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Energetics of a strongly correlated Fermi gas

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ABSTRACT

The energy of the two-component Fermi gas with the s-wave contact interaction is a simple linear functional of its momentum distribution:

$$E_{\text{internal}} = \hbar^2\Omega C/4\pi a m + \sum_{\mathbf{k}\sigma}(\hbar^2k^2/2m)(n_{\mathbf{k}\sigma} - C/k^4)$$

where the external potential energy is not included, a is the scattering length, Ω is the volume, $n_{\mathbf{k}\sigma}$ is the average number of fermions with wave vector $\mathbf{k}$ and spin σ, and $C \equiv \lim_{\mathbf{k}\to\infty} k^4 n_{\mathbf{k}\uparrow} = \lim_{\mathbf{k}\to\infty} k^4 n_{\mathbf{k}\downarrow}$. This result is a *universal identity*. Its proof is facilitated by a novel mathematical idea, which might be of utility in dealing with ultraviolet divergences in quantum field theories. Other properties of this Fermi system, including pair correlations and the dimer–fermion scattering length, are also studied.

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1. Introduction

It is a textbook fact that the energy of a noninteracting two-component Fermi gas is a simple functional of its momentum distribution:

$$E_{\text{noninteracting}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma},$$

where $n_{\mathbf{k}\sigma}$ is the average number of fermions with wave vector $\mathbf{k}$ and spin σ [1], $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$, $\hbar$ is Plank's constant over 2π [2], and m is each fermion's mass. This equation is valid for *any* nonrelativistic state; it is also valid when we have only a few fermions.

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What happens to the above simple formula if a contact interaction between the two components ("spin states") is turned on, characterized by a nonzero s-wave scattering length a? The system's wave function now behaves like

$$\phi = (1/r - 1/a)A + O(r) \tag{1}$$

if the distance r between two fermions in different spin states is small. Here, A depends on the position of the center-of-mass of the two fermions, as well as the positions of the remaining fermions. This system has a superfluid phase with BEC-BCS crossover [3–5] and other interesting properties, and has attracted a lot of experimental and theoretical work. So such a basic question deserves an answer.

Because of the interaction, the momentum distribution now in general only decays like $1/k^4$ at large $\mathbf{k}$ [6], and the kinetic energy diverges [6]. In a real system, a contact interaction is impossible, and the divergence is eventually cut-off at $k \sim 1/r_0$, where r_0 is the range of the interaction [7]. The interparticle interaction energy also depends sensitively on the physics at the short scale r_0. The sum of the two energies (denoted E_{internal} below), however, should be independent of such short-distance physics, when r_0 is much smaller than the other relevant length scales in the problem, including $| a |$.

We show in this paper that there is still a simple relation between the energy and the momentum distribution, which is *independent of the details of the short-range interactions*, except the scattering length a [8]:

$$E_{\text{internal}} = \frac{\Omega C}{4\pi a m} + \lim_{K\to\infty} \sum_{k<K,\sigma} \frac{k^2}{2m}\left(n_{\mathbf{k}\sigma} - \frac{C}{k^4}\right), \tag{2}$$

where

$$C \equiv \lim_{\mathbf{k}\to\infty} k^4 n_{\mathbf{k}\uparrow} = \lim_{\mathbf{k}\to\infty} k^4 n_{\mathbf{k}\downarrow}, \tag{3}$$

Ω is the volume of space [9], $n_{\mathbf{k}\sigma} \equiv \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle$, and $c_{\mathbf{k}\sigma}$ is the standard annihilation operator of a fermion with wave vector $\mathbf{k}$ and spin σ. Eq. (2) holds for any finite-energy states, no matter few-body or many-body, equilibrium or nonequilibrium, zero temperature or finite temperature, superfluid state or normal state. It holds for any populations of the two spin states (balanced or imbalanced) [10].

In the noninteracting limit, namely $k_F a \to 0^-$, $C \propto a^2$ [11], and the first term on the right-hand side of (2) goes to 0. Here, k_F is the Fermi wave number. In the unitarity limit, in which $k_F a \to \infty$ [12], C approaches some finite value, and the first term also vanishes.

Some technical remarks about Eq. (2): (1) here and throughout this paper, "infinite momentum" physically stands for a momentum scale much lower than $1/r_0$, but much higher than any other relevant momentum scales in the problem, namely $1/|a|$, $1/l$, and $1/\lambda_{\text{dB}}$, where l is the typical inter-fermionic distance, and λ_{dB} is the typical de Broglie wave length [13]; (2) E_{internal} is the expectation value of the total energy minus external potential energy [14]; (3) the summation over momentum is understood as $\sum_{\mathbf{k}} \equiv \Omega \int [\mathrm{d}^3 k/(2\pi)^3]$, and there is no infrared divergence.

In Section 2 a generalized function $\Lambda(\mathbf{k})$, called the Lambda function, is introduced. Our motivation is to streamline the formulation of the s-wave contact interaction problem. Properties of $\Lambda(\mathbf{k})$ are discussed. It is then used to study the two-body problem.

In Section 3 another generalized function, $L(\mathbf{k})$, is introduced. This and $\Lambda(\mathbf{k})$ span a two-dimensional linear space. A special element in this space, $\eta(\mathbf{k})$, is defined.

In Section 4 we prove (2) using $\eta(\mathbf{k})$. Physical implications are discussed, including a possible experimental test of (2), and results concerning the pair correlation strength and the one-body reduced density matrix.

In Section 5 we formulate the whole s-wave contact interaction problem (both few-body and many-body) in momentum space in a straightforward and unambiguous way, using the aforementioned generalized functions [15]. Using this formalism, we rederive (2) in a simpler way, and solve the three-body problem for the low energy scattering between a fermion and a weakly bound dimer of fermions.

In Section 6 we summarize our findings, and discuss the possibility of extending the ideas contained in our method to some other important physical systems which appear at first sight to have little to do with the Fermi system considered in this paper.

2. The lambda function

2.1. Introducing $\Lambda(\mathbf{k})$

If the interaction has a range r_0 that is much shorter than the other length scales in the problem (including $|a|$), it can be replaced by the famous pseudopotential [16]

$$V = \frac{4\pi a}{m}\delta(\mathbf{r})\frac{\partial}{\partial r}r, \tag{4}$$

where r is the distance between two fermions in different spin states, and the partial derivative is carried out for fixed center-of-mass location of these two fermions, as well as locations of the remaining particles. When $r_0 \to 0$ but a is kept constant, the pseudopotential becomes exact.

To formulate our current problem in momentum space, we perform a Fourier transform. To be concrete, we first consider two fermions interacting in vacuum. The wave function associated with their relative motion, $\phi(\mathbf{r})$, satisfies a simple Schrödinger equation,

$$E_r\phi = -\frac{\nabla^2}{m}\phi + \frac{4\pi a}{m}\delta(\mathbf{r})\frac{\partial}{\partial r}(r\phi), \tag{5}$$

where E_r is the energy of relative motion. Writing $\phi(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3}\widetilde{\phi}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}$, we get

$$\int \frac{d^3k}{(2\pi)^3}\left(E_r - \frac{k^2}{m}\right)\widetilde{\phi}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{4\pi a}{m}\int \frac{d^3k}{(2\pi)^3}\widetilde{\phi}(\mathbf{k})\delta(\mathbf{r})\frac{\partial}{\partial r}(re^{i\mathbf{k}\cdot\mathbf{r}}). \tag{6}$$

To proceed, we define

$$\delta(\mathbf{r})\frac{\partial}{\partial r}(re^{i\mathbf{k}\cdot\mathbf{r}}) \equiv \delta(\mathbf{r})\Lambda(\mathbf{k}), \tag{7}$$

where $\Lambda(\mathbf{k})$ is so far an unknown function of $\mathbf{k}$. Clearly,

$$\Lambda(\mathbf{k}) = 1 \quad (\text{if } k < \infty), \tag{8a}$$

but also, if we multiply both sides of Eq. (7) by $1/k^2$, and integrate over $\mathbf{k}$, the left side becomes $\propto \delta(\mathbf{r})\frac{\partial}{\partial r}(r/r) = 0$; we are thus led to an equality

$$\int d^3k\frac{\Lambda(\mathbf{k})}{k^2} = 0, \tag{8b}$$

in apparent contradiction with Eq. (8a). This difficulty has hampered the direct application of the pseudopotential in momentum space.

Actually there is no contradiction here at all.

Contradiction can only arise if we force a *third* equality, namely the integral of $\Lambda(\mathbf{k})/k^2$ over the whole $\mathbf{k}$-space is equal to the *limit* of the integral over a *finite* $\mathbf{k}$-space region which expands without bound. If we insist on both (8a) and (8b), as we should, *we must give up this third equality*.

At first sight, this decision is alarming, since the full-space integrals of *all known functions* are defined in terms of such a limit. In fact this is the *standard definition* of full-space integrals in mathematical textbooks. However, if $\Lambda(\mathbf{k})$ is accepted as a special *generalized function*, $\Lambda(\mathbf{k})/k^2$ does not have to obey this rule.

For convenience we postulate one more property for $\Lambda(\mathbf{k})$:

$$\Lambda(-\mathbf{k}) = \Lambda(\mathbf{k}), \tag{8c}$$

whose usefulness will be clear shortly.

Eqs. (8a)–(8c) define a generalized function, $\Lambda(\mathbf{k})$, where $\mathbf{k}$ is a three-dimensional vector.

Eq. (7) is then a corollary of such a definition.

2.2. Mathematical properties of $\Lambda(\mathbf{k})$

Because $\Lambda(c\mathbf{k})$ (where c is any nonzero finite real constant) satisfies the same three basic equations as $\Lambda(\mathbf{k})$ itself,

$$\Lambda(c\mathbf{k}) = \Lambda(\mathbf{k}). \tag{9a}$$

Similarly

$$\Lambda^*(\mathbf{k}) = \Lambda(\mathbf{k}). \tag{9b}$$

For any finite constant vector $\mathbf{k}_0$,

$$\int \mathrm{d}^3k \frac{\Lambda(\mathbf{k})}{(\mathbf{k}-\mathbf{k}_0)^2} = 0. \tag{9c}$$

To prove (9c), we rewrite its left hand side as

$$\int \mathrm{d}^3k \Lambda(\mathbf{k}) \left[\frac{1}{(\mathbf{k}-\mathbf{k}_0)^2} + \frac{c}{k^2}\right]$$

by using (8b). Here, c is *any* finite constant. If $c = -1$, the integrand decays like $1/k^3$ at large $\mathbf{k}$, in a given direction. Without Eq. (8c), we could not determine the integral unambiguously. Using (8c), however, we can take the *average* between the expression in the bracket and its spatial inversion, and get

$$\int \mathrm{d}^3k \Lambda(\mathbf{k}) \left[\frac{1}{2(\mathbf{k}-\mathbf{k}_0)^2} + \frac{1}{2(-\mathbf{k}-\mathbf{k}_0)^2} + \frac{c}{k^2}\right].$$

If $c = -1$, the integrand now decays like $1/k^4$ at large $\mathbf{k}$, and the integral is dominated by a finite region of the $\mathbf{k}$-space (whose size is of the order k_0), so according to Eq. (8a), the Lambda function can now be dropped. The resultant *ordinary* integral turns out to be 0. Eq. (9c) is thus proved. It follows that for any finite constant $\mathbf{k}_0$ and nonzero finite real constant c

$$\Lambda(c\mathbf{k} - \mathbf{k}_0) = \Lambda(\mathbf{k}). \tag{9d}$$

Similarly, it is easy to show, e.g.,

$$\int \frac{\mathrm{d}^3k}{(2\pi)^3} \frac{\Lambda(\mathbf{k})}{(\mathbf{k}-\mathbf{k}_0)^2 + \alpha^2} = -\frac{\alpha}{4\pi} \quad (\alpha \geqslant 0), \tag{9e}$$

which is the $\mathbf{k}$-space representation of the simple fact that the symmetric average of $\mathrm{e}^{-\alpha r + \mathrm{i}\mathbf{k}_0\cdot\mathbf{r}}/4\pi r$ at $\mathbf{r} \to 0$, excluding the $1/4\pi r$ term, is $-\alpha/4\pi$. Eq. (9e) is a generalization of (9c).

A notable corollary of the Lambda function, as illustrated by (9e), is that the full-space integral of a function that is *positive* for all finite $\mathbf{k}$'s may still be *negative*. We will see that this phenomenon is actually *useful* (in Section 4.3).

The integrals involving the Lambda function still obey many familiar rules. The region of integration, for example, can be freely divided into some subregions (with one restriction; see below), and the total integral equals the sum of the integrals over these subregions. For example,

$$\int \mathrm{d}^3k \frac{\Lambda(\mathbf{k})}{k^2} = \int_{k<K} \mathrm{d}^3k \frac{1}{k^2} + \int_{k>K} \mathrm{d}^3k \frac{\Lambda(\mathbf{k})}{k^2} = (+4\pi K) + (-4\pi K) = 0,$$

for any finite $K \geqslant 0$. In the ball region, $\mathbf{k}$ is finite and $\Lambda(\mathbf{k}) = 1$, while in the external region the integral is identical with that of $\Lambda(\mathbf{k})\theta(k-K)/k^2$ over the whole $\mathbf{k}$-space, which can be computed with the same method as is used to derive Eq. (9c). Here, for simplicity we separate the subregions with a sphere, but other arbitrary shapes of the boundaries are equally permissible, *provided* that infinite momentum is contained by *only one* subregion.

Like the delta function, $\Lambda(\mathbf{k})$ can freely participate in operations like addition, multiplication, integration, and Fourier transformation. It also commutes with other functions and quantum

mechanical state vectors and operators, i.e., $\Lambda(\mathbf{k})X = X\Lambda(\mathbf{k})$, where X may or may not depend on $\mathbf{k}$.

2.3. The Fourier transform of $\Lambda(\mathbf{k})$

The Fourier transform of $\Lambda(\mathbf{k})$ is

$$\lambda(\mathbf{r}) \equiv \int \frac{\mathrm{d}^3k}{(2\pi)^3}\Lambda(\mathbf{k})\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}. \tag{10}$$

Since $\Lambda(\mathbf{k})$ is both even and real, so is $\lambda(\mathbf{r})$:

$$\lambda(-\mathbf{r}) = \lambda(\mathbf{r}), \tag{11a}$$
$$\lambda^*(\mathbf{r}) = \lambda(\mathbf{r}). \tag{11b}$$

It follows from Eqs. (9a) and (10) that

$$\lambda(c\mathbf{r}) = \mid c\mid^{-3}\lambda(\mathbf{r}), \tag{11c}$$

a property reminiscent of the three-dimensional delta function. Here, c is any nonzero finite real constant.

Eq. (9c) can be expressed in $\mathbf{r}$-space as $\int \mathrm{d}^3r\lambda(\mathbf{r})\mathrm{e}^{\mathrm{i}\mathbf{k}_0\cdot\mathbf{r}}/r = 0$. Expanding this result in powers of k_0, we get

$$\int \mathrm{d}^3r\lambda(\mathbf{r})\frac{1}{r} = 0, \tag{11d}$$
$$\int \mathrm{d}^3r\lambda(\mathbf{r})\hat{\mathbf{r}} = 0. \tag{11e}$$

The fact that $\Lambda(\mathbf{k})$ is equal to 1 for any finite $\mathbf{k}$ leads to

$$\int \mathrm{d}^3r\lambda(\mathbf{r})f(\mathbf{r}) = f(0), \tag{11f}$$

for any function f which is *finite* and *continuous* in a region containing $\mathbf{r} = 0$. This entails, in particular, that

$$\lambda(\mathbf{r}) = 0 \quad (\text{if } \mathbf{r}\neq 0). \tag{11g}$$

From Eqs. (11d)–(11f), we get

$$\int \mathrm{d}^3r\lambda(\mathbf{r})\frac{g(\mathbf{r})}{r} = 0, \tag{11h}$$

for any function g which is *smooth* in a region containing $\mathbf{r} = 0$. This equation becomes obvious if we write $g(\mathbf{r}) = A + \mathbf{B}\cdot\mathbf{r} + O(r^2)$.

According to Eq. (11g), all the integrals involving $\lambda(\mathbf{r})$, like the ones showed above, can be restricted to a neighborhood of the origin without affecting their values. This is an important similarity between $\lambda(\mathbf{r})$ and $\delta(\mathbf{r})$. The two generalized functions mainly differ in two aspects: (1) $\int \mathrm{d}^3r\lambda(\mathbf{r})/r = 0$ but $\int \mathrm{d}^3r\delta(\mathbf{r})/r$ is divergent; (2) $\int \mathrm{d}^3r\lambda(\mathbf{r})\hat{\mathbf{r}} = 0$ but $\int \mathrm{d}^3r\delta(\mathbf{r})\hat{\mathbf{r}}$ is undefined.

$\lambda(\mathbf{r})$ is related to the operator $\delta(\mathbf{r})(\partial/\partial r)r$:

$$\int \mathrm{d}^3r\delta(\mathbf{r})\frac{\partial}{\partial r}[rf(\mathbf{r})] = \int \mathrm{d}^3r\lambda(\mathbf{r})f(\mathbf{r}), \tag{11i}$$

for any function f for which $\int \mathrm{d}^3r\delta(\mathbf{r})\frac{\partial}{\partial r}[rf(\mathbf{r})]$ is well-defined.

Finally, if we integrate both sides of Eq. (7) over $\mathbf{r}$, and use Eq. (11i), we get

$$\int \mathrm{d}^3r\lambda(\mathbf{r})\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \Lambda(\mathbf{k}), \tag{11j}$$

which is just the Fourier transformation from the $\mathbf{r}$-space to the $\mathbf{k}$-space. This equation is consistent with (10), because the Lambda function is even.

It will be clear that $\Lambda(\mathbf{k})$ and $\lambda(\mathbf{r})$ allow for a much more flexible treatment of the s-wave contact interaction problem than the operator $\delta(\mathbf{r})(\partial/\partial r)r$.

2.4. Two-body problem

The right-hand side of (6) equals $\frac{4\pi a}{m}\int\frac{d^3k'}{(2\pi)^3}\Lambda(\mathbf{k}')\widetilde{\phi}(\mathbf{k}')\delta(\mathbf{r})$ according to (7). Expanding $\delta(\mathbf{r})$ in terms of plane waves, and comparing both sides of Eq. (6), we obtain the $\mathbf{k}$-space representation of (5),

$$E_r\widetilde{\phi}(\mathbf{k}) = \frac{k^2}{m}\widetilde{\phi}(\mathbf{k}) + \frac{4\pi a}{m}\int\frac{d^3k'}{(2\pi)^3}\Lambda(\mathbf{k}')\widetilde{\phi}(\mathbf{k}') \tag{12}$$

or, equivalently,

$$E_r\widetilde{\phi}(\mathbf{k}) = \frac{k^2}{m}\widetilde{\phi}(\mathbf{k}) + \frac{4\pi a}{m\Omega}\sum_{\mathbf{k}'}\Lambda(\mathbf{k}')\widetilde{\phi}(\mathbf{k}').$$

To familiarize ourselves with this formalism, we consider a simple exact solution to (12), namely the bound state ($E_r<0$). Let f denote the second term on the right-hand side of (12). Solving (12) formally, we get

$$\widetilde{\phi}(\mathbf{k}) = -f/(k^2/m - E_r) \quad (f\neq 0) \tag{13}$$

which is smooth for all $\mathbf{k}$. Substituting (45) back into the definition of f, and using (9e), we get $f = fa\sqrt{-mE_r}$. So $a>0$, $E_r=-1/ma^2$, and $\widetilde{\phi}(\mathbf{k})\propto 1/(k^2+a^{-2})$, in perfect agreement with the established wisdom [17].

We can easily extend the above approach to three or more particles (see Section 5.2 for an illustration).

3. Short-range selectors

3.1. $L(\mathbf{k})$

If the connection between $\int d^3k$ and $\lim_{K\to\infty}\int_{|\mathbf{k}|<K} d^3k$ is not universal, nothing can prevent the existence of another generalized function, $L(\mathbf{k})$, defined as follows:

$$L(\mathbf{k}) = 0 \quad (\text{if } k<\infty), \tag{14a}$$

$$\int\frac{d^3k}{(2\pi)^3}\frac{L(\mathbf{k})}{k^2} = 1, \tag{14b}$$

$$L(-\mathbf{k}) = L(\mathbf{k}). \tag{14c}$$

As generalized functions, $\Lambda(\mathbf{k})$ and $L(\mathbf{k})$ can both be approached by ordinary functions. If $\mathbf{k}$ is a wave vector, $L(\mathbf{k})$'s dimension is length, while $\Lambda(\mathbf{k})$ is dimensionless.

3.2. Properties of the L function

$$\int\frac{d^3k}{(2\pi)^3}f(\mathbf{k})L(\mathbf{k}) = \lim_{\mathbf{k}\to\infty}k^2 f(\mathbf{k}) \tag{15a}$$

for any ordinary function $f(\mathbf{k})$.

We now list some other properties of $L(\mathbf{k})$; their proofs are similar to those in Section 2.

$$L(c\mathbf{k}) = |c|^{-1}L(\mathbf{k}) \tag{15b}$$

for any real constant $c\neq 0$.

$$L^*(\mathbf{k}) = L(\mathbf{k}), \tag{15c}$$

$$L(\mathbf{k}-\mathbf{k}_0) = L(\mathbf{k}) \tag{15d}$$

for any constant vector $\mathbf{k}_0$. An integral involving $L(\mathbf{k})$, like that involving $\Lambda(\mathbf{k})$, can be freely divided into many subintegrals (*provided* that infinite momentum is contained by *only one* subregion). $L(\mathbf{k})$ can also freely participate in various operations, and it commutes with other objects.

Now turn to the coordinate representation of the L function,

$$l(\mathbf{r}) \equiv \int \frac{\mathrm{d}^3 k}{(2\pi)^3} L(\mathbf{k}) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}. \tag{16}$$

For any ordinary function $f(\mathbf{r})$,

$$\int \mathrm{d}^3 r l(\mathbf{r}) f(\mathbf{r}) = \lim_{\mathbf{r}\to 0} 4\pi r f(\mathbf{r}). \tag{17a}$$

Other properties of $l(\mathbf{r})$ are listed below.

$$l(\mathbf{r}) = 0 \quad (\text{if } \mathbf{r}\neq 0), \tag{17b}$$

$$l^*(\mathbf{r}) = l(-\mathbf{r}) = l(\mathbf{r}), \tag{17c}$$

$$l(c\mathbf{r}) = |c|^{-2} l(\mathbf{r}) \tag{17d}$$

for any real constant $c\neq 0$. Eq. (17d) is consistent with the dimension of $l(\mathbf{r})$, namely $[\text{length}]^{-2}$.

$$\int \mathrm{d}^3 r l(\mathbf{r}) \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = L(\mathbf{k}). \tag{17e}$$

3.3. Introducing the short-range selectors

Let $f_1(\mathbf{k})$ be any ordinary function satisfying $\int \frac{\mathrm{d}^3 k}{(2\pi)^3} f_1(\mathbf{k}) = 1$. Let $f_2(\mathbf{k}) = 1/k^2 + r'(\mathbf{k})$ be any ordinary function satisfying $\int \frac{\mathrm{d}^3 k}{(2\pi)^3} r'(\mathbf{k}) = 0$. Let $s_1(\mathbf{k}) = \Lambda(\mathbf{k})$ and $s_2(\mathbf{k}) = L(\mathbf{k})$. We have

$$\int \frac{\mathrm{d}^3 k}{(2\pi)^3} s_i^*(\mathbf{k}) f_j(\mathbf{k}) = \delta_{ij}. \tag{18}$$

$f_1(\mathbf{k})$ and $f_2(\mathbf{k})$ span a two-dimensional linear space $\mathcal{F}$. $\Lambda(\mathbf{k})$ and $L(\mathbf{k})$ span another two-dimensional linear space $\mathcal{S}$. Eq. (18) states that $\mathcal{F}$ and $\mathcal{S}$ are *dual linear spaces*. We shall call the elements of $\mathcal{S}$ (short-range) selectors, because for any function $f(\mathbf{k}) = \sum_i c_i f_i(\mathbf{k})$, we can selectively extract the coefficient c_i using an element in $\mathcal{S}$: $\int \frac{\mathrm{d}^3 k}{(2\pi)^3} s_i^*(\mathbf{k}) f(\mathbf{k}) = c_i$.

All these functions can be Fourier-transformed to the $\mathbf{r}$-space. Let $\widetilde{s}_i(\mathbf{r}) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} s_i(\mathbf{k}) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$, $\widetilde{f}_i(\mathbf{r}) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} f_i(\mathbf{k}) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$.

$$\int \mathrm{d}^3 r \widetilde{s}_i^*(\mathbf{r}) \widetilde{f}_j(\mathbf{r}) = \delta_{ij}, \tag{19}$$

which represents a group of nontrivial equations:

$$\begin{aligned} &\int \mathrm{d}^3 r \lambda(\mathbf{r}) = 1, \quad \int \mathrm{d}^3 r \lambda(\mathbf{r})/(4\pi r) = 0, \\ &\int \mathrm{d}^3 r l(\mathbf{r}) = 0, \quad \int \mathrm{d}^3 r l(\mathbf{r})/(4\pi r) = 1. \end{aligned} \tag{20}$$

Also,

$$\widetilde{s}_i(\mathbf{r}) = 0 \quad (\text{if } \mathbf{r}\neq 0). \tag{21}$$

Each short-range selector corresponds to a linear functional which extracts a short-range property of an ordinary function $\widetilde{f}(\mathbf{r})$.

At this point, we have completed a tool which will free us from ill-defined ultraviolet divergences, for the two-component Fermi gas with s-wave contact interaction [1]. In this formalism, no *ad hoc* large momentum cut-offs or dimensional regularizations are needed.

Here, we have presented our approach in a generic form, so that it *might* be possible to extend it to other physical systems involving contact interactions. For the other systems we may need more than two linearly independent short-range selectors. For instance, we may need *three* independent selectors when the two components of the Fermi gas with s-wave contact interaction have a mass ratio exceeding 13.6, so that there is Efimov effect which introduces an additional parameter for the interaction [18,19].

3.4. The η-selector

The η-selector is a particular element in $\mathcal{S}$:

$$\eta(\mathbf{k}) \equiv \Lambda(\mathbf{k}) + \frac{L(\mathbf{k})}{4\pi a}, \tag{22a}$$

$$\widetilde{\eta}(\mathbf{r}) \equiv \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \eta(\mathbf{k}) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \lambda(\mathbf{r}) + \frac{l(\mathbf{r})}{4\pi a}. \tag{22b}$$

This selector will play a crucial role in the s-wave contact interaction problem, because it selectively annihilates the relative wave function of two particles with such interaction:

$$\int \mathrm{d}^3 r \widetilde{\eta}(\mathbf{r})[1/r - 1/a + O(r)] = 0. \tag{23a}$$

On the other hand,

$$\int \mathrm{d}^3 r \widetilde{\eta}(\mathbf{r}) f(\mathbf{r}) = f(0), \tag{23b}$$

for any ordinary function $f(\mathbf{r})$ that is continuous in the neighborhood of the origin, so $\widetilde{\eta}(\mathbf{r})$ behaves like the delta function for nonsingular functions. More properties of the η-selector are listed below.

$$\int \mathrm{d}^3 r \widetilde{\eta}(\mathbf{r}) \hat{\mathbf{r}} = 0, \tag{23c}$$

$$\widetilde{\eta}(\mathbf{r}) = 0 \quad (\text{if } \mathbf{r} \neq 0), \tag{23d}$$

$$\widetilde{\eta}^*(\mathbf{r}) = \widetilde{\eta}(-\mathbf{r}) = \widetilde{\eta}(\mathbf{r}), \tag{23e}$$

$$\eta(\mathbf{k}) = 1 \quad (\text{if } k < \infty), \tag{23f}$$

$$\int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\eta(\mathbf{k})}{k^2} = \frac{1}{4\pi a}, \tag{23g}$$

$$\int \frac{\mathrm{d}^3 k}{(2\pi)^3} \eta(\mathbf{k}) f(\mathbf{k}) = \frac{c}{4\pi a} + \lim_{K\to\infty} \int_{|\mathbf{k}|<K} \frac{\mathrm{d}^3 k}{(2\pi)^3} \left[f(\mathbf{k}) - \frac{c}{k^2} \right], \tag{23h}$$

where $f(\mathbf{k})$ is an ordinary function and $c = \lim_{\mathbf{k}\to\infty} k^2 f(\mathbf{k})$.

4. Energy theorem

4.1. Mathematical formulation

Theorem. *If the system of fermions of equal mass m populating two spin states with s-wave contact interaction and scattering length a is in a smooth external potential* $V_{\mathrm{ext}}(\mathbf{r})$*, and is in a state* $\hat{\rho} = \sum_{i=1}^{\infty} \alpha_i \mid \phi_i\rangle\langle\phi_i \mid$ *(where* $\langle\phi_i \mid \phi_j\rangle = \delta_{ij}$*,* $\alpha_i \geqslant 0$*, and* $\sum_i \alpha_i = 1$*) satisfying two conditions: firstly each* $\mid \phi_i\rangle$ *is a linear combination of energy eigenstates with coefficients of the combination decaying sufficiently fast at large energy such that the wave function* ϕ_i *in the coordinate representation has no singularities other than those introduced by the interfermionic interaction, and secondly the probability* α_i *decays sufficiently fast at large i such that*

$$C = \sum_i \alpha_i C_i, \tag{24}$$

where C [defined by (3)] is associated with the state $\hat{\rho}$, and C_i associated with $|\phi_i\rangle$ [20], then the system's energy expectation value is

$$E = \sum_{\mathbf{k}\sigma} \eta(\mathbf{k}) \frac{k^2}{2m} n_{\mathbf{k}\sigma} + \sum_{\sigma} \int \mathrm{d}^3 r V_{\mathrm{ext}}(\mathbf{r}) \rho_\sigma(\mathbf{r}). \tag{25}$$

Here, $\eta(\mathbf{k})$ is defined in the previous section, $n_{\mathbf{k}\sigma}$ is the momentum distribution, and $\rho_\sigma(\mathbf{r})$ is the spatial density distribution.

Proof. The second term on the right-hand side of (25) is trivial. We will concentrate on the first term, E_{internal}, which is physically the sum of the total kinetic energy and the interfermionic interaction energy, both of which are divergent in the zero-range interaction limit. However, E_{internal} can be unambiguously determined in this limit (with $a \neq 0$ fixed), using the pseudopotential method.

Let us first consider the case in which the system is in a pure state $|\phi\rangle$ having exactly N fermions in the spin up state and M fermions in the spin down state:

$$\begin{aligned} |\phi\rangle = \frac{1}{N!M!} \int \mathrm{d}^3 r_1 \cdots \mathrm{d}^3 r_N \ \mathrm{d}^3 s_1 \cdots \mathrm{d}^3 s_M \phi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{s}_1, \ldots, \mathbf{s}_M) \\ \times \psi_\uparrow^\dagger(\mathbf{r}_1) \cdots \psi_\uparrow^\dagger(\mathbf{r}_N) \psi_\downarrow^\dagger(\mathbf{s}_1) \cdots \psi_\downarrow^\dagger(\mathbf{s}_M) |0\rangle, \end{aligned} \tag{26}$$

where $|0\rangle$ is the particle vacuum, and $\psi_\sigma(\mathbf{r})$ is the standard fermion annihilation operator at spin state σ and spatial location $\mathbf{r}$. The wave function $\phi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{s}_1, \ldots, \mathbf{s}_M)$ is completely antisymmetric under the exchange of any two fermions in the same spin state; it has also been properly normalized:

$$\frac{1}{N!M!} \int \mathrm{d}^3 r_1 \cdots \mathrm{d}^3 r_N \mathrm{d}^3 s_1 \cdots \mathrm{d}^3 s_M \ |\phi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{s}_1, \ldots, \mathbf{s}_M)|^2 = 1, \tag{27}$$

so that $\langle \phi | \phi \rangle = 1$.

The *only role* of the pseudopotential is to *exactly cancel* the delta function singularities arising when the kinetic energy operator (which is just a $3N + 3M$-dimensional Laplace operator divided by $-2m$) acts on the wave function. These delta functions arise when two fermions with opposite spins come together. To understand this, we may examine Eq. (5) closely; note also that this cancelation mechanism is carried over to the arbitrary-body cases, with or without external potentials. The internal energy of the fermions is therefore given by a simple expression,

$$-2m E_{\mathrm{internal}} = \frac{1}{N!M!} \lim_{\epsilon \to 0} \int_{\mathcal{D}(\epsilon)} \mathrm{d}^{3N+3M} R \phi^*(\mathbf{R}) \nabla^2 \phi(\mathbf{R}), \tag{28}$$

where $\mathbf{R}$ is the shorthand for the $3N + 3M$ coordinates of the fermions, and ∇^2 is the $3N + 3M$-dimensional Laplace operator. $\mathcal{D}(\epsilon)$ is a subset of the $3N + 3M$-dimensional configuration space, *excluding* the regions in which any two fermions with opposite spins have a distance *less than* ϵ.

Now define another quantity X,

$$\begin{aligned} -2mX \equiv \frac{1}{N!M!} \int \mathrm{d}^{3N+3M} R \mathrm{d}^3 t \tilde{\eta}(\mathbf{t}) \phi^*(\mathbf{r}_1 \cdots \mathbf{r}_N \mathbf{s}_1 \cdots \mathbf{s}_M) \\ \times \nabla_{\mathbf{t}}^2 \left[\sum_{i=1}^{N} \phi(\mathbf{r}_1 \cdots \mathbf{r}_{i-1}, \mathbf{r}_i + \mathbf{t}, \mathbf{r}_{i+1} \cdots \mathbf{r}_N \mathbf{s}_1 \cdots \mathbf{s}_M) + \sum_{j=1}^{M} \phi(\mathbf{r}_1 \cdots \mathbf{r}_N \mathbf{s}_1 \cdots \mathbf{s}_{j-1}, \mathbf{s}_j + \mathbf{t}, \mathbf{s}_{j+1} \cdots \mathbf{s}_M) \right], \end{aligned} \tag{29}$$

and we want to prove that $X = E_{\mathrm{internal}}$. To do so, we divide the $3N + 3M$-dimensional $\mathbf{R}$-space in this new integral into $\mathcal{D}(\epsilon)$ and $\mathcal{I}(\epsilon)$, where $\mathcal{D}(\epsilon)$ is the same as above, and $\mathcal{I}(\epsilon)$ is complementary to $\mathcal{D}(\epsilon)$. Clearly, in the subregion $\mathcal{D}(\epsilon)$, the integral over $\mathbf{R}$ is finite and continuous, and the result is a continuous function of $\mathbf{t}$ for $t < \epsilon$; then, according to the basic property of $\tilde{\eta}(\mathbf{t})$, it can be treated as the delta function, and we immediately see the integral is exactly equal to the integral in E_{internal}.

We then only need to show that the integral in $\mathcal{I}(\epsilon)$ approaches zero as $\epsilon \to 0$. Since the volume of $\mathcal{I}(\epsilon)$ is proportional to ϵ^3 when ϵ is sufficiently small, $\mathcal{I}(\epsilon)$ can be further divided into NM subregions, in one of which $|\mathbf{r}_1 - \mathbf{s}_1| < \epsilon$. All the other $NM - 1$ subregions are the same as this, due to fermionic

symmetry. We have omitted subregions with volumes of higher orders in ϵ. In the thermodynamic limit, however, even when ϵ is very small, we can still have many pairs of fermions, and the distance between two fermions in each of these pairs is smaller than ϵ. But we note that these pairs are far apart if ϵ is small, so they can be treated *independently*.

So now we only consider the case in which $|\mathbf{r}_1 - \mathbf{s}_1| < \epsilon$, which is representative of the general situation. In this case, only two terms in the big bracket on the right side of Eq. (29) have the possibility of making contributions to the total integral which do not approach zero. One of them is the term in which $\mathbf{r}_1$ is replaced by $\mathbf{r}_1 + \mathbf{t}$, the other being the one in which $\mathbf{s}_1$ is replaced by $\mathbf{s}_1 + \mathbf{t}$. We only discuss the first term, since the logic is the same for the second one.

To treat this term we make a coordinate transformation: $\mathbf{r} = \mathbf{r}_1 - \mathbf{s}_1$ and $\mathbf{r}_0 = (\mathbf{r}_1 + \mathbf{s}_1)/2$, and represent $\mathbf{r}_2, \ldots, \mathbf{r}_N, \mathbf{s}_2, \ldots, \mathbf{s}_M$ with a single $3N + 3M - 6$-dimensional vector $\mathbf{R}'$. We then first do integral over $\mathbf{r}$ (and $r < \epsilon$), then do the integral over $\mathbf{t}$, and finally integrate over $\mathbf{r}_0$ and $\mathbf{R}'$.

Expanding $\phi(\mathbf{R}', \mathbf{r}_0, \mathbf{r})$ in this case as $A(\mathbf{R}', \mathbf{r}_0)(1/r - 1/a) + O(r)$ (according to the short range boundary condition), we write our target integral in the form

$$Y = \int \mathrm{d}^{3N+3M-6}R' \mathrm{d}^3 r_0 \int \mathrm{d}^3 t \tilde{\eta}(\mathbf{t}) \nabla_{\mathbf{t}}^2 K(\mathbf{R}', \mathbf{r}_0, \mathbf{t}),$$

where we have omitted the constant coefficient since it is irrelevant to our question, and

$$K(\mathbf{R}', \mathbf{r}_0, \mathbf{t}) \equiv \int_{r<\epsilon} \mathrm{d}^3 r \left[A^*(\mathbf{R}', \mathbf{r}_0)(1/r - 1/a) + O(r)\right] \times \left[A(\mathbf{R}', \mathbf{r}_0 + \mathbf{t}/2)(1/|\mathbf{r} + \mathbf{t}| - 1/a) + O(|\mathbf{r} + \mathbf{t}|)\right].$$

K should be expanded in powers of the small $\mathbf{t}$, before we can carry out the integral over $\mathbf{t}$; t is regarded as much smaller than ϵ, because $\tilde{\eta}(\mathbf{t})$ is zero for any nonzero $\mathbf{t}$. In such an expansion, any term which contains a factor ϵ raised to any positive power should be omitted. Also, any term which is of the order t^3 or higher should be omitted, since it contributes nothing to the integral $\int \mathrm{d}^3 t \tilde{\eta}(\mathbf{t}) \nabla_{\mathbf{t}}^2 [\cdot]$. We then have $K \sim c_1(t/2 - t^2/6a) + \mathbf{c}_2 \cdot \hat{\mathbf{t}} t^2$, where $c_1 = -4\pi |A(\mathbf{R}', \mathbf{r}_0)|^2$, and $\mathbf{c}_2 = -\pi A^*(\mathbf{R}', \mathbf{r}_0) \nabla_{\mathbf{r}_0} A(\mathbf{R}', \mathbf{r}_0)$. But now $\nabla_{\mathbf{t}}^2 K \sim c_1(1/t - 1/a) + 4\mathbf{c}_2 \cdot \hat{\mathbf{t}}$, and according to the short-range properties of $\tilde{\eta}(\mathbf{t})$, the integral over $\mathbf{t}$ vanishes.

The above analysis shows that the contribution to X from $\mathcal{I}(\epsilon)$ approaches zero as $\epsilon \to 0$, so $X = E_{\text{internal}}$.

Eq. (29) can be easily rewritten in the second-quantized form:

$$-2mX = \left\langle \phi \middle| \sum_\sigma \int \mathrm{d}^3 r \mathrm{d}^3 t \tilde{\eta}(\mathbf{t}) \nabla_{\mathbf{t}}^2 \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r} + \mathbf{t}) \middle| \phi \right\rangle.$$

Expanding $\psi_\sigma(\mathbf{r}) = \Omega^{-1/2} \sum_{\mathbf{k}_1} c_{\mathbf{k}_1 \sigma} \exp(\mathrm{i}\mathbf{k}_1 \cdot \mathbf{r})$ and similarly for $\psi_\sigma(\mathbf{r} + \mathbf{t})$, and carrying out the integration over $\mathbf{r}$ and $\mathbf{t}$, we get

$$-2mX = \left\langle \phi \middle| \sum_{\mathbf{k}\sigma} \eta(\mathbf{k})(-k^2) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \middle| \phi \right\rangle.$$

So $E_{\text{internal}} = \sum_{\mathbf{k}\sigma} \eta(\mathbf{k})(k^2/2m) \langle \phi | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \phi \rangle$.

So far, we have proved (25) for a pure quantum state, with fixed numbers of fermions in the two spin states.

If the pure state is not an eigenstate of particle numbers in the two spin states, we can expand it as a superposition of such eigenstates; since the interaction conserves the number of fermions in each spin state, the off-diagonal matrix elements of the Hamiltonian between these eigenstates are zero, and the theorem remains valid.

If the system is in a mixed state, described by the density operator $\hat{\rho}$, and the different eigenstates of $\hat{\rho}$ independently satisfy the theorem, then the statistical ensemble of these states still satisfies the theorem, provided that (24) holds.

Using Eq. (23h) to reexpress the first term on the right-hand side of (25), we get (2).

From the many-body wave function, we can also prove Eq. (3) by expanding $\langle \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r} + \mathbf{t}) \rangle$ at small $\mathbf{t}$. In this expansion there is a singular term (proportional to t but independent of $\hat{\mathbf{t}}$) that is independent of σ:

$$\langle\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}+\mathbf{t})\rangle = \rho_\sigma(\mathbf{r}) - \frac{C(\mathbf{r})t}{8\pi} + \frac{\mathrm{i}}{\hbar}\mathbf{p}_\sigma(\mathbf{r})\cdot\mathbf{t} + O(t^2), \tag{30}$$

$$C(\mathbf{r}) \equiv \frac{16\pi^2}{(N-1)!(M-1)!}\int \mathrm{d}^{3N+3M-6}R' \mid A(\mathbf{R}', \mathbf{r})|^2, \tag{31}$$

where $A(\mathbf{R}', \mathbf{r}_0)$ is defined in the above proof. Consequently, $\mathbf{n}_{\mathbf{k}\sigma}$ decays like C/k^4 at large $\mathbf{k}$, and

$$\Omega C = \int C(\mathbf{r})\mathrm{d}^3 r \equiv \mathcal{I}. \tag{32}$$

We can also show a result for the *pair correlations*:

$$\langle\hat\rho_\uparrow(\mathbf{r}-\mathbf{t}/2)\hat\rho_\downarrow(\mathbf{r}+\mathbf{t}/2)\rangle = \frac{C(\mathbf{r})}{16\pi^2}\left(\frac{1}{t^2} - \frac{2}{at}\right) + O(t^0) \tag{33}$$

at small $\mathbf{t}$, where $\hat\rho_\sigma(\mathbf{r}) \equiv \psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r})$.

4.2. Other proofs

For those who are not satisfied with the proof of the energy theorem with the η-selector, we have in principle at least two other proofs. One of them is almost identical with the proof presented; instead of directly using the η-selector to annihilate some terms, we may do a detailed analysis of the behavior of $\langle\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}+\mathbf{t})\rangle$ at small $\mathbf{t}$, and, besides the term proportional to t (independent of the direction of $\mathbf{t}$), we also need to analyze the term proportional to t^2 (also independent of $\hat{\mathbf{t}}$). There is also a term proportional to the inner product of $t^2\hat{\mathbf{t}}$ and a direction vector, but it contributes nothing if we do the symmetric integral in momentum space (as is done in Eq. (2)).

The other proof is inspired by what Eq. (2) tells us. Instead of studying an idealized s-wave contact interaction model, we may study a short-range (r_0) attractive interaction potential, and fine-tune the depth of the potential to achieve a specified scattering length ($\mid a \mid \gg r_0$). Then, we can divide the total internal energy in two pieces. One of them is the integral of kinetic energy up to a momentum scale K, where K is much smaller than $1/r_0$ but much larger than the other characteristic momentum scales in the problem. The other piece is the kinetic energy integral from K to much higher than $1/r_0$, *plus* all the interfermionic interaction energy. It is then possible to show that the second piece can be expressed in terms of $C \approx K^4 n_{\mathbf{K}\sigma}$: approximately $[\pi/(2a) - K]\Omega C/(2\pi^2 m) + O(1/K)$, with other errors that vanish in the limit $r_0 \to 0$ (but the scattering length is kept constant). In the two-body case, this approach can work out without much difficulty. In the many-body cases, it is however tricky to give a rigorous proof; but there is a *heuristic* physical picture: at large K, we are effectively probing those fermions each of which is close to another fermion (with distance $\sim 1/K$), and for each of such fermion pair, two-body physics is a good approximation.

4.3. Physical implications

One can measure the momentum distribution $n_{\mathbf{k}\sigma}$ experimentally. A well-known method is to suddenly switch off *both* the interaction between fermions *and* the external confinement potential, to allow the fermionic cloud to expand ballistically. Because particles with different momenta move at different velocities, eventually the spatial density distribution will reflect the momentum distribution. (The spatial distribution can be measured with some imaging technique.) See, e.g., Ref. [21].

From the measured $n_{\mathbf{k}\sigma}$, one can compute a partial kinetic energy, by summing contributions from all $\mathbf{k}$'s up to scale K:

$$T(K) \equiv \sum_{|\mathbf{k}|<K,\sigma} \frac{\hbar^2 k^2}{2m} n_{\mathbf{k}\sigma}, \tag{34}$$

and plot $T(K)$ versus K. Because of the nonzero C [22] (in the C/k^4 tail of the momentum distribution), $T(K)$ does not approach any finite value for $K \ll 1/r_0$, but instead, it approaches a straight line with a positive slope, which is just the *asymptote* of the curve $T(K)$. What Eq. (2) states is simply that *the*

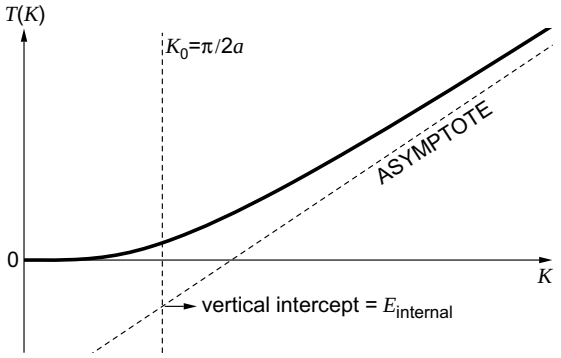

Fig. 1. Partial kinetic energy $T(K)$ versus K. The vertical intercept of the asymptote at $K_0 = \pi/2a$ equals the internal energy, according to (35).

internal energy is exactly equal to the vertical intercept of such an asymptote at $K_0 \equiv \pi/(2a)$. See Fig. 1 for illustration. More specifically,

$$T(K) = E_{\text{internal}} + \frac{\hbar^2 \Omega C}{2\pi^2 m}\left(K - \frac{\pi}{2a}\right) + O(1/K), \tag{35}$$

for K much larger than the other momentum scales in the problem but much smaller than $1/r_0$. This result is *universally valid*, as is stressed in Section 1.

The $O(1/K)$ term on the right-hand side of (35) is related to the second order singularity of the relative wave function of two fermions with opposite spins. The first order singularity is like $1/r$ and the second order is like r. The interference between these two orders gives rise to a term $\propto 1/K$ at large K.

If we plot $T(K)$ all the way up to the scale $1/r_0$, the above asymptote behavior breaks down, and the curve eventually approaches a horizontal line, associated with the total kinetic energy, which is much larger than the internal energy.

It is simple mathematics to confirm the energy theorem in the case of an isolated bound state of two fermions, whose momentum distribution is [17]

$$n_{\mathbf{k}\sigma} = \frac{C}{\left(|\,\mathbf{k} - \mathbf{k}_0|^2 + a^{-2}\right)^2}, \quad C = \frac{8\pi}{a\Omega},$$

where $2\hbar\mathbf{k}_0$ is the total momentum. In this case the first term on the right-hand side of Eq. (2) equals $+2\hbar^2/(ma^2)$, and the second term equals $-3\hbar^2/(ma^2) + (\hbar k_0)^2/m$. The total energy is $-\hbar^2/(ma^2) + (\hbar k_0)^2/m$, simply a sum of the binding energy [17] and the center-of-mass kinetic energy. Note that the total energy is negative if $k_0 < a^{-1}$.

Here, we see that the symbol $\eta(\mathbf{k})$ has to break the conventional law of integral (that the integral over the whole $\mathbf{k}$-space equals the limit of integrals over finite regions of this space), otherwise it would be impossible for the first term on the right-hand side of Eq. (25) to generate any negative number, since $\eta(\mathbf{k})$ is equal to $+1$ for any finite $\mathbf{k}$ and the momentum distribution is also everywhere positive. The negative binding energy is associated with this purely positive momentum distribution. We could of course reject this modified notion of integration, and stick to Eq. (2) only, but then the beautiful structure of the problem, as shown by (25), would be obscured.

The energy theorem takes a particularly simple form in the unitarity limit: when $a \to \infty$, the internal energy is just the intercept of the aforementioned asymptote at *zero momentum*.

The quantum few-body problem in the unitarity limit in a harmonic trap is preliminarily studied in [23]; we may also study the momentum distributions of these few-body systems and relate them to the energies, using Eq. (35).

Eqs. (32) and (33) imply that the expectation of the number of pairs of fermions with diameters smaller than a *small* distance s is

$$N_{\text{pair}} = \frac{\Omega C s}{4\pi} \tag{36}$$

if s is still much larger than r_0. More specifically, the expectation of the number of pairs of fermions located in a volume element $\mathrm{d}^3 r$, with diameters smaller than a small distance s is

$$\mathrm{d}N_{\text{pair}} = \frac{C(\mathbf{r}) s}{4\pi} \mathrm{d}^3 r. \tag{37}$$

For these reasons, we shall call $C(\mathbf{r})$ *local contact intensity*, $\mathcal{I} = \int C(\mathbf{r}) \mathrm{d}^3 r = \Omega C$ *integrated* contact intensity, and C *average* contact intensity (over volume Ω).

In a trapped Fermi gas, when the Thomas–Fermi approximation is valid, we may also have an approximate concept of local momentum distribution, valid within the limit set by Heisenberg uncertainty principle. Here, we are using the term "Thomas–Fermi approximation" in its broadest sense, namely the fermionic cloud is divided into many portions: each portion is *both* so small that it is roughly uniform, *and* so large that it can be treated as in the thermodynamic limit, so that all the thermodynamic quantities are meaningful.

Even when the Thomas–Fermi approximation is invalid (e.g., in few-body systems), the local contact intensity $C(\mathbf{r})$ is still an *exact* concept. The resolution δk of the momentum distribution within a local spatial region is of the order the inverse size of the region. In the large momentum part, where we can use a large unit for momentum, δk is negligible, and a tail $C(\mathbf{r})/k^4$ is well-defined.

We also have a concept of *local internal energy density* $\epsilon_{\text{internal}}$, inspired by an intermediate step in the proof of the energy theorem:

$$\epsilon_{\text{internal}}(\mathbf{r}) \equiv -\sum_{\sigma} \int \mathrm{d}^3 s \widetilde{\eta}(\mathbf{s}) \frac{\hbar^2 \nabla_{\mathbf{s}}^2}{2m} \left\langle \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r}+\mathbf{s}) \right\rangle, \tag{38}$$

and the total internal energy is exactly

$$E_{\text{internal}} = \int \epsilon_{\text{internal}}(\mathbf{r}) \mathrm{d}^3 r. \tag{39}$$

The above results concerning local pair correlations and local energy densities can help us to address a fundamental problem for a finite number of fermions, namely how to construct a systematically improvable perturbation theory, with the Thomas–Fermi approximation as the zeroth order approximation. The problem is important for two reasons: (1) ultracold atomic Fermi gases realized so far typically contain hundreds of thousands of atoms, for which the Thomas–Fermi approximation has detectable errors, and (2) if we want to use a quantum few-body system to simulate the many-body thermodynamic limit (see, e.g., [23]), finite size corrections must be taken into account. In fact few-body calculations are *all that we can do*. BCS theory, for example, is all about the two-fermion correlations in the presence of a many-body *mean field*. Quantum Monte-Carlo simulations are restricted to a small number of particles. In fact we can not solve Schrödinger equation for more than a handful of particles (except for the noninteracting systems or some very special systems).

In the thermodynamic limit, the behavior of C or the complete momentum distribution on the entire $(-1/k_{\text{F}}a, T/T_{\text{F}})$ plane (for balanced populations of the two spin states) is worth studying. Here, T is temperature, and $T_{\text{F}} = \hbar^2 k_{\text{F}}^2 / 2mk_{\text{B}}$ the Fermi temperature. Since the energy does not change smoothly across the phase transition line, the energy theorem implies that the momentum distribution also has some unsmooth change.

Another implication of the energy theorem concerns a common dynamic process: the Fermi gas is initially confined in a trap, and then the trap potential is suddenly turned off (but the scattering length is not changed), so that the gas expands in the presence of interactions. During the expansion, the contact intensity continuously decreases, in such a way that the vertical intercept [at $K_0 = \pi/(2a)$] of the *asymptote* of the function $T(K)$ remains constant because of energy conservation. This is a *constraint* on the instantaneous momentum distributions.

If the Fermi gas is in a motion (or if we are looking at a *local portion* of the expanding cloud in the local approximation), and the momentum distribution is roughly symmetric around $\mathbf{k} = \mathbf{k}_0$, it is better to use the following alternative formula to evaluate the internal energy

$$E_{\text{internal}} = \frac{\hbar^2 \Omega C}{4\pi a m} + \lim_{K\to\infty} \sum_{|\mathbf{k}-\mathbf{k}_0|<K,\sigma} \left[\frac{\hbar^2 k^2}{2m} n_{\mathbf{k}\sigma} - \frac{\hbar^2 C}{2m(\mathbf{k}-\mathbf{k}_0)^2} \right], \tag{40}$$

and $C = \lim_{\mathbf{k}-\mathbf{k}_0\to\infty} |\mathbf{k}-\mathbf{k}_0|^4 n_{\mathbf{k}\sigma}$. These two formulas are equivalent to Eqs. (2) and (3), in the contact-interaction limit. But now k_0 can exceed $1/r_0$ without leading to any problems, provided that the typical *relative* energy of these fermions is much smaller than $\hbar^2/(mr_0^2)$.

5. Many-body problem in momentum space

5.1. Basic formulation

Many-body theories are often studied in momentum space, because in the thermodynamic limit, we often have translational symmetry, and the exploitation of this symmetry in momentum space simplifies many things.

The s-wave contact interaction problem, however, lacks a satisfactory momentum representation to date. The peculiar contact interaction causes ultraviolet divergence problems, which some authors deal with by using concepts like "bare" coupling constants and renormalized ones; the shortcoming of these approaches is that the bare constants are ill-defined divergent quantities, and the sum of them and the divergent counterterms are ambiguous.

Here, we write down the momentum formulation of the problem, using the short-range selectors.

We start from the coordinate space. The many-body Hamiltonian is

$$H = H_{\text{internal}} + \int \mathrm{d}^3 r \sum_\sigma V_{\text{ext}}(\mathbf{r}) \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r}), \tag{41}$$

$$H_{\text{internal}} = -\frac{1}{2m} \int \mathrm{d}^3 r \sum_\sigma \psi_\sigma^\dagger(\mathbf{r}) \nabla^2 \psi_\sigma(\mathbf{r}) + \frac{4\pi a}{m} \int \mathrm{d}^3 r \mathrm{d}^3 r' \lambda(\mathbf{r}') \psi_\uparrow^\dagger(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) \psi_\downarrow(\mathbf{r}-\mathbf{r}'/2) \psi_\uparrow(\mathbf{r}+\mathbf{r}'/2). \tag{42}$$

Note the similarity between the above equation and Eqs. (1) and (2) of Ref. [16], where the hard-sphere *Bose* gas is studied; but in our context, in the contact interaction limit, the pseudopotential Hamiltonian is exact. Any *right-hand side eigenstate* $|\phi\rangle$ of the Hamiltonian (satisfying $H|\phi\rangle = E|\phi\rangle$), or any linear combinations of such eigenstates (with an upper bound in energy), automatically satisfy the short-range boundary condition

$$\int \mathrm{d}^3 r' \tilde{\eta}(\mathbf{r}') \psi_\downarrow(\mathbf{r}-\mathbf{r}'/2) \psi_\uparrow(\mathbf{r}+\mathbf{r}'/2) |\phi\rangle = 0. \tag{43}$$

All the state vectors which satisfy this boundary condition form a subspace of the Hilbert space, and we call it the *physical subspace*, and represent it with $\mathcal{P}$ [24].

Eqs. (42) and (43) can be rewritten in the momentum space:

$$H_{\text{internal}} = \sum_{\mathbf{k}\sigma} \frac{k^2}{2m} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{4\pi a}{m\Omega} \sum_{\mathbf{q}\mathbf{k}\mathbf{k}'} \Lambda(\mathbf{k}') c_{\mathbf{q}/2+\mathbf{k}\uparrow}^\dagger c_{\mathbf{q}/2-\mathbf{k}\downarrow}^\dagger c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow}, \tag{44}$$

$$\sum_{\mathbf{k}} \eta(\mathbf{k}) c_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2+\mathbf{k}\uparrow} |\phi\rangle = 0 \quad (\text{for any } \mathbf{q}). \tag{45}$$

All the ultraviolet divergence problems disappear, when $\Lambda(\mathbf{k}')$ is restored in the Hamiltonian. No divergent bare constants, no *ad hoc* regularizations, no renormalizations. Everything can be formulated *simply* and *exactly*.

We now describe how to compute the expectation value of H_{internal} under any state $|\phi\rangle \in \mathcal{P}$. The rule is very simple:

$$\langle H_{\text{internal}} \rangle = \sum_{\mathbf{k}} \left\{ \sum_\sigma \frac{k^2}{2m} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle + \frac{4\pi a}{m\Omega} \sum_{\mathbf{q}\mathbf{k}'} \Lambda(\mathbf{k}') \langle c_{\mathbf{q}/2+\mathbf{k}\uparrow}^\dagger c_{\mathbf{q}/2-\mathbf{k}\downarrow}^\dagger c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow} \rangle \right\}, \tag{46}$$

that is, the two terms should be grouped in the above way. Now the energy is finite, so the summation over $\mathbf{k}$ is convergent and the summand decays faster than $1/k^3$ at large $\mathbf{k}$. Consequently, we can insert the η-selector, according to (23h):

$$\langle H_{\text{internal}}\rangle = \sum_{\mathbf{k}} \eta(\mathbf{k}) \left\{ \sum_{\sigma} \frac{k^2}{2m} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle + \frac{4\pi a}{m\Omega} \sum_{\mathbf{q}\mathbf{k}'} \Lambda(\mathbf{k}') \langle c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow}\rangle \right\}.$$

Distributing $\eta(\mathbf{k})$ to the two terms, we get

$$\langle H_{\text{internal}}\rangle = \sum_{\mathbf{k}\sigma} \eta(\mathbf{k}) \frac{k^2}{2m} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle + \frac{4\pi a}{m\Omega} \sum_{\mathbf{q}\mathbf{k}\mathbf{k}'} \eta(\mathbf{k}) \Lambda(\mathbf{k}') \langle \phi \mid c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow} \mid \phi\rangle / \langle \phi \mid \phi\rangle,$$

but the second term must vanish, since the Hermitian conjugate of Eq. (45) is $\sum_{\mathbf{k}} \eta(\mathbf{k}) \langle \phi \mid c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} = 0$. Therefore,

$$\langle H_{\text{internal}}\rangle = \sum_{\mathbf{k}\sigma} \eta(\mathbf{k}) \frac{k^2}{2m} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle,$$

which is precisely the energy theorem.

It is tempting to use this approach as the simplest way to derive the energy theorem. However, it is not explained why the terms should be grouped in the way as in Eq. (46), even though it is a very natural grouping. It is the logical proof of the energy theorem in the last section that supports this way of grouping the terms.

The inner product of Eq. (45) with any quantum state is zero. This gives us many useful identities. The simplest of them is

$$\sum_{\mathbf{k}} \eta(\mathbf{k}) \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle = 0, \tag{47}$$

which is a constraint on the pairing amplitude in the superfluid state. We have also seen the constraint on the two-body reduced density matrix, and we exploited it to rederive the energy theorem above. Similar constraints are present on the three-body, four-body,..., reduced density matrices.

The internal Hamiltonian (44), although not Hermitian in the whole Hilbert space, *is* Hermitian in the physical subspace. This can be easily shown from the energy theorem, which indicates that the expectation value of H_{internal} under any state in $\mathcal{P}$ is real. For any $\mid \phi_1\rangle, \mid \phi_2\rangle \in \mathcal{P}$, and any angle θ, $\mid \phi_1\rangle + \mathrm{e}^{\,\mathrm{i}\theta} \mid \phi_2\rangle$ is also in $\mathcal{P}$, and the expectation values of H_{internal} under all these states are real. It then follows that $\langle \phi_1 \mid H_{\text{internal}} \mid \phi_2\rangle = \langle \phi_2 \mid H_{\text{internal}} \mid \phi_1\rangle^*$.

One might worry about the divergence of a in the unitarity limit, in which the second term on the right-hand side of (44) appears ill-defined. We can show, however, that there is no real problem here. Before a becomes divergent, we should use the physical subspace condition to replace $\Lambda(\mathbf{k}')$ with $\Lambda(\mathbf{k}') + j\eta(\mathbf{k}')$, where j is an arbitrary constant. Choosing $j = -1$ we get

$$H_{\text{internal}} \mid \phi\rangle = \sum_{\mathbf{k}\sigma} \frac{k^2}{2m} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \mid \phi\rangle - \frac{1}{m\Omega} \sum_{\mathbf{q}\mathbf{k}\mathbf{k}'} L(\mathbf{k}') c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow} \mid \phi\rangle, \tag{48}$$

and the second term is now explicitly well-behaved in the unitarity limit. This equation is valid for *any* scattering length, no matter finite or divergent. To calculate the inner product of this equation with any state vector, we should use Eq. (15a) to convert the integral over $\mathbf{k}'$ to a limit at large $\mathbf{k}'$.

Note that in the unitarity limit the η-selector is equal to the Λ-selector, making many expressions particularly simple.

5.2. Few-body physics: an example

All the few-body physics is clearly contained by our second-quantized formulation.

To show that the formalism presented in this paper is a streamlined *working method* (and not only a formal framework), and to show that few-body physics and many-body physics can be treated with

this very *same* formalism, we demonstrate a simple example, the low energy scattering of a fermionic dimer and a free fermion, in which case $a > 0$ necessarily. This calculation can be compared with Ref. [25] in which the same problem is studied.

It is desirable to work in momentum space because of spatial translational symmetry. The system is in a quantum state

$$|\phi\rangle = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} \phi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} c^\dagger_{\mathbf{k}_1\uparrow} c^\dagger_{\mathbf{k}_2\uparrow} c^\dagger_{\mathbf{k}_3\downarrow} |0\rangle, \tag{49}$$

where the wave function is antisymmetric under the exchange of $\mathbf{k}_1$ and $\mathbf{k}_2$, and is zero if $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 \neq 0$. Substituting (49) into Schrödinger equation $H|\phi\rangle = E|\phi\rangle$, where H is given by (44) (assuming $V_{\text{ext}} = 0$), we get

$$\left(\frac{k_1^2 + k_2^2 + k_3^2}{2m} - E\right)\phi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \frac{4\pi a}{m\Omega}\left[\sum_{\mathbf{k}'_1\mathbf{k}'_3} \Lambda(\mathbf{k}'_1 - \mathbf{k}'_3)\phi_{\mathbf{k}'_1\mathbf{k}_2\mathbf{k}'_3} + \sum_{\mathbf{k}'_2\mathbf{k}'_3} \Lambda(\mathbf{k}'_2 - \mathbf{k}'_3)\phi_{\mathbf{k}_1\mathbf{k}'_2\mathbf{k}'_3}\right] = 0. \tag{50}$$

We define

$$f_{\mathbf{k}_2} \equiv \frac{1}{\Omega}\sum_{\mathbf{k}'_1\mathbf{k}'_3} \Lambda(\mathbf{k}'_1 - \mathbf{k}'_3)\phi_{\mathbf{k}'_1\mathbf{k}_2\mathbf{k}'_3}, \tag{51}$$

which is a function of just the *length* of $\mathbf{k}_2$, in the case of low energy s-wave scattering. If the relative momentum of the dimer and the fermion approaches 0, $E = -1/(ma^2) < 0$, and Eq. (50) can be formally solved:

$$\phi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \frac{4\pi a(f_{\mathbf{k}_1} - f_{\mathbf{k}_2})}{(k_1^2 + k_2^2 + k_3^2)/2 + 1/a^2}, \tag{52}$$

for $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0$. Substituting this back to the definition of $f_{\mathbf{k}_2}$, and writing $\mathbf{k}_2 = \mathbf{k}$, $\mathbf{k}'_1 = -\mathbf{k}/2 + \mathbf{k}'$, and $\mathbf{k}'_3 = -\mathbf{k}/2 - \mathbf{k}'$, we get

$$f_{\mathbf{k}} = 4\pi a \int \frac{\mathrm{d}^3k'}{(2\pi)^3} \Lambda(\mathbf{k}') \frac{f_{-\mathbf{k}/2+\mathbf{k}'} - f_{\mathbf{k}}}{k'^2 + 3k^2/4 + a^{-2}}, \tag{53}$$

where the integral of the second term on the right-hand side can be immediately evaluated, using (9e). In the first term, however, $\Lambda(\mathbf{k}')$ can be dropped, because the integrand decays faster than $1/k'^3$ for $\mathbf{k}' \to \infty$. If this were not the case, $f_{\mathbf{k}}$ would have to decay like $1/k$ or even slower at large k, and according to Eq. (52), $\phi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ would have to decay like $1/K^3$ or slower, when k_1, k_2, and k_3 are all of the order $K \to \infty$, making the wave function unnormalizable at short distances [26]. We thus get

$$\left(\sqrt{3k^2/4 + a^{-2}} - a^{-1}\right) f_{\mathbf{k}} + 4\pi \int \frac{\mathrm{d}^3k'}{(2\pi)^3} \frac{f_{\mathbf{k}'}}{k'^2 + \mathbf{k}\cdot\mathbf{k}' + k^2 + a^{-2}} = 0, \tag{54}$$

where $\mathbf{k}'$ has been shifted.

The Fourier transform of $f_{\mathbf{k}}$ is proportional to the relative wave function of the fermion and the dimer at large distances, and must be of the form $1 - a_{\text{fd}}/r$ for $r \to \infty$. Here, a_{fd} is the fermion–dimer scattering length, whose value we shall determine. Consequently, $f_{\mathbf{k}}$ is of the form $(2\pi)^3\delta(\mathbf{k}) - 4\pi a_{\text{fd}}/k^2$ plus regular terms at small $\mathbf{k}$.

Let $f_{\mathbf{k}} \equiv F(t)$, where $t \equiv (ka)^2$ is dimensionless. Eq. (54) is easily simplified to

$$\left(\sqrt{1 + \frac{3t}{4}} - 1\right) F(t) + \frac{1}{\pi\sqrt{t}} \int_0^\infty F(t') \ \operatorname{arctanh}\frac{\sqrt{tt'}}{1 + t + t'} \mathrm{d}t' = 0. \tag{55}$$

It can be shown that $F(t) \propto -\pi\delta(t)/\sqrt{t} + (a_{\text{fd}}/a)/t$ plus a *smooth* function for all $t \geqslant 0$ (including the neighborhood of $t = 0$), and that $F(t) \propto c_0 t^{\mu_0/2} + c_1 t^{(\mu_0-1)/2}$ plus higher order terms at $t \to \infty$, where

$$\mu_0 = -4.16622197664779257337, \quad \text{and} \quad c_1/c_0 = 0.30268913080233667524.$$

Exploiting these properties, we can discretize the integral equation in an appropriate way, and solve it extremely accurately. The resultant fermion–dimer scattering length turns out to be

$$a_{\mathrm{fd}} = 1.1790662349a. \tag{56}$$

To make an extremely accurate prediction for a *real* system (e.g., ultracold atoms), we have to take various corrections to the idealized s-wave contact interaction into account, a topic beyond the scope of this paper.

6. Summary and outlook

To solve a paradox arising in the formulation of the s-wave contact interaction problem of ultracold fermions in momentum space, we modified the conventional notion of integrals. This unexpectedly led us to a simple relation between the energy and the momentum distribution of these fermions.

The new notion is that while the integral of an ordinary function over the whole space is always equal to the limit of integrals over finite regions of space, some generalized functions do not obey this rule. For them, certain full-space integrals are specified beforehand, in a way that is compatible with their other properties and with conventional mathematics.

Our approach is *very different* from the ones used by some people in some relativistic quantum field theories (in which they force integrals like $\int \mathrm{d}^4k k^{-2} = 0$), even though one might form this false impression if one only reads Section 2 of this paper. In our approach, for example, $\Lambda(\mathbf{k})/k^2$ and $\eta(\mathbf{k})/k^2$ are equal for all finite $\mathbf{k}$'s, but their full-space integrals are different. The infinitely many possibilities form a *linear space*, called the *selector space*, in which each point corresponds to certain values of some integrals. Also, in our approach, integrals of ordinary functions which are divergent remain divergent forever (for example, $\int \mathrm{d}^4k k^{-2} = \infty$), and the generalized functions and ordinary ones *coexist*, forming a coherent system.

We discussed the physical implications of our calculations. In particular, if we measure the momentum distribution of fermions with s-wave contact interactions, and plot the result in a certain way, a simple asymptote appears, and the height of such an asymptote at a certain horizontal coordinate is equal to the internal energy. This result is the generalization of a simple property of noninteracting particles, in the context of strongly interacting ultracold quantum gases with resonant interactions ($|\, a \,| \gg r_0$).

We also discussed the application of the results to confined quantum gases, and found that the energy of the system can be extracted from the equal-time *one-body reduced density matrix* only. This is of course completely different from the density functional theory of electrons, in which the explicit form of the functional is *unknown*.

We formulated the s-wave contact interaction problem of ultracold fermions in a simple and coherent way, and can now freely transform the problem between coordinate space and momentum space. This is a streamlined formalism for studying many concrete problems, including few-body ones.

Full applications of this formalism to the many-body problem are a topic of future research. Because of the peculiar structure of this system, we can not predict whether there will be further surprises awaiting us. The short-range boundary condition of the many-body wave function, essentially the definition of the scattering length, appears to be a highly nontrivial constraint. Can we construct a series of approximations to reduce discrepancies with this constraint in a progressive way, and to minimize the system's free energy at the same time? It is possible.

The BCS wave function is of course not consistent with this constraint. For example, $\sum_{\mathbf{k}'} \eta(\mathbf{k}') \langle \phi_{\mathrm{BCS}} \mid c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow} \mid \phi_{\mathrm{BCS}} \rangle \neq 0$ at $\mathbf{q} \neq 0$.

I hope to extend some essential ideas in this paper to *all* systems with contact interactions, including the Standard Model of particle physics. If there are R independent "renormalized" constants that must be determined by experiments (or by a higher energy theory) in a low energy effective theory, is the dimension of the associated selector space equal to $R + 1$? We have this tentative guess, because in the nonrelativistic s-wave contact interaction problem considered in this paper, we have only one "renormalized" constant, the scattering length, and our selector space is two-dimensional. Another

conjecture is that the selector spaces of those other theories may have some nontrivial algebraic properties; for example, the momentum translation of one selector may lead to mixtures with other ones. It may also be interesting to investigate how these selectors evolve (*inside the selector space*) under the continuous scaling transformation, to see whether or how the conventional notion of renormalization group flow is incorporated. In the two-dimensional selector space described in this paper, $\Lambda(\mathbf{k})$ is unchanged if $\mathbf{k}$ is rescaled, but $L(\mathbf{k})$ undergoes a simple scaling transformation, and a generic selector [linear combination of $\Lambda(\mathbf{k})$ and $L(\mathbf{k})$] generally changes after a scaling transformation.

If such a universal approach is realized, certain developments will follow. The most important of them will probably be related to some nonperturbative properties of interacting quantum fields. Even if we can not determine all the properties quantitatively, we may still find some exact relations and/or qualitative features.

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References

[1] In this paper "spin" denotes any of the two alternative internal states of the fermion, or two fermionic species (each has one internal state only). To a heteronuclear Fermi mixture ($m_\uparrow \neq m_\downarrow$), the results in this paper can be easily generalized. But note that when the mass ratio $m_\uparrow/m_\downarrow$ (or $m_\downarrow/m_\uparrow$) exceeds 13.6, the three-body Efimov effect appears [18], the two-body pseudopotential is no longer sufficient, and the formalism in this paper can no longer be applied without qualitative modifications and/or extensions.
[2] We let $\hbar = 1$ for conciseness, and the term "wave vector" is used interchangeably with "momentum". $\hbar$ is restored when contact with experiments is made.
[3] D.M. Eagles, Phys. Rev. 186 (1969) 456.
[4] A.J. Leggett, Modern Trends in the Theory of Condensed Matter, Springer Verlag, Berlin, 1980. pp. 13–27.
[5] The BEC-BCS crossover is not restricted to a Fermi gas with resonant contact interaction characterized by the s-wave scattering length, although the latter system is the most popular, and this paper is restricted to this minimal model.
[6] See, e.g., L. Viverit et al., Phys. Rev. A 69, 013607 (2004), in particular its footnote 31.
[7] A practical definition of r_0 is in terms of the two-body scattering amplitude $F_l(k)$, where k is the magnitude of the relative momentum, and l is the relative orbital angular momentum quantum number. $1/r_0$ is the lowest momentum scale at which either $-F_0(k)^{-1} = a^{-1} + ik$ becomes a bad approximation, or $F_l(k)$ ($l \geqslant 1$) is no longer negligible.
[8] Since we are assuming that the interaction is characterized by the scattering length only, the theory in this paper is not directly applicable to Fermi gases near narrow Feshbach resonances, where there can be a length scale R^* which may be comparable to or larger than $|a|$ [27]. But to broad Feshbach resonances, where R^* is small, our calculations are directly applicable.
[9] Periodic boundary condition is used. In the case of a uniform gas, Ω is the volume of the uniform system; in the case of a confined gas, Ω is any volume which greatly exceeds the actual spatial extension of the gas.
[10] The system is assumed to be in a smooth external potential (may be zero), so that the C/k^4 tail of $n_{k\sigma}$ is solely caused by interparticle interactions.
[11] To appreciate this general feature, it is instructive to consider two interacting fermions confined in a box.
[12] The concept of the unitarity limit of the Fermi gas was first introduced by G.F. Bertsch, as indicated by G.A. Baker Jr., Phys. Rev. C 60 (1999) 054311. See, e.g., T.L. Ho, Phys. Rev. Lett. 92 (2004) 090402 and references therein for an updated introduction to it.
[13] A convenient definition of the "typical de Broglie wave length is $1/m\lambda_{\mathrm{dB}}^2 \sim \epsilon_1$, where ϵ_1 is the total internal energy (kinetic energy plus interfermionic interaction energy) divided by the number of fermions, in the center-of-mass frame of the Fermi gas.
[14] The "internal energy" , E_{internal}, discussed in this paper includes the bulk kinetic energy, if the whole system is in a motion.
[15] There are other attempts to formulate the same problem. Most of them are aimed at a mean-field approximation, in contrast with this paper. An alternative approach that is of the same simplicity has yet been seen.
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[17] A.J. Leggett, Rev. Mod. Phys. 73 (2001) 307. in particular, its Section IV.B.
[18] D.S. Petrov, Phys. Rev. A 67 (2003) 010703.
[19] E. Braaten, H.-W. Hammer, Available from: <cond-mat/0410417>.
[20] The mixed state $\hat{\rho} = \sum_k C_\uparrow (k^2 + a^{-2})^{-2} \mid k\rangle\langle k \mid$, where $\mid k\rangle = c_{k\uparrow}^\dagger \mid 0\rangle$ is a single-fermion momentum eigenstate, violates both the second equality in (3) and (24). This counterexample shows the necessity of the condition that the probability α_i (in $\hat{\rho} = \sum_i \alpha_i \mid \phi_i\rangle\langle\phi_i \mid$) decays sufficiently fast at large i.
[21] M. Greiner et al, Phys. Rev. Lett. 94 (2005) 110401.
[22] In the contact-interaction model, there are many "interactionless" states, where any two fermions with opposite spins have precisely zero probability to be in the s-wave orbital channel, so that $C = 0$ even though $a \neq 0$. For many-body systems, such states are difficult to realize experimentally, unless some unexpected technique is invented.
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[24] The vacuum state and the single-fermion states also belong to the physical subspace. Any linear combination of any two states which belong to $\mathcal{P}$ also belongs to $\mathcal{P}$ and is physically allowed.
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D.S. Petrov, C. Salomon, G.V. Shlyapnikov, Phys. Rev. A 71 (2005) 012708.
[26] The wave function is of course not normalizable at long distances in the scattering state. But when the three fermions cluster in a small region of size $r \to 0$, the wave function must be smaller than $O(1/r^3)$; consequently its momentum representation must decay faster than $1/K^3$, if all the three momenta of the fermions are of the order $K \to \infty$.
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