\left[-(Z - \alpha)(r_1 + r_2)\right]. \tag{40}$$

We are led to the Shannon information

$$S_F = -6 \ln (Z - \alpha) + 6 + 2 \ln \pi \tag{41}$$

that can also be written as

$$S_F = -3 \ln T_s - 3 \ln 2 + 6 + 2 \ln \pi. \tag{42}$$

We mention here that Massen and Panos [26] proposed a relationship between the phase-space Shannon information and the kinetic energy.

The idempotent one-matrix for the He isoelectronic series can be written as :

$$\gamma = 2\phi_{1s}(r_1)\phi_{1s}(r_2), \tag{43}$$

where ϕ_{1s} is the one-electron orbital. The Shannon information has the the form

$$S_F = -2 \int n_{1s}(r) \ln (n_{1s}(r)) d\mathbf{r}, \tag{44}$$

where $n_{1s} = (\phi_{1s})^2$ is the one-electron density. The Shannon information S_n constructed from the electron density n (Eq. (5) can be related to the S_F:

$$S_F = S_n + 2 \ln 2. \tag{45}$$

Fig. 1 presents S_n and T_s. S_n has been numerically obtained using the analytical Hartree-Fock wave functions of Koga et al. [27] for the He isoelectronic series ($Z = 2$-9). The values of T_s have been obtained from reference [28]. We have fitted these values obtaining (with a c. c. of 0.95) that

$$S_n = -3.07 \ln T_s + 7.25 \tag{46}$$

in good agreement with Eq. (42) that can be written in terms of S_n as

$$S_n = -3 \ln T_s + 6.90. \tag{47}$$

Eq. (45) is valid only for a one-level, two-electron system. In other cases Eq. (27) should be used and the relationship between S_n and T_s cannot be described by expressions (46) or (47). It will be the subject of further research. Finally, we can utilize expression for the lower bound of S_n derived by Gadre and Bendale [18]:

$$S_n \geq 3N(1 + \ln \pi)/2 + (N \ln N)/2 - 3N \ln (3N/4T_s)/2. \tag{48}$$

Substituting T_s from Eq. (19) into Eq. (48) the inequality for S_n is expressed by the Fisher information I_F:

$$S_n \geq 3N(1 + \ln \pi)/2 + (N \ln N)/2 - 3N \ln (N/12I_F)/2. \tag{49}$$

In summary, a six-dimentional distribution function is constructed from the one-matrix of a non-interacting system. For double occupied orbitals and real one-matrix, the Fisher information obtaineed from the six-dimentional distribution function is proportional to the non-interacting kinetic energy. A local six-dimensional wave-vector q is defined that establishes a link between the Shannon and Fisher information: the local wave-vector is the gradient of the Shannon information per particle and the square of the local wave-vector is the Fisher information per particle. A relationship is explored between the non-interacting kinetic energy and the local wave-vector.
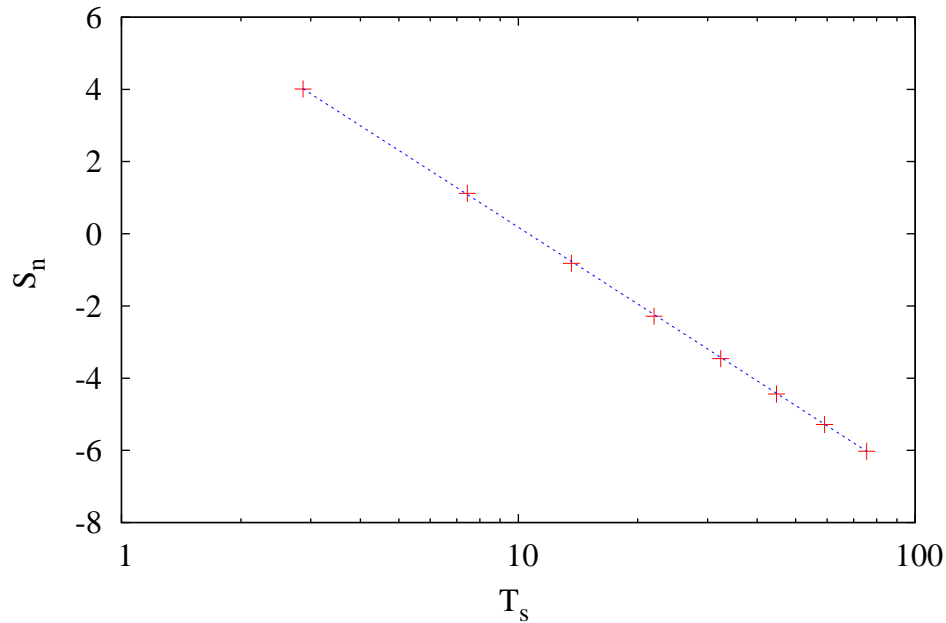
FIG. 1: S_n in terms of T_s for He-like ions. The crosses correspond to the Hartree-Fock values for the ions with nuclear charge $Z = 2 - 9$. The dashed line corresponds to equation (46). All the data are in atomic units.

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