Bounds for kinetic and exchange energies of fermion systems

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We show that the physical quantities of an A-fermion system expressed by means of integrals of powers of the single-particle density $\rho(\mathbf{r})$ are bounded by any kth moment around the origin $\langle r^k\rangle$ of ρ and A in a simple manner. As applications, the kinetic and semiclassical exchange energies of a neutral atom ($A=Z$) turn out to be bounded from below by $0.2184Z^{5/3}\langle r^{-1}\rangle^2$ and from above by $0.3046Z^{4/3}\langle r\rangle$, respectively. Comparison of these bounds with the microscopic values of the corresponding quantities is made. Similar bounds for the same quantities in nuclei are also given and analyzed.

I. INTRODUCTION

Single-particle density is a physical observable which plays a basic role in the quantum description of many fermion systems. There are many physical properties of atomic, molecular, and nuclear systems which can be interpreted in terms of the fermion density of the system. For instance, in the case of an atom at the ground state, the electron density fully characterizes[1,2] the system: All properties are functionals of the density.

It is also known[3–6] that the functionals of various physical quantities of fermionic systems (such as, e.g., the kinetic, Coulomb, and exchange energies) are, at least to the leading order, integrals of powers of the fermion density ρ. Or, using a rigorous statistical language, there exist some physical quantities which are frequency moments[7] of integer or fractional order of the density ρ. The aim of this work is to obtain bounds for any physical quantity of this type in terms of the total fermion number and an arbitrary moment around the origin of positive or negative order of the density ρ of the system. It will be argued that the moments of negative (positive) order give the best bounds for electronic (nucleonic) systems.

The paper is structured as follows. Section II contains the method to obtain the general expressions for the lower bounds of an arbitrary frequency moment of ρ. These expressions are used in Sec. III to find lower bounds for the Thomas-Fermi kinetic energy of atoms and nuclei. Here the Thomas-Fermi kinetic energy means the energy obtained via substituting an approximate Hartree-Fock charge density into the Thomas-Fermi appropriate functional. Emphasis will be put on atoms since a paper on the nuclear bounds has already been published.[8] In Sec. IV, the Dirac exchange energy of atoms and nuclei is bounded from above and not from below due to its global negative sign. Comparison with the exact or some approximate values obtained for these quantities by various authors is also done in Secs. III and IV.

II. METHOD AND GENERAL RESULTS

In Ref. 8, the authors have shown that for an A-particle system the frequency moment of order n (not necessarily integer but greater than or equal to 1) of the single-particle density $\rho(\mathbf{r})$, i.e.,

$$w_n=\int[\rho(\mathbf{r})]^n d\mathbf{r}\ , \tag{1}$$

is bounded from below as

$$w_n\geq\frac{nk}{(k+3)n-3}A^n\left[\frac{k\left[\frac{3n-3}{(k+3)n-3}\right]^{3/k}}{4\pi B\left[\frac{n}{n-1},\frac{3}{k}\right]\langle r^k\rangle^{3/k}}\right]^{n-1} \tag{2}$$

for $k=1,2,3,\ldots$. Here the B symbol denotes the β function defined by

$$B(x,y)=\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}=\int_0^1 t^{x-1}(1-t)^{y-1}dt$$

and $\langle r^k\rangle$ is the (positive) kth moment around the origin of the normalized $\rho(\mathbf{r})$, i.e.,

$$\langle r^k\rangle=A^{-1}\int r^k\rho(\mathbf{r})d\mathbf{r}\ . \tag{3}$$

Here we want to show that the frequency moment w_n given by Eq. (1) can also be bounded from below in terms of the negative moments $\langle r^{-k}\rangle$ of the density ρ. It is found that

$$w_n\geq\frac{nk}{n(3-k)-3}A^n\left[\frac{k\left[\frac{n(3-k)-3}{3n-3}\langle r^{-k}\rangle\right]^{3/k}}{4\pi B\left[\frac{3}{k}-\frac{1}{n-1},\frac{n}{n-1}\right]}\right]^{n-1} \tag{4}$$

for $k=1,2,\ldots$ and provided that

$$k<(3n-3)/n\ . \tag{5}$$

To prove the inequality (4) we will consider an arbitrary density function $\rho(\mathbf{r})$ and denote by w_n its nth frequency moment defined by (1). Now, let us search for a function $f(\mathbf{r})$ such that (a) its norm and moment around the origin $\langle r^{-k}\rangle$ are equal to the corresponding norm and moment of $\rho(\mathbf{r})$, and (b) its frequency moment w_n^* minimizes the corresponding moment w_n of $\rho(\mathbf{r})$. To do that, we minimize the quantity $\int[f(\mathbf{r})]^n d\mathbf{r}$ subject to the conditions

$$A=\int f(\mathbf{r})d\mathbf{r}\ , \tag{6}$$

$$\langle r^{-k}\rangle = A^{-1}\int r^{-k}f(\mathbf{r})d\mathbf{r}\,, \tag{7}$$

i.e., we take variations in the form

$$\delta\left[\int [f(\mathbf{r})]^n d\mathbf{r} - \lambda\int r^{-k}f(\mathbf{r})d\mathbf{r} - \mu\int f(\mathbf{r})d\mathbf{r}\right] = 0\,,$$

where λ and μ are Lagrange's multipliers. Then one obtains

$$f(r) = [(\lambda r^{-k} + \mu)/n]^{1/(n-1)} \tag{8}$$

provided that $f(\mathbf{r}) = f(r)$ and $r \geq 0$. Assuming μ negative, then $\lambda \geq 0$. So the support interval of the density $f(r)$ is $[0, (-\lambda/\mu)^{1/k}]$. This expression transforms with an appropriate change of scale onto

$$f(r) = \begin{cases} C(r^{-k} - b^k)^{1/(n-1)} & \text{if } 0 \leq r \leq 1/b\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{9}$$

The C factor can be calculated from the normalization condition (6). One easily obtains

$$C = Ak\left[4\pi b^{k/(n-1)-3}B\left(\frac{3}{k} - \frac{1}{n-1}, \frac{n}{n-1}\right)\right]^{-1}$$

provided that k is less than $3n-3$. Similarly, the moment around the origin $\langle r^{-k}\rangle$ and the frequency moment w_n^* of the function $f(r)$ given by (9) are

$$\langle r^{-k}\rangle = \frac{3n-3}{n(3-k)-3}b^k\,,$$

$$w_n^* = \frac{nk}{n(3-k)-3}A^n\left[\frac{k\left[\dfrac{n(3-k)-3}{3n-3}\langle r^{-k}\rangle\right]^{3/k}}{4\pi B\left(\dfrac{3}{k} - \dfrac{1}{n-1}, \dfrac{n}{n-1}\right)}\right]^{n-1}$$

provided that $k < (3n-3)/n$ and $n \geq 1$. It only remains to show that w_n^* is a lower bound of the frequency moment w_n of $\rho(\mathbf{r})$. This can be easily done operating in a fully analogous and parallel way as we do in Ref. 8 to prove the inequality (2).

III. LOWER BOUNDS FOR KINETIC ENERGY

Recently Lieb and Thirring[9] have proved that the kinetic energy T of a system of A fermions with q spin states available to each particle ($q=2$ for electrons) is bounded as

$$T \geq 1.643Kq^{-2/3}\int [\rho(\mathbf{r})]^{5/3}d\mathbf{r} \tag{10}$$

with $K = 3(3\pi/2)^{2/3}/10$. Moreover, Lieb has conjectured[5] that the Thomas-Fermi kinetic value T_{TF} is a lower bound for the exact A-fermion kinetic energy, i.e.,

$$T \geq T_{\mathrm{TF}} = (4\pi)^{2/3}Kq^{-2/3}\int [\rho(\mathbf{r})]^{5/3}d\mathbf{r} \text{ a.u.}$$
$$= \tfrac{3}{10}(6\pi^2)^{2/3}q^{-2/3}w_{5/3} \text{ a.u.}\,, \tag{11}$$

where the notation (1) has been used. Atomic units will be used throughout the paper. One sees that the Thomas-Fermi kinetic energy is, apart from a constant, the frequency momentum of order $\frac{5}{3}$ of the fermion density of the system.

Here we want to find lower bounds to the kinetic energy T_{TF}. A straightforward use of Eq. (2) for $n = \frac{5}{3}$ leads to the following set of lower bounds for T_{TF}:

$$T_{\mathrm{TF}} \geq C_q G_k \frac{A^{5/3}}{\langle r^k\rangle^{2/k}}, \quad k = 1,2,\ldots \tag{12a}$$

with

$$C_q = \tfrac{3}{10}(6\pi^2)^{2/3}q^{-2/3} \tag{12b}$$

and

$$G_k = \frac{5k}{5k+6}\left[\frac{k\left[\dfrac{6}{5k+6}\right]^{3/k}}{4\pi B\left[\dfrac{5}{2}, \dfrac{3}{k}\right]}\right]^{2/3}. \tag{12c}$$

Also Eqs. (4) and (5) produce an additional lower bound

$$T_{\mathrm{TF}} \geq C_q \frac{5}{36}\left[\frac{4}{\pi^2}\right]^{2/3}\langle 1/r\rangle^2 A^{5/3}\,. \tag{13}$$

For atoms ($q=2$), the bounds (12) and (13) take on the values

$$T_{\mathrm{TF}} \geq 2.8712G_k\langle r^k\rangle^{-2/k}A^{5/3}, \quad k = 1,2,\ldots \tag{14}$$

and

$$T_{\mathrm{TF}} \geq 0.2184\langle 1/r\rangle^2 A^{5/3}\,, \tag{15}$$

respectively. The bound (15) can also be readily found from a well-known relationship[10]

$$T \geq \frac{Z^2}{4|\epsilon_0|}\langle r^{-1}\rangle^2\,,$$

where ϵ_0 is the (exactly known) leading term of the Z^{-1} perturbation series, whose asymptotic expansion is[11]

$$-\epsilon_0(A) = (3A/2)^{1/3}[1 - \tfrac{1}{2}(3A/2)^{-1/3} + O(A^{-2/3})]\,.$$

Notice that the inequality (15) can be accordingly improved for $A = Z$ as

$$T \geq \tfrac{1}{4}(2/3)^{1/3}Z^{5/3}\langle r^{-1}\rangle^2[1 + \tfrac{1}{2}(3Z/2)^{-1/3} + \cdots]\,.$$

It can be shown that the bound (15) is much more accurate that those given by inequality (14). The bound (15) gives the exact kinetic energy in the original Thomas-Fermi model of a neutral atom ($A = Z$) which considers a pure Coulomb potential, $-Z/r$, the reason being that the electronic density is of the form $(1/r - c)^{3/2}$ which coincides with Eq. (9) for $k=1$. In this case the inequality (14) gives a bound which for $k=1$, 2, and 3 is such that the relative error with respect to the exact kinetic energy is 0.526, 0.603, and 0.649, respectively; for $k > 3$, the error is bigger. Moreover, taking the values $\langle 1/r\rangle$ and $\langle r\rangle$ of a phenomenological realistic electronic density such as[12] $\rho(r) \propto [4\pi r(a+r)^4]^{-1}$, $a = (9/2Z)^{1/3}$, into the inequalities (14) and (15), one easily finds two lower bounds with relative errors of 0.865 and 0.099, respectively. The same remains true for theoretically well-founded realistic electronic densities of atoms. Then, henceforth we will refer only to the lower bound (15) in our discussion on the atomic kinetic energy.

The goodness of the bound (11)—(15) is numerically analyzed in Tables I and II for various neutral atoms.

TABLE I. Comparison between the lower bound given by (15) and the Thomas-Fermi kinetic energy for various neutral atoms as explained in text. Atomic units are used everywhere.

Z	$\langle 1/r \rangle$	Lower bound	T_{TF}	ϵ_r
3	1.91	4.97	6.70	0.258
4	2.099	9.70	13.13	0.261
5	2.275	16.53	21.97	0.248
6	2.447	25.91	33.61	0.229
7	2.619	38.37	48.63	0.211
8	2.783	54.13	67.22	0.195
9	2.947	73.86	90.07	0.180
10	3.113	98.24	117.77	0.166

TABLE II. Comparison between the lower bound (15) using nonrelativistic values for $\langle 1/r \rangle$ and the total kinetic energy quoted in Ref. 15 for various neutral atoms. Atomic units are used.

Z	$\langle 1/r \rangle$	Lower bound	T	ϵ_r
6	2.5	25.97	37.66	0.310
12	3.34	153.24	199.62	0.232
18	3.87	404.39	526.82	0.232
28	4.59	1187.98	1506.82	0.212
48	5.65	4485.97	5465.13	0.179
64	6.27	8792.0	10820.1	0.187
74	6.77	13056.2	15287.4	0.146
82	6.91	16151.6	19524.0	0.173

Table I shows the comparison between the lower bound calculated with the values $\langle 1/r \rangle$ obtained by means of the atomic wave functions of Clementi and Roetti,[13] and the (Thomas-Fermi) leading term of the kinetic energy obtained[14] with the same atomic wave functions. One observes that the relative error of the bound is at most 0.26, which occurs for $Z=4$, and then it rapidly decreases for bigger atomic numbers.

In Table II the lower bound (15) obtained with the $\langle 1/r \rangle$ values given by Desclaux[15] is compared with the total kinetic energy. Both values have been taken from the nonrelativistic calculations quoted in Ref. 15. One observes that for intermediate and heavy atoms the relative error of the bound is always smaller than 0.18.

Finally it is interesting to point out that the combination of the expression[16]

$$\langle 1/r \rangle \geq 1.3956 Z^{1/3}[1-O(Z^{-1/3})] , \tag{16}$$

based on the virial theorem, and the inequality (15) allows us to write that

$$T_{TF} \geq 0.4254 Z^{7/3} .$$

This lower bound is exceedingly simple and already has the well-known $Z^{7/3}$ dependence of the atomic kinetic energy, but it is not very accurate because the minimal estimation for $\langle 1/r \rangle$ given by (16) has been used.

In nuclear systems, the bounds (12) are, for positive k values, much better than (13). Essentially this is because a f function of the form $f(r) \propto (r^k - a)^{3/2}$ is much closer to the phenomenological nucleonic densities with positive k values than with $k=-1$. Besides, it has been shown[17] that the use of the values for the moments $\langle r^k \rangle$, $k>0$, and $\langle 1/r \rangle$ obtained from phenomenological single-particle densities (Fermi, modified Gaussian) in the inequalities (12) and (13) also leads to the same conclusion.

To study the goodness of the bounds (12), let us calculate them within a nuclear model where the kinetic energy can be determined exactly. For example, in the simple harmonic-oscillator shell model where the single-particle wave functions are pure harmonic-oscillator functions, the kinetic energy per particle is given by[18] $T = C/\langle r^2 \rangle$ MeV, where C is a constant which depends on the nucleus under consideration (e.g., 104.8 for ^{16}O and 565.2 for ^{208}Pb). For $k=2$, the bounds (12) give the values $95.8/\langle r^2 \rangle$ and $529.6/\langle r^2 \rangle$ MeV for ^{16}O and ^{208}Pb, respectively. The corresponding relative error is of 0.09 for oxygen and 0.06 for lead.

In Hartree-Fock and nonrenormalized Brueckner-Hartree-Fock theories, it is also possible to know the exact value of the average kinetic energy per particle, $\langle T \rangle$, from the binding energy per particle B/A and the single-particle energies ε_λ via the sum rule[18]

$$B/A = \tfrac{1}{2}\langle T \rangle + \frac{1}{2A}\sum_\lambda \varepsilon_\lambda .$$

The comparison between the values of $\langle T \rangle$ obtained within these models and the bound (12) for $k=2$ is shown in Table III for two nuclei. One observes that the relative

TABLE III. Comparison between the lower bound given by Eq. (12) with $k=2$ and the kinetic energy obtained in several self-consistent calculations for the nuclei ^{16}O and ^{208}Pb.

Nuclei	Type of calculation	$\langle r^2 \rangle^{1/2}$ (fm)	T (MeV)	Lower bound (MeV)	ϵ_r
^{16}O	HF[a]	2.54	16.88	14.84	0.12
	BHF[b]	2.46	17.39	15.8	0.09
^{208}Pb	HF[c]	5.32	20.01	18.71	0.07
	BHF[b]	4.60	25.99	25.02	0.04

[a]Reference 27.
[b]Reference 28.
[c]Reference 29.

TABLE IV. Values in atomic units of the exchange energy for several atoms. The upper bound given by Eq. (19) is compared with the exchange energy obtained by means of the Schwinger's semiempirical value, E_{ex}(Sch), and using the Clementi-Roetti wave functions, E'_{ex}, as explained in text.

Z	$\langle r \rangle$	Upper bound	E_{ex}(Sch)	E'_{ex}	ϵ_r
6	1.198	−2.772	−4.375	−4.603	0.366
12	1.019	−8.212	−13.888	−14.811	0.409
18	0.889	−16.163	−27.297	−28.233	0.408
28	0.778	−33.288	−57.007	−59.290	0.416
48	0.694	−76.564	−139.981	−142.962	0.453
82	0.614	−176.731	−341.735		0.483

error of the bound is, as before, around 0.1 with respect to the exact value. Further details and more complete discussion of these and other comparisons for these nuclei are given in Refs. 8 and 17.

IV. UPPER BOUNDS FOR EXCHANGE ENERGY

The Dirac or semiclassical exchange energy of a fermionic system is given by[5]

$$E_{ex} = -C_e \int [\rho(\mathbf{r})]^{4/3} d\mathbf{r} \equiv -C_e w_{4/3} , \tag{17}$$

where $C_e = 3(3/\pi)^{1/3}/4$. In writing the second equality, we have used the definition (1). Then the exchange energy E_{ex} is related to the frequency moment of order $\frac{4}{3}$ of the fermionic density (electronic if atoms, protonic if nuclei) of the system.

The inequalities (2), (4) and (5) give no lower but upper bounds to E_{ex} because of the negative sign in Eq. (17). Moreover, the restriction (5) is not fulfilled for $n = \frac{4}{3}$ so that the exchange energy cannot be bounded in terms of the quantities $\langle r^{-k} \rangle$. However, the expressions (2) and (17) allow us to obtain upper bounds to the exchange energy of an A-fermion system in terms of the moments of positive order, $\langle r^k \rangle$, of the single-fermion density. These bounds are

$$E_{ex} \leq -C_e K_k \frac{A^{4/3}}{\langle r^k \rangle^{1/k}}, \quad k = 1,2,\ldots \tag{18a}$$

where

$$K_k = \frac{4k}{4k+3} \left[\frac{k[3/(4k+3)]^{3/k}}{4\pi B\left[4, \frac{3}{k}\right]} \right]^{1/3} . \tag{18b}$$

For neutral atoms ($A = Z$) one can easily see, as in Sec. III, that the best bound is given[17] for $k = 1$, that is, by means of the centroid of the single-particle density, $\langle r \rangle$. This is

$$E_{ex} \leq -C_e \frac{12}{49} \left[\frac{15}{\pi} \right]^{1/3} \frac{Z^{4/3}}{\langle r \rangle} = -0.3046 \frac{Z^{4/3}}{\langle r \rangle} \text{ a.u.} \tag{19}$$

Taking into account that $\langle r \rangle$ is proportional[12] to $Z^{-1/3}$, one observes from this bound that the exchange energy is itself proportional to $Z^{5/3}$ as one would expect.[19] On the other hand, an idea of the goodness of this bound can be obtained by comparing it with the values of the exchange energy given by the Schwinger's semiempirical expression (Ref. 20) $E_{ex}(\text{Sch}) = -0.2208 Z^{5/3}$ a.u. and the relation (Ref. 21) $E'_{ex} = -C_e 4(3\pi^2)^{-1/3} \langle p \rangle = -0.3183 \langle p \rangle$ a.u., where the expectation value of the single-particle momentum was calculated[22] by using the Clementi-Roetti wave functions.[13] This comparison is shown in Table IV, where the first and second columns give the $\langle r \rangle$ values[15] and the bound (19), respectively. The third and fourth columns contain the magnitudes E_{ex}(Sch) and E'_{ex}, respectively, and the last one collects the relative error of the bound with respect to E_{ex}(Sch). One observes that the bound (19) is certainly not good since the relative error oscillates between ~0.37 and ~0.48.

For nuclei and with $k = 2$, the inequality (18a) gives the following upper bound for the exchange energy:

$$E_{ex} \leq -C_e \frac{2}{11} \left[\frac{3}{11} \right]^{1/2} \left[\frac{315}{\pi} \right]^{1/3} \frac{Z^{4/3}}{\langle r^2 \rangle^{1/2}} \text{ a.u.}$$
$$= -0.469\,16 \frac{Z^{4/3}}{\langle r^2 \rangle^{1/2}} \text{ MeV} . \tag{20}$$

TABLE V. Values in MeV of the Coulomb exchange energy for various nuclei. The upper bound given by (20) is compared with two different microscopic values obtained by Titin-Schneider and Quentin (Ref. 23), E'_{ex}, and Rosati and Schiavilla (Ref. 24), E''_{ex}.

Nuclei	$\langle r^2 \rangle^{1/2}$ (fm)	Upper bound (MeV)	E'_{ex} (MeV)	E''_{ex} (MeV)	ϵ_r
^{16}O	2.71	−2.77	−2.87	−2.4	0.035
^{20}Ne	3.00	−3.33	−3.64		0.074
^{24}Mg	3.08	−4.19	−4.44		0.058
^{28}Si	3.10	−5.11	−5.24		0.025
^{32}S	3.263	−5.80	−6.0		0.034
^{40}Ca	3.48	−7.28	−7.52	−6.8	0.027
^{208}Pb	5.52	−30.28		−33.8	

In Table V this bound (see column 2) is compared with the exchange energy given by the two following models: (i) exact Hartree-Fock calculations of Eq. (17) using the Skyrme III forces,[23] E'_{ex}, and (ii) exact microscopic calculations[24] in terms of the two-proton distribution function calculated in the local-density approximation by solving the FHNC/O (Fermi hypernetted chain calculations) equations[25] for infinite, nonsymmetric, nuclear matter with the nucleons interacting via the so-called OMY potential,[26] E''_{ex}. From this comparison, one realizes that the relative error of the bound (20) with respect to the microscopic values, E'_{ex}, of the exchange energy is always less than 0.1.

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