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# EXACT KINETIC ENERGY FUNCTIONAL OF NONINTERACTING FERMIONS

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The exact expression of kinetic energy as a functional of the density for a system of noninteracting fermions, which has been searched for many years, is derived based on the direct method.

One of the greatest challenges in density functional theory of many-fermion system is the explicit expression of the kinetic energy that is a functional of the density of the system.[1,2] Since the inception of Thomas–Fermi[3,4] statistical model of electrons in atoms, the precursor of modern density functional theory, much effort has been put to search after the kinetic energy functional. The Hohenberg–Kohn[5] theorem confirms the existence of kinetic energy functional $T[n]$, but it cannot tell us what the exact form of $T[n]$ is. Although the conventional gradient expansion[6–8] has been explored extensively to approximate $T[n]$ in a systematic way and has witnessed some success, it is essentially semiclassical.[9,10] The author[11] has shown that an *ab initio* gradient expansion of the kinetic energy functional is divergent. Thus the observation[12] that the conventional gradient expansion could not improve the kinetic energy systematically is explained. In this letter, we first derive a formulation for $T[n]$ by Taylor functional expansion, which contains unknown higher order functional derivatives of $T[n]$ with respect to the density $n(\mathbf{r})$ for a uniform system. We then establish relations between these functional derivatives and the response functions whose exact expressions are available. Inserting the functional derivatives of $T[n]$ expressed in terms of response functions into the formulation of $T[n]$, we arrive at an explicit, exact expression of the kinetic energy as a functional of density. Some possible approximations to the exact but complicated kinetic energy functional are pointed out. For brevity, we always use the term *system* for the system of noninteracting fermions in the following.

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Starting with the functional Taylor expansion of $T[n]$ at zero density, we are able to write

$$T[n] = \sum_{m=1}^{\infty} \frac{1}{m!} \int \cdots \int C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; 0) n(\mathbf{r}_1) \cdots n(\mathbf{r}_m) d\bar{r}_1 \cdots d\bar{r}_m \,, \tag{1}$$

where $C_0^{(m)}$ is the $m$th order functional derivative of $T[n]$ with respect to $n(\mathbf{r})$ for a uniform system and the integration (also in the following if not explicitly indicated) is taken over the entire space.

After its counterpart of classical fluids, we call $C^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; [n(\mathbf{r})])$, the functional derivative of $T[n]$ with respect to $n(\mathbf{r})$, direct correlation function (DCF). The DCFs of noninteracting fermions are due to the Pauli correlation.

For the uniform system, $C_0^{(m)}$ satisfies the sum rule

$$\begin{aligned} \frac{\partial}{\partial n} C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; n) &= \int \frac{\delta C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; n)}{\delta n(\mathbf{r}_{m+1})} d\bar{r}_{m+1} \\ &= \int C_0^{(m+1)}(\mathbf{r}_1, \ldots, \mathbf{r}_{m+1}; n) d\bar{r}_{m+1} \,. \end{aligned} \tag{2}$$

This relation allows us to derive the following Taylor expansion:

$$\begin{aligned} C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; 0) &= \sum_{p=0}^{\infty} \frac{1}{p!} (-n)^p \left(\frac{\partial}{\partial n}\right)^p C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; n) \\ &= \sum_{p=0}^{\infty} \frac{1}{p!} (-n)^p \int \cdots \int C_0^{(m+p)}(\mathbf{r}_1, \ldots, \mathbf{r}_{m+p}; n) \\ &\quad \times d\bar{r}_m \cdots d\bar{r}_{m+p} \\ &= \sum_{p=0}^{\infty} \frac{1}{p!} [-n(r_1)]^p \int \cdots \int C_0^{(m+p)}(\mathbf{r}_1, \ldots, \mathbf{r}_{m+p}; n(\mathbf{r}_1)) \\ &\quad \times d\bar{r}_m \cdots d\bar{r}_{m+p} \,, \end{aligned} \tag{3}$$

thus transforming Eq. (1) to

$$\begin{aligned} T[n] = \sum_{m=1}^{\infty} \int \cdots \int C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; n(\mathbf{r}_1)) \Bigg[ \sum_{i=1}^{m} \frac{(-1)^{m-i}}{(m-i)!i!} \\ \cdot n(\mathbf{r}_1)^{m-i+1} n(\mathbf{r}_2) \cdots n(\mathbf{r}_i) \Bigg] d\bar{r}_1 \cdots d\bar{r}_m \,. \end{aligned} \tag{4}$$

The above derivation of the expression of $T[n]$ follows from Percus' idea[13] of the direct method. A rigorous treatment based on the functional integral method can be found in Ref. 14.

The first order DCF and the second order (in $k$ space) DCF of a $d$-D uniform system with density $n$ are well-known,[15,16] namely,

$$\begin{aligned} C_0^{(1)}(n) &= \frac{\partial t_{\mathrm{TF}}}{\partial n} \\ &= 2^{1-2/d}\left[\Gamma\left(\frac{d}{2}+1\right)\right]^{2/d} n^{2/d}\,, \end{aligned} \tag{5}$$

$$\begin{aligned} \tilde{C}_0^{(2)}(k;\, n) &= -\frac{1}{\tilde{R}_0^{(1)}(k;\, \mu)} \\ &= \frac{k_{\mathrm{F}}^2}{dn}\,\frac{1}{F\left[1,\, 1-\frac{d}{2};\, \frac{3}{2};\, \left(\frac{\mathbf{k}}{2k_{\mathrm{F}}}\right)^2\right]}\,, \end{aligned} \tag{6}$$

where $t_{\mathrm{TF}}$ is the Thomas–Fermi kinetic energy density, $\tilde{R}_0^{(1)}(k;\, \mu)$ is the first order response function in $k$ space (the Lindhard function in 3D case), $\mu$ is the chemical potential, $\Gamma(\alpha)$ is the gamma function, $F(\alpha,\, \beta;\, \gamma;\, z)$ is the hypergeometric function, and $k_{\mathrm{F}}$ is determined by

$$k_{\mathrm{F}} = 2^{1-1/d}\pi^{1/2}\left[\Gamma\left(\frac{d}{2}+1\right)\right]^{1/d} n^{1/d}\,.$$

But the expressions of higher order DCFs are not known yet and so, the kinetic energy functional in Eq. (4) as it stands is only a formal one. To acquire an explicit formulation of $T[n]$, the exact higher order DCFs are required. We now show how the DCF is related with the response function.

Applying variational principle of Hohenberg and Kohn to the studied system, we reach the Euler–Lagrange equation

$$\frac{\partial T[n]}{\partial n} + V(\mathbf{r}) = \mu\,, \tag{7}$$

where $V(\mathbf{r})$ is the external potential and $\mu$ the chemical potential.

By functional differentiating Eq. (7) and noting that the chemical potential is fixed for uniform system, we obtain immediately

$$C_0^{(m)}(\mathbf{r}_1,\, \ldots\,,\, \mathbf{r}_m;\, n) = -\left.\frac{\delta^{m-1}V(\mathbf{r}_1)}{\delta n(\mathbf{r}_2)\cdots\delta n(\mathbf{r}_m)}\right|_{n(\mathbf{r})=n}\,. \tag{8}$$

The response function is defined as

$$R^{(m)}(\mathbf{r}_1,\, \ldots\,,\, \mathbf{r}_m;\, [V]) \equiv \frac{\delta^m n(\mathbf{r}_1)}{\delta V(\mathbf{r}_2)\cdots\delta V(\mathbf{r}_m)}\,, \tag{9}$$

and their expressions for 1, 2, and 3D uniform systems have already been derived:[17–19]

$$R_0^{(m)} = (-1)^m \frac{k_{\mathrm{F}} m!}{\pi} \int_{\sum_{i=1}^{m+1} R_i}^{\infty} \int_{s_m}^{\infty} \cdots \int_{s_2}^{\infty} \mathrm{j}_0(k_{\mathrm{F}} s_1) ds_1 \cdots ds_m , \quad \text{if } d = 1 ,$$

$$R_0^{(m)} = (-1)^m \frac{k_{\mathrm{F}}^2 m!}{\pi^{m+2}} \int_0^{\infty} \cdots \int_0^{\infty} \mathrm{j}_1\left( k_{\mathrm{F}} \sum_{i=1}^{m+1} R_i \cosh s_i \right) ds_1 \cdots ds_{m+1} , \quad \text{if } d = 2 ,$$

$$R_0^{(m)} = (-1)^m \frac{k_{\mathrm{F}}^2}{2\pi^2} \frac{m!}{(2\pi)^m} \frac{\mathrm{j}_1(k_{\mathrm{F}} \sum_{i=1}^{m+1} R_i)}{\prod_{j=1}^{m+1} R_j} , \quad \text{if } d = 3 ,$$

where $R_i = |\mathbf{r}_{i+1} - \mathbf{r}_i|$, $R_{m+1} = |\mathbf{r}_1 - \mathbf{r}_{m+1}|$, and $\mathrm{j}_i$ is the spherical Bessel function.

With the chain rule of functional differentiation, there yields from the definitions of DCF and response function:[20]

$$\int C^{(2)}(\mathbf{r}_1, \mathbf{r}_2; [n]) R^{(1)}(\mathbf{r}_2, \mathbf{r}_3; [V]) d\bar{r}_2 = -\delta(\mathbf{r}_1 - \mathbf{r}_3) . \tag{10}$$

For uniform system, Eq. (10) reads

$$\tilde{C}_0^{(2)}(k; n) = -\frac{1}{\tilde{R}_0^{(1)}(k; \mu)} \tag{11}$$

in $k$ space, which is a well-known result from linear response theory.

Employing the chain rule of functional differentiation repeatedly, we obtain the third and fourth order DCFs:

$$\begin{aligned} C_0^{(3)} = &-\int\int\int R_0^{(2)}(\mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6) C_0^{(2)}(\mathbf{r}_4, \mathbf{r}_1) \\ &\cdot C_0^{(2)}(\mathbf{r}_5, \mathbf{r}_2) C_0^{(2)}(\mathbf{r}_6, \mathbf{r}_3) d\bar{r}_4 d\bar{r}_5 d\bar{r}_6 , \end{aligned} \tag{12}$$

$$\begin{aligned} C_0^{(4)} = &-\int\int\int\int R_0^{(3)}(\mathbf{r}_5, \mathbf{r}_6, \mathbf{r}_7, \mathbf{r}_8) C_0^{(2)}(\mathbf{r}_5, \mathbf{r}_1) C_0^{(2)}(\mathbf{r}_6, \mathbf{r}_2) C_0^{(2)}(\mathbf{r}_7, \mathbf{r}_3) \\ &\cdot C_0^{(2)}(\mathbf{r}_8, \mathbf{r}_4) d\bar{r}_5 d\bar{r}_6 d\bar{r}_7 d\bar{r}_8 - \int\int\int R_0^{(2)}(\mathbf{r}_5, \mathbf{r}_6, \mathbf{r}_7) \Big[ C_0^{(3)}(\mathbf{r}_5, \mathbf{r}_1, \mathbf{r}_4) \\ &\cdot C_0^{(2)}(\mathbf{r}_6, \mathbf{r}_2) C_0^{(2)}(\mathbf{r}_7, \mathbf{r}_3) + C_0^{(3)}(\mathbf{r}_6, \mathbf{r}_2, \mathbf{r}_4) C_0^{(2)}(\mathbf{r}_5, \mathbf{r}_1) C_0^{(2)}(\mathbf{r}_6, \mathbf{r}_2) \\ &+ C_0^{(3)}(\mathbf{r}_7, \mathbf{r}_3, \mathbf{r}_4) C_0^{(2)}(\mathbf{r}_5, \mathbf{r}_1) C_0^{(2)}(\mathbf{r}_6, \mathbf{r}_2) \Big] d\bar{r}_5 d\bar{r}_6 d\bar{r}_7 . \end{aligned} \tag{13}$$

If we define the Fourier transform of the DCF as

$$\begin{aligned} \tilde{C}_0^{(m)}(\mathbf{k}_1, \ldots, \mathbf{k}_{m-1}) \equiv &\int \cdots \int C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m) \\ &\cdot \exp[-i\mathbf{k}_1 \cdot (\mathbf{r}_2 - \mathbf{r}_1) - \cdots - i\mathbf{k}_m \cdot (\mathbf{r}_m - \mathbf{r}_1)] \, d\bar{r}_2 \cdots d\bar{r}_m , \end{aligned} \tag{14}$$

where $m \geq 2$, then in $k$ space, the relation between the DCF and the response function becomes simple:

$$\tilde{C}_0^{(3)}(\mathbf{k}_1, \mathbf{k}_2) = -\tilde{R}_0^{(2)}(\mathbf{k}_1, \mathbf{k}_2)\tilde{C}_0^{(2)}(\mathbf{k}_1)\tilde{C}_0^{(2)}(\mathbf{k}_2)\tilde{C}_0^{(2)}(\mathbf{k}_1 + \mathbf{k}_2)\,, \tag{15}$$

$$\begin{aligned}\tilde{C}_0^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = -\tilde{R}_0^{(2)}(\mathbf{k}_1, \mathbf{k}_2)[\tilde{C}_0^{(3)}(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3) + \tilde{C}_0^{(3)}(\mathbf{k}_1 + \mathbf{k}_3, \mathbf{k}_2) \\ + \tilde{C}_0^{(3)}(\mathbf{k}_2 + \mathbf{k}_3, \mathbf{k}_1)] - \tilde{R}_0^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)\tilde{C}_0^{(2)}(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \\ \cdot \tilde{C}_0^{(2)}(\mathbf{k}_1)\tilde{C}_0^{(2)}(\mathbf{k}_2)\tilde{C}_0^{(2)}(\mathbf{k}_3)\,.\end{aligned} \tag{16}$$

For the 1D system, we can write down the explicit higher order DCF explicitly. For example, the third order one reads

$$\tilde{C}_0^{(3)} = -\pi^2[f(\eta_1)f(\eta_1 + \eta_2) + f(\eta_2)f(\eta_1 + \eta_2) - f(\eta_1)f(\eta_2)]\,, \tag{17}$$

with

$$f(x) = \frac{1}{\ln\left|\dfrac{1+x}{1-x}\right|}\,, \tag{18}$$

and $\eta_1 = k_1/(2k_{\mathrm{F}})$ and $\eta_2 = k_2/(2k_{\mathrm{F}})$.

Other DCFs of homogeneous system are easily determined in the same way, and they are expressed as functionals of the response functions and the lower order DCFs.

Substituting the DCFs derived above into Eq. (4), we obtain an exact expression of the kinetic energy functional.

Starting with the integral form of the virial theorem[21]

$$T[n] = -\frac{1}{2}\int n(\mathbf{r})\mathbf{r} \cdot \nabla(\mu - V(\mathbf{r}))d\bar{r}\,, \tag{19}$$

Kugler[20] was able to derive an exact hierarchy for the kinetic energy functional

$$T[n] = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m!} \int \cdots \int C^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; [n]) \prod_{i=1}^{m} [n(\mathbf{r}_i)d\bar{r}_i]\,. \tag{20}$$

Although Eqs. (4) and (20) look similar, there is an essential difference between them: in the former, only the expression of the DCF for the *uniform* system is required but in the latter, the form of the DCF for *general* system is required. Obviously, the practical value of Kugler's kinetic energy functional is strongly limited since we do not know the DCF for nonhomogeneous systems. Moreover, Kugler's theory is tedious too. To derive the explicit form of $T[n]$ by Kugler's method, we need the information of the DCF of any order, or all the functional derivatives of $T[n]$ with respect to $n(\mathbf{r})$, which is not necessary. In fact, the knowledge of the first order DCF is sufficient to help us derive $T[n]$ itself by direct functional integration along a linear path,[22] which is the idea of escalation method.[13] Simple calculation yields

$$T[n] = \int n(\mathbf{r}) \int_0^1 \frac{\delta T[n_\lambda]}{\delta n_\lambda(\mathbf{r})} d\lambda d\bar{r}$$
$$= \int n(\mathbf{r}) \int_0^1 C^{(1)}(\mathbf{r}, [n_\lambda]) d\lambda d\bar{r} , \tag{21}$$

where $n_\lambda(\mathbf{r}) = \lambda n(\mathbf{r})$. Hence, if the expression of the first order DCF were known, an exact kinetic energy would immediately be formed.

Let us apply the formulation (4) to the uniform system. Suppose that the density of a uniform system is $n_0$. We consider the kinetic energy of a part of this system, which is confined in a volume $\Omega$. From Eq. (4), we find

$$T[n_0] = \sum_{m=1}^{\infty} \sum_{i=1}^{m} \frac{(-1)^{m-i}}{(m-i)!i!} \int_\Omega \int \cdots \int C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; 0) n_0^m d\bar{r}_1 \cdots d\bar{r}_m$$
$$= \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m!} n_0^m \int_\Omega \int \cdots \int C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; 0) d\bar{r}_1 \cdots d\bar{r}_m , \tag{22}$$

where the integration of function of $\mathbf{r}_1$ is taken over $\Omega$. In deriving 22, we used the identity

$$\sum_{i=1}^{m} \frac{(-1)^{m-i}}{(m-i)!i!} = \frac{(-1)^{m+1}}{m!} .$$

Via the sum rule applied to Eq. (22), one has

$$T[n_0] = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m!} n_0^m \int_\Omega \frac{\partial^{m-1}}{\partial n_0^{m-1}} C_0^{(1)}(n_0) d\bar{r}_1 . \tag{23}$$

Thus, one gets the kinetic energy density

$$t[n_0] = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m!} n_0^m \frac{\partial^{m-1}}{\partial n_0^{m-1}} C_0^{(1)}(n_0) . \tag{24}$$

Replacing $C_0^{(1)}$ on the RHS by Eq. (5), we obtain

$$t[n_0] = 2^{1-2/d}\pi \left[\Gamma\left(\frac{d}{2}+1\right)\right]^{2/d} n_0^{2/d+1}(1+S) , \tag{25}$$

where

$$S = 1 + \sum_{m=2}^{\infty} \frac{(-1)^{m+1}}{m!} \frac{2}{d}\left(\frac{2}{d}-1\right) \cdots \left(\frac{2}{d}-m+2\right)$$
$$= \frac{d}{2+d} .$$

Therefore, the final result reads

$$t[n_0] = \frac{d}{d+2}\,\frac{2\pi}{2^{d/2}}\left[\Gamma\left(\frac{d}{2}+1\right)\right]^{2/d} n_0^{2/d+1}\,, \tag{26}$$

which is the correct kinetic energy density.

Although the uniform system is a trivial model, the demonstration that verifies the internal consistency of the formulation is not. Moreover, the newly derived kinetic energy functional may help us to work out nontrivial results. Certainly, because of the complexity of DCF, it is difficult to implement our exact formulation of $T[n]$ in practice. However, some rational approximation is possible. For instance, keeping $j$th and lower order exact DCFs, one can use the following ansatz

$$C_0^{(m)} = \left.\frac{\partial C_0^{(m-1)}}{\partial n(\mathbf{r}_m)}\right|_{n(\mathbf{r})=n} \delta(\mathbf{r}_m - \mathbf{r}_{m-1}) \tag{27}$$

to approximate higher order DCFs. An approximate kinetic energy functional is then obtained:

$$\begin{aligned} T[n] = {} & \sum_{m=1}^{j} \int \cdots \int C_0^{(m)}(\mathbf{r}_1, \ldots, \mathbf{r}_m; n(\mathbf{r}_1)) \Bigg[\sum_{i=1}^{m} \frac{(-1)^{m-i}}{(m-i)!i!} \\ & \cdot n(\mathbf{r}_1)^{m-i+1} n(\mathbf{r}_2) \cdots n(\mathbf{r}_i)\Bigg] d\bar{r}_1 \cdots d\bar{r}_m \\ & + \sum_{m=j+1}^{\infty} \int \cdots \int \left(\frac{\partial}{\partial n(\mathbf{r}_1)}\right)^{m-j} C_0^{(j)}(\mathbf{r}_1, \ldots, \mathbf{r}_j; n(\mathbf{r}_1)) \Bigg[\sum_{i=1}^{m} \frac{(-1)^{m-i}}{(m-i)!i!} \\ & \cdot n(\mathbf{r}_1)^{m-i+1} n(\mathbf{r}_2) \cdots n(\mathbf{r}_j)^{m-j}\Bigg] d\bar{r}_1 \cdots d\bar{r}_j\,. \end{aligned} \tag{28}$$

The approximate kinetic energy functional is nonlocal except for the case of $j$ being chosen as one. In the latter situation, one rediscovers the Thomas–Fermi model. It is expected that the bigger $j$ in this scheme one chooses, the more accurate kinetic energy functional will be obtained and the more complicated $T[n]$ will become at the same time. Therefore, one has to make a reconciliation between accuracy and complexity when dealing with $T[n]$.

The gradient expansion can be introduced into the exact formulation of $T[n]$. Taking the spread density $n(\mathbf{r}_i)$ $(i \geq 2)$ as a series in $\nabla$ from Taylor expansion, i.e.

$$n(\mathbf{r}_i) = n(\mathbf{r}_1) + \sum_{k=1}^{\infty} \frac{1}{k!}\left[(\mathbf{r}_i - \mathbf{r}_1)\cdot\nabla\right]^k n(\mathbf{r}_1)\,, \tag{29}$$

then substituting into Eq. (4), we may identify the coefficient function of any order term in $\nabla$ for the kinetic energy density. Since all the odd order terms in $\nabla$ of the kinetic energy density vanish, then the kinetic energy functional can be written as

$$T[n] = \sum_{i=0}^{\infty} T_{2i}[n]\,, \tag{30}$$

where $T_{2i}$ stands for the part of kinetic energy resulted from $2i$th order in $\nabla$.

One can show that $T_0$ is Thomas–Fermi kinetic energy and that

$$T_2 = \left(\frac{1}{24} - \frac{1}{12d}\right) \frac{[\nabla n(\mathbf{r})]^2}{n(\mathbf{r})}\,, \tag{31}$$

which is equivalent to the result by the conventional gradient expansion.[16] On the RHS of Eq. (31), a Laplacian term that does not contribute to the total energy is neglected. However, unlike the conventional or semiclassical theory, our gradient expansion shows that the higher order terms in $\nabla$ of the kinetic energy density have infinite coefficients besides that of the 2D system. For a 2D system, the gradient expansion of kinetic energy functional results in only one term, the Thomas–Fermi kinetic energy, which is confirmed by both our *ab initio* method and the semiclassical one.

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