Particle distribution tail and related energy formula

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We present a simple derivation of the energy formula found by Tan, relative to the single-channel Hamiltonian relevant for ultracold Fermi gases. This derivation is generalized to particles with different masses, to arbitrary mixtures, and to two-dimensional space. We show how in a field-theoretic approach, the $1/k^4$ tail in the momentum distribution and the energy formula arise in a natural way. As a specific example, we consider quantitative calculations of the energy from different formulas within the ladder diagram approximation in the normal state. The comparison of the results provides an indication on the quality of the approximation.

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I. INTRODUCTION

The remarkable progress in the field of ultracold atomic gases has provided access to a number of systems which may display quite new physical properties. One of the most striking example is provided by ultracold fermionic gases [1] and the Bose-Einstein condensate (BEC)–BCS crossover. While the physics of BECs is known from superfluid ^{4}He (and from ultracold bosonic atomic gases) and that of BCS condensates is known from superconductors, fermionic gases provide systems which display a smooth continuous evolution between these two extremes. This is made possible by the existence of Feshbach resonances which allow control of the value of the scattering length a merely by changing the applied magnetic field. For ultracold gases the kinetic energy of the atoms is so small that only s-wave scattering is relevant, and it is fully characterized by the scattering length. Since Pauli principle forbids s-wave scattering between identical fermions, the scattering length corresponds in most of the experiments performed so far to scattering between atoms in different hyperfine states of a same element. These hyperfine states are often called for convenience "spin up" and "spin down." In the case of a wide Feshbach resonance (as it occurs, for example, for ^{6}Li and ^{40}K), the closed channel responsible for the Feshbach resonance may be omitted and the system is described by a single-open-channel Hamiltonian, where the interaction is characterized by the single parameter a. With the densities produced in experiments this interaction has quite a small range compared to the interatomic distance. This single-channel Hamiltonian is particularly interesting because it is at the same time very simple and highly nontrivial, and moreover it is realized with an excellent precision in these ultracold fermionic gases. Hence we may hope, in getting full control and understanding of this Hamiltonian, to gain knowledge which may be applicable to more complex Hamiltonians, such as those encountered in condensed-matter physics or in quark matter [2].

In this context a simple general expression for the energy of a system described by this Hamiltonian was found by Tan [3], which involves only the momentum distribution $n_\sigma(k)$ of the particles together with their large-k behavior. However the details raise unanswered mathematical difficulties. Nevertheless the expression can be checked in limiting cases (see Appendix A for details). This expression is of high interest since it is quite nontrivial. It is directly related to the well-known problem that for a contact interaction, the kinetic energy presents a formal divergence, because the momentum distribution $n_\sigma(k)$ behaves as $1/k^4$ for large momentum (as found, for example, in the perturbative calculation of Belyakov [4]), a feature merely linked to two-body physics. Naturally there is no divergence in the energy itself, because the interaction energy comes in to compensate for this feature from the kinetic energy. This is easily seen from a simple finite-range interaction model (for example, the square-well potential), with range r_0. The momentum distribution decreases more rapidly than $1/k^4$ for momentum beyond $1/r_0$, which acts as a cutoff in momentum space. The apparently singular situation is found when one lets $r_0 \to 0$, which should be taken as the definition of the contact interaction. In the formula found by Tan [3], the total energy appears essentially as the kinetic energy with this divergence problem removed. Indeed the high-momentum part, responsible for the divergence, is subtracted out and an additional explicit contribution which contains the scattering length appears.

This matter was taken up recently by Braaten and Platter [5], who made use of the operator product expansion developed by Wilson. In this way they derived the energy relation in a compact and formal way. In contrast with the Tan approach, the interaction comes in explicitly. Braaten and Platter [5] also obtained the expression of the known [6] adiabatic relation for this contact potential Hamiltonian. This convenient expression in terms of the scattering length and of the coefficient of the $1/k^4$ tail in the momentum distribution was pointed out by Tan [7]. Quite recently it has been used [8] to obtain the number of closed-channel molecules in the two-channel model. Also very recently it was derived and studied in detail by Zhang and Leggett [9].

In this paper we present first a derivation of this energy formula, which is simple, explicit, and fairly short and avoids unnecessary and uncontrolled mathematical complications. It is in line with the Tan approach, in that it deals only with the kinetic energy. This is done in a careful way in order to avoid divergences. Our treatment is similar in spirit to Ref. [9]. This simple proof allows straightforward generalizations to more complicated situations, with unequal masses, several kinds of particles, and two-dimensional (2D) space. Next we show how, in a field-theoretic approach, the

$1/k^4$ tail in the momentum distribution and the energy formula arise in a natural way. Finally, as a specific example, we consider also quantitative calculations within the ladder diagram approximation in the normal state. There are different ways to obtain the energy and we can compare the various approximate results, which gives an indication on the quality of the approximation.

II. DETAILED DERIVATION

In this paragraph we consider the case where we have only two kinds of particles which are ultracold fermions. The volume of the system is assumed to be unity. Namely, we have $n_\uparrow$ particles with mass $m_\uparrow$ and $n_\downarrow$ particles with mass $m_\downarrow$. We consider directly the case where the masses $m_\uparrow$ and $m_\downarrow$ are different since it does not make any problem. The positions of the $\uparrow$ particles are denoted $\mathbf{r}_i$, while those of the $\downarrow$ particles are $\boldsymbol{\rho}_j$. For these ultracold fermions only s-wave scattering has to be taken into account. Hence only interactions between $\uparrow$ and $\downarrow$ particles have to be considered. Generalizations are considered in Sec. III. The Hamiltonian reads $H=H_c+\mathcal{V}$, with (we take $\hbar=1$)

$$H_c=-\frac{1}{2m_\uparrow}\sum_{i=1}^{n_\uparrow}\Delta_{\mathbf{r}_i}-\frac{1}{2m_\downarrow}\sum_{j=1}^{n_\downarrow}\Delta_{\boldsymbol{\rho}_j} \tag{1}$$

and

$$\mathcal{V}=\sum_{i,j}V(\mathbf{r}_i-\boldsymbol{\rho}_j). \tag{2}$$

We assume the interaction potential $V(\mathbf{r})$ to be short range. For clarity and simplicity we assume that it has a definite range r_0 and satisfies $V(\mathbf{r})=0$ for $r>r_0$. However, just as in standard scattering theory [6], the results will hold for physical short-range potentials where the interaction decreases rapidly enough with interparticle distance.

We consider an eigenfunction $|\Phi\rangle$ of this Hamiltonian, having, for example, in mind the ground-state wave function. However this is not necessary and we can as well consider excited states, which leads to the extension of the results to nonzero temperature, as pointed out by Tan [3]. Let $\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})$ be the corresponding wave function, with proper symmetrization and normalization to unity. We want to calculate the energy corresponding to this state:

$$E=\langle\Phi|H|\Phi\rangle=\int d\mathbf{r}_i d\boldsymbol{\rho}_j\Phi^*(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})(H_c+\mathcal{V})\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\}), \tag{3}$$

where $d\mathbf{r}_i d\boldsymbol{\rho}_j$ is for $\Pi_{i,j}d\mathbf{r}_i d\boldsymbol{\rho}_j$, with $i=1,\ldots,n_\uparrow$ and $j=1,\ldots,n_\downarrow$.

We follow the basic principle put forward by Tan [3]. In Eq. (3) the potential $V(\mathbf{r})$ comes in only in the regions of the integration domain where $|\mathbf{r}_m-\boldsymbol{\rho}_n|<r_0$, where $m=1,\ldots,n_\uparrow$ and $n=1,\ldots,n_\downarrow$. The overlap between these regions is negligible for dilute gases where r_0 is small compared with the mean interparticle distance d. In particular, since the domain corresponding to three particles being close together is negligible, this means that we will not deal directly with three-body problems. [However three-body and more generally many-body effects appear indirectly in the value of the many-body wave function $\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})$.] There are $n_\uparrow n_\downarrow$ such regions satisfying $|\mathbf{r}_m-\boldsymbol{\rho}_n|<r_0$. Compared to the total integration domain, the domain of these regions is of order $(r_0/d)^3$. For equal populations $n_\uparrow=n_\downarrow\equiv k_F^3/6\pi^2$, this would be of order $(k_F r_0)^3$. Since we have $H\Phi=E\Phi$ also inside these regions, and that Φ inside these regions has no singular behavior (this can be checked explicitly since this behavior is obtained from a one-body Schrödinger equation, as we use below), we may neglect the contribution of these regions. Actually this has to be done for consistency since [9] keeping only s-wave scattering for ultracold gases implies that terms of order $(k_F r_0)^2$, corresponding to higher angular momenta, are neglected. Hence the energy is simply obtained by calculating the kinetic energy outside these regions:

$$E=\int_{|\mathbf{r}_m-\boldsymbol{\rho}_n|>r_0}d\mathbf{r}_i d\rho_j\Phi^*(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})H_c\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\}). \tag{4}$$

We introduce now the Fourier transform $\varphi(\{\mathbf{k}_i\},\{\mathbf{q}_j\})$ of $\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})$ with respect to all variables:

$$\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})=\sum_{\{\mathbf{k}_i\},\{\mathbf{q}_j\}}\exp\left(i\sum_i\mathbf{k}_i\cdot\mathbf{r}_i+i\sum_j\mathbf{q}_j\cdot\boldsymbol{\rho}_j\right)\varphi(\{\mathbf{k}_i\},\{\mathbf{q}_j\}), \tag{5}$$

where we use the notation $\Sigma_{\mathbf{k}}\equiv(2\pi)^{-3}\int d\mathbf{k}$. The one-particle density distributions $n_\uparrow(k)$ and $n_\downarrow(k)$ are given by

$$n_\uparrow(k_1)=n_\uparrow\sum_{\{\mathbf{k}_i,i\neq1\},\{\mathbf{q}_j\}}|\varphi(\{\mathbf{k}_i\},\{\mathbf{q}_j\})|^2,$$

$$n_\downarrow(q_1)=n_\downarrow\sum_{\{\mathbf{k}_i\},\{\mathbf{q}_j,j\neq1\}}|\varphi(\{\mathbf{k}_i\},\{\mathbf{q}_j\})|^2. \tag{6}$$

This leads to

$$E=\sum_{\{\mathbf{k}_i'\},\{\mathbf{q}_j'\}}\varphi^*(\{\mathbf{k}_i'\},\{\mathbf{q}_j'\})\times\sum_{\{\mathbf{k}_i\},\{\mathbf{q}_j\}}\left[\frac{1}{2m_\uparrow}\sum_{M=1}^{n_\uparrow}k_M^2+\frac{1}{2m_\downarrow}\sum_{N=1}^{n_\downarrow}q_N^2\right]\varphi(\{\mathbf{k}_i\},\{\mathbf{q}_j\})\int_{|\mathbf{r}_m-\boldsymbol{\rho}_n|>r_0}d\mathbf{r}_i d\boldsymbol{\rho}_j\exp\left\{i\sum_i(\mathbf{k}_i-\mathbf{k}_i')\cdot\mathbf{r}_i+i\sum_j(\mathbf{q}_j-\mathbf{q}_j')\cdot\boldsymbol{\rho}_j\right\}. \tag{7}$$

If we did not have the restrictions $|\mathbf{r}_m-\boldsymbol{\rho}_n|>r_0$ in the last integral, it would give a factor proportional to $\Pi_i\delta(\mathbf{k}_i-\mathbf{k}_i')\Pi_j\delta(\mathbf{q}_j-\mathbf{q}_j')$ and we would find the standard expression for the kinetic energy:

$$E_c=\frac{1}{2m_\uparrow}\sum_{\mathbf{k}_1}k_1^2n_\uparrow(k_1)+\frac{1}{2m_\downarrow}\sum_{\mathbf{q}_1}q_1^2n_\downarrow(q_1), \tag{8}$$

which displays a divergence for large wave vector. Hence the restriction is crucial in order to avoid the divergence.

However, since we want to have the standard expression for the kinetic energy appearing, we will write

$$\int_{|\mathbf{r}_m-\boldsymbol{\rho}_n|>r_0}d\mathbf{r}_id\boldsymbol{\rho}_j=\int d\mathbf{r}_id\boldsymbol{\rho}_j-\sum_{m,n}\int_{|\mathbf{r}_m-\boldsymbol{\rho}_n|<r_0}d\mathbf{r}_id\boldsymbol{\rho}_j, \tag{9}$$

where for simplicity we have not written explicitly the exponential integrand appearing in Eq. (7). As long as all the k_i and q_j integrations are not performed in Eq. (7), no singularity appears so we can handle the various terms in Eq. (9) separately. As we have just mentioned the first one leads to the standard kinetic-energy expression, so we have just to handle the other terms quite carefully since the limit $r_0\to 0$ is singular. Note that in the regions $|\mathbf{r}_m-\boldsymbol{\rho}_n|<r_0$, we will deal with the analytic continuation of the expression of the wave function for $|\mathbf{r}_m-\boldsymbol{\rho}_n|>r_0$, which we will discuss below. This is naturally quite different from its physical value in these regions, since for this last one, the interaction $V(\mathbf{r})$ has to be taken into account.

Let us consider the term $m=n=1$ in Eq. (9). In Eq. (7) only the terms $(1/2m_\uparrow)k_1^2+(1/2m_\downarrow)q_1^2$ in the bracket will be relevant, and for now on we consider only these ones. Basically we will deal carefully with this two-body problem. Accordingly it is convenient to think, as long as we are not back to the many-body problem, that only these two particles scatter. Equivalently we could handle all the $\{m,n\}$ terms simultaneously, but this is much more cumbersome presentation. Since they are more convenient for expressing the condition $|\mathbf{r}_1-\boldsymbol{\rho}_1|<r_0$, we introduce the relative position $\mathbf{r}=\mathbf{r}_1-\boldsymbol{\rho}_1$ and the center-of-mass position $\mathbf{R}=(m_\uparrow\mathbf{r}_1+m_\downarrow\boldsymbol{\rho}_1)/M$, together with their conjugate variables the total momentum $\mathbf{K}=\mathbf{k}_1+\mathbf{q}_1$ and the relative momentum $\mathbf{k}=(m_\downarrow\mathbf{k}_1-m_\uparrow\mathbf{q}_1)/M$, with $M=m_\uparrow+m_\downarrow$. We have

$$\frac{1}{2m_\uparrow}k_1^2+\frac{1}{2m_\downarrow}q_1^2=\frac{1}{2\mu}k^2+\frac{1}{2M}K^2, \tag{10}$$

where $\mu=m_\uparrow m_\downarrow/(m_\uparrow+m_\downarrow)$ is the reduced mass. The difficulties arise from the $k^2/2\mu$ term in the large-k limit.

It is convenient for the discussion to introduce the Fourier transform $\bar{\varphi}(\mathbf{k},\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})$ of the wave function with respect to the variables $\mathbf{r}$ and $\mathbf{R}$, instead of $\mathbf{r}_1$ and $\boldsymbol{\rho}_1$. It is merely given by

$$\bar{\varphi}(\mathbf{k},\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})=\varphi\left(\mathbf{k}+\frac{m_\uparrow}{M}\mathbf{K},-\mathbf{k}+\frac{m_\downarrow}{M}\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\}\right). \tag{11}$$

Making use, in Eqs. (7) and (9), of $(\mathbf{k}_1-\mathbf{k}_1')\cdot\mathbf{r}_1+(\mathbf{q}_1-\mathbf{q}_1')\cdot\boldsymbol{\rho}_1=(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}+(\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}$, together with $d\mathbf{r}_1d\boldsymbol{\rho}_1=d\mathbf{r}d\mathbf{R}$ and $d\mathbf{k}_1d\mathbf{q}_1=d\mathbf{k}d\mathbf{K}$, we find that for the $k^2/2\mu$ term in Eq. (10), we have to deal with

$$\sum_{\mathbf{K},\mathbf{kq}_2}\sum_{\mathbf{k},\mathbf{k}'}\bar{\varphi}^*(\mathbf{k}',\mathbf{K},\mathbf{kq}_2)k^2\bar{\varphi}(\mathbf{k},\mathbf{K},\mathbf{kq}_2)\int_{r<r_0}d\mathbf{r}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}, \tag{12}$$

where $\mathbf{kq}_2$ is shorthand for $\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\}$. We have used the fact that integration over all unrestricted position variables gives corresponding δ functions for the corresponding wave-vector variables, as we have mentioned above. The problem for large k in this expression is directly linked to the behavior of the wave function for small relative distance r, which we consider now.

When the relative distance r is small compared to the mean interparticle distance d, the dependence of the wave function $\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})$ on $\mathbf{r}$ is given by the solution of the relative motion of the two-body problem. For ultracold gases the energy corresponding to this motion is nearly zero and the corresponding wave function is, for $r>r_0$, proportional to $\psi(r)$ with $\psi(r)\equiv 1/r-1/a$, where a is the scattering length [1]. This form is actually valid provided r is small compared to a typical particle wavelength, that is, $r\ll d$. Since we have $r_0\ll d$, there is a range of validity for this form for $r>r_0$. We are also interested in the case of large positive a, where a two-body bound state exists with wave function proportional to $\exp(-r/a)/r$. In this case the above form requires $r\ll a$. There is again a range of validity for this condition for $r>r_0$ since we are in practice interested in physical situations where the scattering length a is large compared to the potential range r_0. Hence for small r we have

$$\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})=\psi(r)\bar{\Phi}(\mathbf{R},\{\mathbf{r}_2,\ldots\},\{\boldsymbol{\rho}_2,\ldots\}). \tag{13}$$

Since in the evaluation of the $\int_{r<r_0}$ term of Eq. (9), we will let $r_0\to 0$; only large values of $\mathbf{k}$ are relevant. Indeed if we considered only bounded values $k<k_c$, this term would go to zero for $r_0\to 0$ (and the k integral would converge because of the cutoff k_c). Hence we have to consider $k\to\infty$. In this case the dependence of $\bar{\varphi}(\mathbf{k},\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})$ on k is entirely linked to the short-distance behavior on r of $\Phi(\{\mathbf{r}_i\},\{\boldsymbol{\rho}_j\})$ given by Eq. (13). We have in this limit

$$\bar{\varphi}(\mathbf{k},\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})=\psi_F(k)\bar{\Phi}_F(\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\}), \tag{14}$$

where $\psi_F(k)$ and $\bar{\Phi}_F(\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})$ are the Fourier transform of $\psi(r)$ and $\bar{\Phi}(\mathbf{R},\{\mathbf{r}_2,\ldots\},\{\rho_2,\ldots\})$, respectively.

As well known, the Fourier transform of $1/r$ is $4\pi/k^2$. On the other hand, for the calculation of $k^2\bar{\varphi}(\mathbf{k},\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})$ in expression (12), we do not have to take into account the constant $-1/a$ in the wave function since it gives zero when we apply on it the kinetic-energy operator $\Delta_{\mathbf{r}}$ (corresponding to the factor k^2). All this Fourier-transform calculation can be done quite carefully by multiplying the wave function $\psi(r)$ by a convergence factor $e^{-\eta r}$, then letting $\eta\to 0_+$. This confirms the above results. Finally, when handling expression (12), we have merely $k^2\bar{\varphi}(\mathbf{k},\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})=4\pi\bar{\Phi}_F(\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})$.

Physically,

$$p(k) \equiv \sum_{\mathbf{K},\mathbf{kq}_2} |\bar{\varphi}(\mathbf{k},\mathbf{K},\mathbf{kq}_2)|^2 \tag{15}$$

is the isotropic probability distribution of wave vector $\mathbf{k}$ in the relative motion of the two $\uparrow$ and $\downarrow$ particles we are considering. We have found that its leading behavior for $k \to \infty$ is p_4/k^4, with

$$p_4 = (4\pi)^2 \sum_{\mathbf{K},\mathbf{kq}_2} |\bar{\Phi}_F(\mathbf{K},\mathbf{kq}_2)|^2. \tag{16}$$

On the other hand, with respect to $\mathbf{k}'$ integration in expression (12), it is more convenient to go back to $\mathbf{r}$ space through $\Sigma_{\mathbf{k}'} e^{-i\mathbf{k}'\cdot\mathbf{r}} \psi_F^*(k') = \psi(r)$, which gives a factor of $\psi(r)\bar{\Phi}_F^*(\mathbf{K},\{\mathbf{k}_2,\ldots\},\{\mathbf{q}_2,\ldots\})$. Since $\psi(r)$ is isotropic, we can perform explicitly the angular $\mathbf{r}$ integration $\int d\Omega_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sin(kr)/kr$. Finally, for expression (12), we are left with the calculation of $\int_0^{r_0} dr r \sin(kr)\psi(r)$. This r integration is easily performed, leading to

$$k\int_0^{r_0} dr r \sin(kr)\left(\frac{1}{r} - \frac{1}{a}\right) = 1 - \left[\left(1 - \frac{r_0}{a}\right)\cos(kr_0) + \frac{1}{ka}\sin(kr_0)\right] \equiv 1 - f(k,r_0). \tag{17}$$

We write now, with this result, the partial contribution E_{11k} to energy equation (7), coming from the term $m=n=1$ in Eq. (9) and where we retain only the $k^2/2\mu$ term in Eq. (10). We obtain

$$E_{11k} = -\frac{1}{2\mu}\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{k^2} p_4[1 - f(k,r_0)] = -\frac{1}{4\pi^2\mu}\int_0^{k_c} dk p_4 + \frac{p_4}{4\pi^2\mu}\int_0^{\infty} dk f(k,r_0). \tag{18}$$

In the first term in the right-hand side, we have put a cutoff k_c since this integral diverges when $k_c \to \infty$. This divergence will just compensate in the final result for the above-mentioned divergence in Eq. (8). Hence the global result will be convergent as expected.

If in the last integral of Eq. (18) we were setting $r_0=0$, we would get $f(k,r_0)=1$ and a divergent result. Instead this integral is perfectly convergent when we calculate it explicitly for $r_0 \neq 0$ and then take properly the $r_0 \to 0$ limit. Indeed we see that it is not divergent because $f(k,r_0)$ involves oscillatory functions. The $\cos(kr_0)$ term merely gives a result proportional to $\delta(r_0)$, where $\delta(x)$ is the Dirac distribution. Since $r_0 \neq 0$ the contribution of this $\cos(kr_0)$ term is zero. On the other hand, owing to

$$\int_0^{\infty} dx \frac{\sin x}{x} = \frac{\pi}{2}, \tag{19}$$

the $\sin(kr_0)$ term gives a contribution $\pi/2a$ to the integral, leading to a contribution $p_4/8\pi\mu a$ to E_{11k}. As we have mentioned above, we could improve the presentation of our handling of the k integration, to deal with perfectly defined integrals, by introducing a convergence factor $\exp(-\eta k)$ and then let $\eta \to 0_+$. Physically this would correspond to regularization of the wave function in the $r \to 0$ limit. This would confirm our above results.

We have not yet taken into account the $K^2/2M$ term in Eq. (10), because there is no singular behavior associated with it. The corresponding contribution E_{11K} of the term $m=n=1$ in Eq. (9) goes to zero as $r_0 \to 0$, as it is obvious directly and can be checked by following the same procedure as above. Finally one sees easily that for all the other kinetic-energy terms $(1/2m_\uparrow)\Sigma_{m=2}^{n_\uparrow} k_m^2 + (1/2m_\downarrow)\Sigma_{n=2}^{n_\downarrow} q_n^2$ in the bracket of Eq. (7), the contribution from the term $m=n=1$ in Eq. (9) also goes to zero when $r_0 \to 0$. Hence the total contribution E_{11} of the $m=n=1$ term is merely $E_{11}=E_{11k}$.

We rewrite now the sum E_{11} in terms of the variables corresponding to particles $\uparrow$ and $\downarrow$, instead of the relative and center-of-mass variables. We have

$$E_{11} = -\frac{1}{2\mu}\sum_{\mathbf{k},\mathbf{K}} \frac{P_4(\mathbf{K})}{k^2} + \frac{p_4}{8\pi\mu a}, \tag{20}$$

with again a cutoff k_c understood for the summation over $\mathbf{k}$, and where we have introduced

$$P_4(\mathbf{K}) = (4\pi)^2 \sum_{\mathbf{kq}_2} |\bar{\Phi}_F(\mathbf{K},\mathbf{kq}_2)|^2 \tag{21}$$

related to p_4 by $p_4 = \Sigma_{\mathbf{K}} P_4(\mathbf{K})$. With $1/\mu = 1/m_\uparrow + 1/m_\downarrow$, we have

$$E_{11} = -\frac{1}{2m_\uparrow}\sum_{\mathbf{k},\mathbf{K}} \frac{P_4(\mathbf{K})}{k^2} - \frac{1}{2m_\downarrow}\sum_{\mathbf{k},\mathbf{K}} \frac{P_4(\mathbf{K})}{k^2} + \frac{p_4}{8\pi\mu a}. \tag{22}$$

We make use of Eq. (10) to go back to the $\mathbf{k}_1$ and $\mathbf{q}_1$ variables. In the first term we change the summation variables from $\{\mathbf{K},\mathbf{k}\}$ to $\{\mathbf{K},\mathbf{k}_1 = \mathbf{k} + (m_\uparrow/M)\mathbf{K}\}$, making use of $d\mathbf{k}d\mathbf{K} = d\mathbf{k}_1 d\mathbf{K}$. In particular we have $1/k^2 = 1/[\mathbf{k}_1 - (m_\uparrow/M)\mathbf{K}]^2$. However we can use the identity

$$\int d\mathbf{r}\left[\frac{1}{(\mathbf{r}-\mathbf{A})^2} - \frac{1}{(\mathbf{r}+\mathbf{A})^2}\right] = 0, \tag{23}$$

where $\mathbf{A}$ is any fixed vector (this result is obvious by changing $\mathbf{r}$ into $-\mathbf{r}$), to write $\Sigma_{\mathbf{k}_1}[1/k^2 - 1/k_1^2] = 0$ at fixed $\mathbf{K}$. Proceeding in the same way with the second term of Eq. (22), we obtain

$$E_{11} = -\frac{1}{2m_\uparrow}\sum_{\mathbf{k}_1} \frac{p_4}{k_1^2} - \frac{1}{2m_\downarrow}\sum_{\mathbf{q}_1} \frac{p_4}{q_1^2} + \frac{p_4}{8\pi\mu a}, \tag{24}$$

with a cutoff k_c understood for the summation over $\mathbf{k}_1$ and $\mathbf{q}_1$.

In conclusion we have calculated all the contributions coming from the presence of the term $m=n=1$ in Eq. (9). These are just the three terms, proportional to p_4, in Eq. (24). To summarize, for the expression of the energy, we are back to Eq. (7) with the restriction $|\mathbf{r}_1 - \rho_1| > r_0$ removed, and the above three p_4 terms added.

We have just to repeat the same argument for all the other restrictions $|\mathbf{r}_i-\rho_j|>r_0$. In this way we obtain $n_\uparrow n_\downarrow$ analogous p_4 terms, which are naturally all equivalent after a change of variables. Taking Eq. (8) into account, this leads to the final expression for the energy:

$$E=\frac{1}{2m_\uparrow}\sum_{\mathbf{k}}\left[k^2n_\uparrow(k)-\frac{n_4}{k^2}\right]+\frac{1}{2m_\downarrow}\sum_{\mathbf{q}}\left[q^2n_\downarrow(q)-\frac{n_4}{q^2}\right]+\frac{n_4}{8\pi\mu a}, \tag{25}$$

where $n_4=n_\uparrow n_\downarrow p_4=\lim_{k\to\infty}k^4n_\uparrow(k)=\lim_{k\to\infty}k^4n_\downarrow(k)$. Indeed, from Eq. (6), $n_\uparrow(k)$ and $n_\downarrow(k)$ behave in this way for large k since, for example, $\mathbf{k}_1$ scatters with all the $\mathbf{q}_j$, and each scattering brings a contribution p_4/k^4. That is, any of the $n_\uparrow$ particles scatters with any of the $n_\downarrow$ particles. Hence the summations in Eq. (25) are perfectly convergent. This formula is the simple generalization of the formula found by Tan [3] to the case where the two species of involved particles have different masses.

In this derivation we introduced a cutoff to manipulate separately each contribution. This makes an easier presentation for the derivation. However this is just a convenience. We could avoid it by handling all the terms simultaneously. The presentation would be much awkward, but we would only deal with well-defined convergent integrals, without any need for a cutoff.

III. SIMPLE GENERALIZATIONS

It is first worthwhile to note that the above derivation did not make use of the statistics of the particles. Hence the result is valid for bosons as well as for fermions. Naturally it is artificial for bosons to consider only scattering between different species, although it might just happen that this scattering is the dominant one. Nevertheless for bosons there is no reason to exclude scattering between particles belonging to the same species. If we consider first the case of a single bosonic species, with n particles of mass m in the unit volume and with scattering length a, we can follow the same procedure as in Sec. II. We can write the equivalent of Eq. (7) for a single species, with a restriction $|\mathbf{r}_i-\mathbf{r}_j|>r_0$ working now between any of the $n(n-1)/2$ couples of particles. Taking care of the restrictions in the same way as in Sec. II, we end up with

$$E=\frac{1}{2m}\sum_{\mathbf{k}}\left[k^2n(k)-\frac{n_4}{k^2}\right]+\frac{n_4}{8\pi ma}, \tag{26}$$

with $n_4=n(n-1)p_4=\lim_{k\to\infty}k^4n(k)$. We note that the physics associated with the Efimov effect [10] does not appear explicitly in this result because, as we have argued in Sec. II below Eq. (3), three-body effects have not to be considered directly in our derivation which applies to the dilute limit $r_0\to 0$. However Efimov physics could still appear indirectly through its effect on the many-body wave function, from which $n(k)$ and n_4 have to be calculated.

We can then generalize this result to any mixture of N boson species with n_i particles of mass m_i in the unit volume $(i=1,\ldots,N)$ and interaction between species i and j characterized by scattering lengths a_{ij}. We find in the same way

$$E=\sum_{i=1}^{N}\frac{1}{2m_i}\sum_{\mathbf{k}}\left[k^2n_i(k)-\frac{n_{4i}}{k^2}\right]+\frac{1}{16\pi}\sum_{i,j}\frac{n_{4ij}}{\mu_{ij}a_{ij}}, \tag{27}$$

where $\mu_{ij}=m_im_j/(m_i+m_j)$ is the reduced mass for the i-j scattering, $n_{4i}=\lim_{k\to\infty}k^4n_i(k)$, and $n_{4i}=\Sigma_j n_{4ij}$. Naturally the formula is more complex for these mixtures, since it requires the knowledge of the $N(N+1)/2$ constants $n_{4ij}=n_{4ji}$ associated with the i-j scattering. The same result works for ultracold fermionic mixtures, except that we have to set $n_{4ii}=0$ because of Pauli principle.

IV. 2D CASE

While in one-dimensional (1D) situations the kinetic energy converges, and indeed in exact solutions of many-body problems the energy is precisely calculated by evaluating the kinetic energy, there is in two dimensions a divergence analogous to the three-dimensional (3D) case, except that the divergence is logarithmic in the 2D case. We show here how the procedure followed in three dimensions can be extended to this 2D case. Actually there is not so much difference since the space dimensionality does not appear in the principle of the procedure. The changes appear only when one comes to practical matters. We keep the same notations for the variables, but naturally we have to deal now with two-dimensional variables and integrations.

First the expression of the wave function $\psi(r)$ for the relative motion at small distance $r>r_0$ is modified into $\psi(r)\equiv\ln(a/r)$, which is solution of the 2D equation $\Delta\psi(r)=0$. The length a for which $\psi(a)=0$ plays the role of the scattering length and is naturally obtained from the interaction potential. The Fourier transform of $\psi(r)$ is $\psi_F(k)=2\pi/k^2$, omitting the irrelevant Fourier transform of $\ln a$. Similarly the large-k behavior of $p(k)$ is p_4/k^4, with $(2\pi)^2$ appearing in Eq. (16) instead of $(4\pi)^2$. Then the 2D angular integration gives $\int_0^{2\pi}e^{i\mathbf{k}\cdot\mathbf{r}}=2\pi J_0(kr)$, where $J_0(x)$ is the first kind Bessel function. Hence, instead of Eq. (18), we obtain

$$E_{11k}=-\frac{p_4}{2\mu}\int\frac{d\mathbf{k}}{(2\pi)^2}\int_0^{r_0}drr\ln\frac{a}{r}J_0(kr)=-\frac{p_4}{4\pi\mu}\int_0^{k_c}\frac{dk}{k}\int_0^{kr_0}dxx\ln\frac{ka}{x}J_0(x), \tag{28}$$

where in the last expression we have changed to the variable $x=kr$, and we have naturally to take the cutoff $k_c\to\infty$ at the end of the calculation, when the standard kinetic-energy term is included, as we have done in Sec. II. The logarithmic divergence arising in this standard term is expected to be compensated for by the contributions of all the terms similar to Eq. (28). Indeed, integrating by parts, we have

$$\int_0^{k_c} \frac{dk}{k} \int_0^{kr_0} dxx \ln xJ_0(x) = \left[\ln k \int_0^{kr_0} dxx \ln xJ_0(x) \right]_0^{k_c} - r_0^2 \int_0^{k_c} dkk \ln k \ln(kr_0) J_0(kr_0). \tag{29}$$

To evaluate the first term we use [11] (when the integral is not absolutely convergent, we define it as above with an exponential convergence factor, with an extremely weak decreasing behavior)

$$\int_0^{\infty} dxx^{\mu} J_0(x) = 2^{\mu} \frac{\Gamma\left(\frac{1+\mu}{2}\right)}{\Gamma\left(\frac{1-\mu}{2}\right)} \tag{30}$$

[where $\Gamma(x)$ is the standard Euler gamma function] together with $\ln x = \lim_{\epsilon \to 0}(x^{\epsilon}-1)/\epsilon$. Note in particular that $\int_0^{\infty} dxxJ_0(x)=0$. This gives $\int_0^{\infty} dxx \ln xJ_0(x)=-1$, which is also consistent with the fact that the Fourier transform of $\ln r$ is $-(2\pi)/k^2$. Hence we find indeed that Eq. (29) provides the required compensating term to avoid a divergent result. The other terms lead to constants, so we may take immediately in their expression the limit $k_c \to \infty$. First, except for the prefactor $-p_4/(4\pi\mu)$, the factor of $\ln a$ in the second term of the integral in Eq. (28) is

$$\int_0^{\infty} \frac{dk}{k} \int_0^{kr_0} dxxJ_0(x) = \int_0^{\infty} \frac{dy}{y} \int_0^{y} dxxJ_0(x) = -\int_0^{\infty} dyy \ln yJ_0(y) = 1 \tag{31}$$

by the change of variable $y=kr_0$ and by integrating by parts. This means that the divergent contribution of the second term in Eq. (28) is proportional to $\ln(k_c a)$, as could be expected from dimensional analysis.

Finally in Eq. (28) we have still a contribution proportional to $\ln k$,

$$-\int_0^{\infty} \frac{dk}{k} \ln k \int_0^{kr_0} dxxJ_0(x) = \frac{r_0^2}{2} \int_0^{\infty} dkk \ln^2 kJ_0(kr_0), \tag{32}$$

again by integrating by parts. Gathering this term and the second term in Eq. (29), we have

$$-r_0^2 \int_0^{\infty} dkk \ln k \ln(kr_0) J_0(kr_0) + \frac{r_0^2}{2} \int_0^{\infty} dkk \ln^2 kJ_0(kr_0) = -\frac{1}{2} \int_0^{\infty} d(kr_0)(kr_0) \ln^2(kr_0) J_0(kr_0), \tag{33}$$

where in the last step for the term proportional to $\ln^2 r_0$, we have used again $\int_0^{\infty} dxxJ_0(x)=0$. The remaining integral is calculated again by making use of Eq. (30) and is found to be $(1/2)\int_0^{\infty} dxx \ln^2 xJ_0(x) = C - \ln 2 \simeq -0.116$, where $C = 0.577\,216\cdots$ is the Euler constant. Gathering the above results we obtain

$$E_{11k} = -\frac{p_4}{4\pi\mu} \ln(k_c a) + p_4 \frac{\ln 2 - C}{4\pi\mu}. \tag{34}$$

Finally, just as for the 3D case, we want to go back to the variables corresponding to particles $\uparrow$ and $\downarrow$. It may be seen that this does not lead to additional contributions. This leads us finally to

$$E = \frac{1}{2m_{\uparrow}} \lim_{k_c \to \infty} \left[\sum_{\mathbf{k}}^{k<k_c} k^2 n_{\uparrow}(k) - \frac{n_4}{2\pi} \ln(k_c a) \right] + \frac{1}{2m_{\downarrow}} \lim_{q_c \to \infty} \left[\sum_{\mathbf{q}}^{q<q_c} q^2 n_{\downarrow}(q) - \frac{n_4}{2\pi} \ln(q_c a) \right] + n_4 \frac{\ln 2 - C}{4\pi\mu}, \tag{35}$$

where we recall that $n_4 = n_{\uparrow} n_{\downarrow} p_4 = \lim_{k \to \infty} k^4 n_{\uparrow}(k) = \lim_{k \to \infty} k^4 n_{\downarrow}(k)$. This result can be checked explicitly in the molecular case (see Appendix A).

V. FIELD-THEORETIC APPROACH

Let us see now how the above expression for the energy arises in the field-theoretic formalism. To be specific we will restrict ourselves for simplicity to the case of major interest, namely, the one of two fermionic species with equal populations, so that $n_{\uparrow}(k) = n_{\downarrow}(k) \equiv n(k)$. Since all the $\uparrow$ and $\downarrow$ quantities are equal, we do not write explicitly this index. We consider also the nonzero-temperature case since it does not make any problem. We deal first with the case of a normal system, and then extend the results to the superfluid case.

A. Normal state

We consider first the large-k dependence of $n(k)$. For free fermions at temperature T, the density distribution has an exponential tail proportional to $e^{-k^2/2mT}$. However, as pointed out in Ref. [5], interactions modify this behavior and give rise on general grounds to a $1/k^4$ dependence which dominates the exponential tail. This is explicit in the weak-coupling domain where the interaction can be treated perturbatively and the scattering length a is small, as was done by Belyakov [4] at zero temperature:

$$n(k) = \left(\frac{2}{3\pi} k_F a \right)^2 \frac{k_F^4}{k^4}, \tag{36}$$

where k_F is the Fermi momentum, $n_{\uparrow} = n_{\downarrow} = k_F^3/6\pi^2$.

In the general case the distribution $n(k)$ is obtained from the temperature Green's function $G(\mathbf{k}, i\omega_n)$, where $\omega_n = (2n+1)\pi T$ (with n as an integer and $k_B = 1$) is the Matsubara frequency, by

$$n(k) = T \sum_n G(\mathbf{k}, i\omega_n) e^{i\omega_n \tau}, \tag{37}$$

where $\tau \to 0_+$. We separate out in this equation the free-particle contribution by writing the Dyson equation:

$$G(\mathbf{k},i\omega_n) = G_0(\mathbf{k},i\omega_n) + G_0(\mathbf{k},i\omega_n)\Sigma(\mathbf{k},i\omega_n)G(\mathbf{k},i\omega_n), \tag{38}$$

where G_0 is the free-particle Green's function $G_0(\mathbf{k},i\omega_n) = [i\omega_n - \epsilon_\mathbf{k} + \mu]^{-1}$, with $\epsilon_\mathbf{k} = k^2/2m$ as the free-particle kinetic energy, and $\Sigma(\mathbf{k},i\omega_n)$ as the self-energy. The first term in Eq. (38) gives in Eq. (37) the free-particle contribution, namely, the Fermi distribution. For large k its exponential tail mentioned above is completely dominated by the algebraic decay $1/k^4$ that we will obtain. Hence we are left only with the second term. For large k, implying a large kinetic energy for the particle, we expect the effect of interaction to be small in the same spirit as the Born approximation in this regime. Since $\Sigma(\mathbf{k},i\omega_n)$ describes this effect we expect it to be small. Hence we may to lowest order replace in this second term G with G_0. On the other hand we replace, in a standard way [12], the summation over Matsubara frequencies by a frequency integration over a contour $\mathcal{C}$ encircling the imaginary axis in the anticlockwise direction. This leads to the following expression for the dominant contribution to $n(k)$ at large k:

$$n(k) = -\frac{1}{2i\pi}\int_\mathcal{C} d\omega f\left(\frac{\omega}{T}\right)\frac{\Sigma(\mathbf{k},\omega)}{(\omega - \epsilon_k + \mu)^2}, \tag{39}$$

where $f(x) = 1/(e^x + 1)$ is the Fermi distribution function. The contour can be deformed into the sum of a contour enclosing the positive frequency Re $\omega > 0$ half plane and another contour enclosing the negative frequency Re $\omega < 0$ half plane, both being in the clockwise direction. Closing the contour at infinity in the Re $\omega > 0$ half plane is allowed by the presence of the Fermi distribution $f(\omega/T)$, and closing it at infinity in the Re $\omega < 0$ half plane by the presence of the $e^{\omega\tau}$ factor, which is then omitted since it does not play any other role.

Now contributions from the double pole at $\omega = \epsilon_k - \mu$ will contain from the Fermi distribution a factor of $e^{-k^2/2mT}$ which makes them negligible. Similarly $\Sigma(\mathbf{k},\omega)$ has also singularities with frequencies which are large and positive, when k is large. The Fermi distribution $f(\omega/T)$ will again make their contribution exponentially small. On the other hand, as shown in detail in Appendix B, $\Sigma(\mathbf{k},\omega)$ has a pole at $\omega \approx -\epsilon_k$ for large k, that is, deep in the Re $\omega < 0$ half plane. Roughly speaking this pole appears since a $\uparrow$ particle with large $\mathbf{k}$ and ω will scatter with a $\downarrow$ particle with essentially opposite parameters $-\mathbf{k}$ and $-\omega$. This happens because, just as in Sec. II the large values occur for the relative motion, but not for the center-of-mass motion. Then the $\downarrow$ particle propagator has a pole at $\omega \simeq -\epsilon_k$, which produces a pole for $\Sigma(\mathbf{k},\omega)$ at the same frequency.

For this pole, we have merely $(\omega - \epsilon_k + \mu)^2 \simeq (2\epsilon_k)^2 = k^4/m^2$ and $f(-\epsilon_k/T) \simeq 1$. If we call R_Σ the corresponding residue of $\Sigma(\mathbf{k},\omega)$, we obtain in this way

$$n(k) \simeq m^2 R_\Sigma \frac{1}{k^4}. \tag{40}$$

Hence we see that the $1/k^4$ dependence of $n(k)$ at large k emerges quite naturally in this approach. We note that our analysis may seem inconsistent, since we have first argued that $\Sigma(\mathbf{k},\omega)$ should be small for large k, but then considered a pole of $\Sigma(\mathbf{k},\omega)$, in the vicinity of which it is large. The justification is that as long as the contour is far away from the pole, $\Sigma(\mathbf{k},\omega)$ is indeed small everywhere on the contour. Making use of the pole is then a convenient way to calculate the contour integral.

We consider now the expression of the energy. It can be written in terms of the Green's function by a standard formula [12] which bears from the start a strong analogy with the expression found by Tan [3]:

$$E = T\sum_{\mathbf{k},n} (i\omega_n + \mu + \epsilon_k)G(\mathbf{k},i\omega_n)e^{i\omega_n\tau}, \tag{41}$$

where again $\tau \to 0_+$. This equation includes an overall factor of 2, coming from summation over spin. The essence of this formula is that calculating $i\omega_n G(\mathbf{k},i\omega_n)$ by Heisenberg equations of motion, one finds $E_c + 2E_{\text{int}}$, that is, the kinetic energy E_c plus twice the interaction energy E_{int}. Adding the kinetic energy E_c, which gives the ϵ_k term in Eq. (41), leads to $2E = 2(E_c + E_{\text{int}})$. In practice Eq. (41) is not so useful since one has to deal carefully with the divergent behavior occurring for large ω_n and large k, which is quite painful numerically. In this respect number equation (37) is much more convenient.

Now, to single out clearly the kinetic-energy contribution, we can rewrite Eq. (41) as

$$E = 2T\sum_{\mathbf{k},n} \epsilon_k G(\mathbf{k},i\omega_n)e^{i\omega_n\tau} + T\sum_{\mathbf{k},n} (i\omega_n + \mu - \epsilon_k)G(\mathbf{k},i\omega_n)e^{i\omega_n\tau}. \tag{42}$$

The first term is just the kinetic energy $E_c = 2\Sigma_\mathbf{k}\epsilon_k n(k)$. In the second term, which is just E_{int}, we can again replace the Matsubara frequency summation by the same contour integrals as above. Moreover the quantity appearing in this summation is just $G_0^{-1}(\mathbf{k},\omega)G(\mathbf{k},\omega) = 1 + \Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega)$. However the term 1 gives a zero contribution to these closed contour integrals. Hence we are left with

$$E = E_c - \frac{1}{2i\pi}\sum_\mathbf{k}\int_\mathcal{C} d\omega f\left(\frac{\omega}{T}\right)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega). \tag{43}$$

We can now analyze the behavior of the interaction energy term for large k, as we have done above for the particle number. In this range $\Sigma(\mathbf{k},\omega)$ is small so we may replace $G(\mathbf{k},\omega)$ with $G_0(\mathbf{k},\omega)$. Hence we have to deal with the same expression as in Eq. (36), except that $G_0(\mathbf{k},\omega)$ is not squared. Following the same arguments we obtain for large k

$$-\frac{1}{2i\pi}\int_\mathcal{C} d\omega f\left(\frac{\omega}{T}\right)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega) \simeq -\frac{mR_\Sigma}{k^2}. \tag{44}$$

Hence we have shown explicitly that the large-k behavior of the interaction energy comes in to cancel the divergent behavior of the kinetic energy. Naturally this is the expected result. Accordingly we may write

$$E = 2\sum_{\mathbf{k}} \left[\frac{k^2}{2m} n(k) - \frac{mR_\Sigma}{2k^2} \right] + \sum_{\mathbf{k}} \left[\frac{mR_\Sigma}{k^2} - \frac{1}{2i\pi} \int_C d\omega f\left(\frac{\omega}{T}\right) \Sigma(\mathbf{k},\omega) G(\mathbf{k},\omega) \right], \tag{45}$$

where, from Eqs. (40) and (44), both brackets give convergent integrals for large k. The first term is just the kinetic energy from which, according to Eq. (40), the large-k behavior has been subtracted. By comparison with Eq. (25), the second term in Eq. (45) is just $mR_\Sigma/4\pi a$, a result by no means obvious.

B. Numerical calculations in the ladder approximation

We are now in a situation where we can calculate the energy from three different formulas, as we explain just below. For the exact theory they would naturally give the same result. However if we use an approximate scheme, the results are expected to be different. The differences can, in some rough way, be seen as a measure of the errors resulting from the approximation. Hence it is of interest to make such a comparison.

Specifically we have taken as an example the ladder approximation [13,14] at unitarity and we have performed numerical calculations of the energy as a function of temperature in this approximation. The ladder approximation has been used in variety of contexts, in particular for high-T_c superconductivity [13]. In the context of ultracold gases, with a short-range potential, it has been used both in the normal state and in the superfluid state (using its natural extension in this regime). In all cases it has proved to be a quite reasonable approximation both qualitatively and quantitatively. In the normal state it can be checked [14] to give in a number of different limiting situations the exact results known from other calculations. In the superfluid state it has been shown to give results in quite good agreement with experiments [15] and it has been checked [16] that for the equation of state, it is again in fairly good agreement with results obtained from Monte Carlo calculations as well as from experiments.

We use three different ways to obtain the energy. Our first expression for the energy is the general one [Eqs. (43) and (45)]. The second one is the energy formula found by Tan [3], that is, Eq. (25), with equal masses. Finally we use the noninteracting gas scaling relation $E=-(3/2)\ \Omega$ between the grand potential Ω and the energy E, which is also valid at unitarity [17] due to the lack of any microscopic energy scale. We calculate the grand potential itself via the density $n(\mu,T)$ [obtained by integration of $n(k)$] using the thermodynamic relation $\Omega(\mu,T)/V=-\int_{-\infty}^{\mu} d\mu' n(\mu',T)$. (We have used the fact that Ω goes to 0 in the high-temperature regime $\mu/T\to-\infty$.) As noted above this last method is much more convenient numerically than the two others, since there are no convergence problems for large k in the $\mathbf{k}$ summation.

The results of these numerical calculations are shown in Fig. 1. We have checked that we recover the proper high-temperature behavior (virial expansion) with the three methods, as it should be. This common evolution toward the virial result is clearer in the inset, where the results are shown with an extended scale, but this convergence is fairly slow. The results of the three methods are fairly close, which is coherent with the fact that we expect the ladder approximation to be reasonably good, mostly toward higher temperatures. Indeed at lower temperature the differences between the three results grow, mostly for the result of the Tan formula. This is clearly due to the proximity of the superfluid critical temperature, which occurs at $T/T_F \simeq 0.243$ in this approximation.

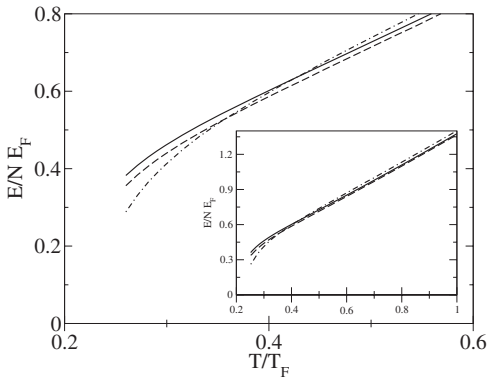

FIG. 1. Energy of the gas at unitarity as a function of reduced temperature, obtained from Eq. (45) (dashed line), Eq. (25) (dashed-dotted line), and from the scaling relation (full line) $E=-(3/2)\ \Omega$, with the grand potential Ω obtained by integrating the particle density. The inset shows the results with an extended scale.

The major numerical problem with the use of Eq. (25) is obtaining the proper coefficient of $1/k^4$ in the large-momentum behavior of $n(k)$. This requires in particular to be sure that the asymptotic regime is reached numerically. The same problem arises in Eq. (45) since one must find numerically that for large k, the kinetic energy is exactly balanced by the interaction energy. In the present case of the ladder approximation, we can check that the asymptotic regime has been reached since we have analytical expressions. In order to check numerically this large-momentum behavior of the contributions coming into the two brackets of Eq. (45), we have performed, as we indicate specifically below, an expansion of the occupation number $n(k)$ and of the interaction energy term up to orders k^{-6} and k^{-4}.

As indicated in Sec. V A the self-energy is small in the large-momentum and -frequency limit and we can expand the Green's function in powers of the self-energy. Hence we have for the occupation number and the interaction energy term the following:

$$n(k) = -\frac{1}{2\pi i} \int_C d\omega f\left(\frac{\omega}{T}\right) [G_0(\mathbf{k},\omega) + G_0(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)G_0(\mathbf{k},\omega) + O(\Sigma^2)] \tag{46}$$

$$-\frac{1}{2\pi i}\int_C d\omega f\left(\frac{\omega}{T}\right)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega)$$
$$=-\frac{1}{2\pi i}\int_C d\omega f\left(\frac{\omega}{T}\right)[\Sigma(\mathbf{k},\omega)G_0(\mathbf{k},\omega)+O(\Sigma^2)]. \quad (47)$$

We start from Eq. (B1) and following the arguments given above and detailed in Appendix B, we neglect the contribution coming from the pole of the Green's function, which gives exponentially small terms, and we only consider the contribution from the cut of the vertex $\Gamma(\mathbf{K},\Omega)$ on the real-frequency axis. Following [14], we call this self-energy contribution Σ_Γ:

$$\Sigma_\Gamma(\mathbf{k},\omega)=\frac{1}{\pi}\sum_{\mathbf{K}}\int_{\Omega_{\min}}^{\infty}d\Omega b\left(\frac{\Omega}{T}\right)\mathrm{Im}\,\Gamma(\mathbf{K},\Omega+i\epsilon)$$
$$\times G_0(\mathbf{K}-\mathbf{k},\Omega-\omega) \quad (48)$$

with $\Omega_{\min}=\frac{K^2}{4m}-2\mu$, and $\epsilon\to 0_+$.

The Bose distribution effectively limits the frequency Ω to be at most a few T and the K integral is therefore effectively bounded. Similarly to what is done in Appendix B, we consider the singularities of the self-energy located at $\omega\approx-\epsilon_{\mathbf{k}}$. In the large-momentum $\mathbf{k}$ and large-frequency ω limit, we expand the free Green's function in Eq. (48) in powers of $(\omega+\epsilon_{\mathbf{k}}+\mu)^{-1}$, leading to

$$\Sigma_\Gamma(k,\omega)=\sum_{p=0}^{\infty}\frac{C_p(k)}{(\omega+\epsilon_{\mathbf{k}}+\mu)^{p+1}}, \quad (49)$$

where

$$C_p(k)=-\frac{1}{\pi}\sum_{\mathbf{K}}\int_{\Omega_{\min}}^{\infty}d\Omega b\left(\frac{\Omega}{T}\right)\mathrm{Im}\,\Gamma(\mathbf{K},\Omega+\epsilon)$$
$$\times\left(\frac{\mathbf{k}\cdot\mathbf{K}}{m}+\Omega-\frac{K^2}{2m}+2\mu\right)^p. \quad (50)$$

In this limit, the contribution to the self-energy due to the cut of the vertex $\Gamma(\mathbf{K},\Omega)$ is a sum of poles of order $p+1$ located at $\omega=-\epsilon_{\mathbf{k}}-\mu$. In Eq. (46), only the second term is of interest, since the first one gives the Fermi distribution which does not contribute to the algebraic tail. So we use expansion (49) in Eq. (46) and find the following expansion for large wave vector k:

$$n(k)\simeq-\frac{1}{2\pi i}\int_C d\omega f\left(\frac{\omega}{T}\right)[G_0(\mathbf{k},\omega)]^2\Sigma(\mathbf{k},\omega)$$
$$\simeq\sum_{p=0}^{\infty}(p+1)\frac{C_p(k)}{(k^2/m)^{p+2}}. \quad (51)$$

The first three terms of this expansion give the dominant contribution. Indeed, it is easily checked that the term of order Σ^2 in Eq. (46) give contributions at least of order k^{-8}. C_0 does not depend on $\mathbf{k}$, while the $\mathbf{k}$ dependence of C_1 vanishes after angular integration. For the coefficient C_2 we can write $C_2(k)=A_2\frac{k^2}{m}+B_2$. Finally we find for the particle distribution in the large-momentum limit:

$$n(k)=C_0\frac{m^2}{k^4}+(2C_1+3A_2)\frac{m^3}{k^6}+O\left(\frac{m^4}{k^8}\right). \quad (52)$$

Comparing with Eq. (40) we see that C_0 is identical to the coefficient R_Σ defined in Sec. V A. We have checked the numerical convergence in the large-k limit by comparing the second term in our expansion (52) with our numerical results. The coefficients are identical with a precision of less than 1%.

We can perform the same analysis for the interaction energy term in Eq. (47) and we find the following expansion:

$$-\frac{1}{2\pi i}\int_C d\omega f\left(\frac{\omega}{T}\right)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega)$$
$$=-C_0\frac{m}{k^2}-(C_1+A_2)\frac{m^2}{k^4}+O\left(\frac{m^3}{k^6}\right). \quad (53)$$

Here also we have checked the numerical convergence with a precision of less than 1%.

C. Superfluid state

Compared to the normal state, we have now to modify Dyson equation (38) to take into account [12] the anomalous self-energy $\Delta(\mathbf{k},i\omega_n)$ and the anomalous propagator $F^+(\mathbf{k},i\omega_n)$. We have

$$G(\mathbf{k},i\omega_n)=G_0(\mathbf{k},i\omega_n)+G_0(\mathbf{k},i\omega_n)\Sigma(\mathbf{k},i\omega_n)G(\mathbf{k},i\omega_n)$$
$$+G_0(\mathbf{k},i\omega_n)\Delta(\mathbf{k},i\omega_n)F^+(\mathbf{k},i\omega_n), \quad (54)$$

$$F^+(\mathbf{k},i\omega_n)=G_0(-\mathbf{k},-i\omega_n)\Sigma(-\mathbf{k},-i\omega_n)F^+(p)$$
$$-G_0(-\mathbf{k},-i\omega_n)\Delta^*(\mathbf{k},i\omega_n)G(\mathbf{k},i\omega_n). \quad (55)$$

Again for large k, we have to lowest order $G(\mathbf{k},i\omega_n)\simeq G_0(\mathbf{k},i\omega_n)$ and $\Sigma(\mathbf{k},i\omega_n)$ small. For such a large k we expect this normal self-energy $\Sigma(\mathbf{k},i\omega_n)$ to behave as in the normal state, discussed in Sec. V B. On the other hand the anomalous self-energy is expected to go to a constant, without any singular behavior. This implies from Eq. (55) that $F^+(\mathbf{k},i\omega_n)$ is small. In this case the first term in the right-hand side of Eq. (55) is negligible and from the second term we have

$$F^+(\mathbf{k},i\omega_n)\simeq-G_0(-\mathbf{k},-i\omega_n)\Delta^*(\mathbf{k},i\omega_n)G_0(\mathbf{k},i\omega_n). \quad (56)$$

Substitution into Eq. (54) gives

$$G(\mathbf{k},i\omega_n)\simeq G_0(\mathbf{k},i\omega_n)+G_0^2(\mathbf{k},i\omega_n)[\Sigma(\mathbf{k},i\omega_n)$$
$$-G_0(-\mathbf{k},-i\omega_n)|\Delta(\mathbf{k},i\omega_n)|^2]. \quad (57)$$

Hence, in addition to the pole at $\omega\approx-\epsilon_k$ coming as discussed above in $\Sigma(\mathbf{k},i\omega_n)$, the last term gives also a pole at the same place from the explicit factor $G_0(-\mathbf{k},-i\omega_n)$. This leads to the large-k behavior:

$$n(k) \simeq m^2[R_\Sigma + |\Delta_\infty|^2]\frac{1}{k^4}, \tag{58}$$

where $\Delta_\infty = \lim_{k\to\infty} \Delta(\mathbf{k}, -\epsilon_k)$. Actually the additional term is well known in the case of BCS theory which gives indeed, with standard notations, $n_k = v_k^2 = (1/2)(1-\xi_k/E_k) \simeq m^2\Delta^2/k^4$ for large k.

Going now to the expression for the energy, there is naturally no modification in Eq. (42). On the other hand we have now, in the second term of Eq. (42) involving $G_0^{-1}G$, to make use of the appropriate Dyson equation (54). This leads, instead of Eq. (43), to

$$E = E_c - \frac{1}{2i\pi}\sum_{\mathbf{k}} \int_{\mathcal{C}} d\omega f\left(\frac{\omega}{T}\right)[\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega) + \Delta(\mathbf{k},i\omega)F^+(\mathbf{k},i\omega)]. \tag{59}$$

Now the large-k analysis goes essentially as in the normal state, and is similar to the one for the particle distribution since there is only a factor of G_0 which is different in the two calculations. This factor leads to a factor of $-k^2/m$ in the present case, compared to the particle distribution. That is, we have for large k

$$-\frac{1}{2i\pi}\int_{\mathcal{C}} d\omega f\left(\frac{\omega}{T}\right)[\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega) + \Delta(\mathbf{k},i\omega)F^+(\mathbf{k},i\omega)] \simeq -m[R_\Sigma + |\Delta_\infty|^2]\frac{1}{k^2}, \tag{60}$$

and the generalization of Eq. (45) is

$$E = 2\sum_{\mathbf{k}}\left[\frac{k^2}{2m}n(k) - \frac{m[R_\Sigma + |\Delta_\infty|^2]}{2k^2}\right] + \sum_{\mathbf{k}}\left[\frac{m[R_\Sigma + |\Delta_\infty|^2]}{k^2} - \frac{1}{2i\pi}\int_{\mathcal{C}} d\omega f\left(\frac{\omega}{T}\right)[\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega) + \Delta(\mathbf{k},i\omega)F^+(\mathbf{k},i\omega)]\right]. \tag{61}$$

VI. CONCLUSION

In this paper we have investigated the large-momentum algebraic tail in the particle distribution and the energy formula found by Tan [3] associated with this tail. We have provided a simple derivation of this energy formula, which rests on the fact that in evaluating this energy for the short-range potential under consideration, the interaction energy contribution is zero in most of phase space, which makes it negligible. Hence only the kinetic energy has to be calculated. The basis of the derivation is the careful subtraction of the kinetic-energy-divergent contribution for interparticle distance less than the potential range. This derivation is easily generalized to particles with different masses, to arbitrary mixtures, and to two-dimensional space. We have then shown how the algebraic tail arises naturally in the field-theoretic many-body approach, from the analytic structure of the self-energy. Making use of these ingredients we have shown how, starting from a standard general expression of the energy in terms of the Green's function, one obtains a formula with a kinetic-energy part which has the same structure as in the formula found by Tan. This has been done both in the normal and in the superfluid state. Finally we have taken the various exact formulas allowing to obtain the energy, and we have compared in the normal state at unitarity the resulting numerical values obtained within the ladder approximation.

Note added in proof. We have recently learned that S. Tan has also considered the two-dimensional case [19].

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APPENDIX A: LIMITING CASES

In the BEC limit $a \to 0_+$, one is led to consider the problem of a single molecule. The normalized wave function is $\psi(r) = (2\pi a)^{-1/2}e^{-r/a}/r$ and the density distribution is given by the square of its Fourier transform $n_\uparrow(k) = n_\downarrow(k) = 8\pi a^{-1}/(k^2 + a^{-2})^2$. The coefficient of the k^{-4} tail is $n_4 = 8\pi a^{-1}$. One checks that indeed the energy $E = 2\Sigma_k(k^2/2m)[n(k) - n_4/k^4] + n_4/(4\pi ma) = -1/ma^2$ gives the proper binding energy $E_b = 1/ma^2$.

In the weak-coupling limit $a \to 0_-$ the energy (per unit volume) can be expanded in powers of $k_F a$ (the contributions which would come from BCS pairing are exponentially negligible). To second order [12],

$$E = n\frac{k_F^2}{m}\left[\frac{3}{10} + \frac{k_F a}{3\pi} + b_2(k_F a)^2\right], \tag{A1}$$

where $n = k_F^3/3\pi^2$ and $b_2 = 2(11 - 2\log 2)/35\pi^2 \simeq 0.055\,661\,3$. Second-order perturbation gives also

$$n_\uparrow(k) = n_\downarrow(k) = \theta(k_F - k) + (k_F a)^2\tilde{n}^{(2)}(k/k_F), \tag{A2}$$

where $n^{(2)}(k)$ is a lengthy analytical expression given in Refs. [4,18]. For large k, $(k_F a)^2\tilde{n}^{(2)}(k/k_F) \simeq n_4^{(2)}/k^4$, with $n_4^{(2)} = (2k_F^3 a/3\pi)^2$. Since there is no first-order correction to the density distribution, the first-order correction to the energy, in energy relation (25), is merely given by the last explicit term, $n_4^{(2)}/4\pi ma = \pi a n^2/m$, which coincides indeed with the (mean-field) first-order term in Eq. (A1).

To check this relation to second order, we need the coefficient $n_4^{(3)}$ of the tail in the third-order contribution $(k_F a)^3\tilde{n}^{(3)}(k/k_F)$ to the density distribution, which is not available. However we can extract it from the adiabatic relation [5,7,9] $n_4 = 4\pi m a^2(dE/da)$, which gives $n_4^{(3)} = 8\pi b_2 n k_F^4 a^3$. Hence we have to check that

$$2\sum_k \frac{k^2}{2m}\left[(k_F a)^2 \tilde{n}^{(2)}\left(\frac{k}{k_F}\right) - \left(\frac{2k_F^3 a}{3\pi}\right)^2 \frac{1}{k^4}\right] + \frac{2b_2 n k_F^4 a^2}{m}$$
$$= b_2 n \frac{k_F^2}{m}(k_F a)^2, \tag{A3}$$

which implies

$$\int_0^\infty dx\left[x^4 \tilde{n}^{(2)}(x) - \frac{4}{9\pi^2}\right] = -\frac{2}{3}b_2. \tag{A4}$$

We have checked numerically this equation with a seven-digit precision corresponding to all the digits given above for b_2.

Finally in the 2D case, in the BEC limit, one has again a single-molecule problem. The normalized wave function of the bound state with energy $E=-1/2\mu\alpha^2$ is $\psi(r)=(\alpha\sqrt{\pi})^{-1}K_0(r/\alpha)$. For small x the Bessel function $K_0(x)\simeq \ln(2e^{-C}/x)$, so that $a=2\alpha e^{-C}$. The density distribution is $n_\uparrow(k)=n_\downarrow(k)=4\pi\alpha^2/[1+(k\alpha)^2]^2$, so that $n_4=4\pi/\alpha^2$. With these ingredients Eq. (35) is easily checked.

APPENDIX B: ANALYTIC STRUCTURE OF THE SELF-ENERGY

We discuss here in detail the analytic structure of $\Sigma(\mathbf{k},\omega)$ in order to justify the assumptions we have made above in Sec. V A. It is useful to consider first the case of the ladder approximation [12,14], where the structure is explicit. In this case the self-energy is given by

$$\Sigma(\mathbf{k},i\omega_n) = T\sum_{\mathbf{K},\nu}\Gamma(\mathbf{K},i\omega_\nu)G_0(\mathbf{K}-\mathbf{k},i\omega_\nu - i\omega_n)$$
$$= \frac{1}{2i\pi}\int_{\mathcal{C}} d\Omega b\left(\frac{\Omega}{T}\right)\sum_{\mathbf{K}}\Gamma(\mathbf{K},\Omega)G_0(\mathbf{K}-\mathbf{k},\Omega - i\omega_n), \tag{B1}$$

where in the last step we have replaced the summation over bosonic Matsubara frequencies $\omega_\nu=2\pi\nu T$, with ν as an integer, by an integral over the contour $\mathcal{C}$ introduced above, and with $b(x)=1/(e^x-1)$ as the Bose distribution function. The vertex $\Gamma(\mathbf{K},\Omega)$ is given by

$$\Gamma^{-1}(\mathbf{K},\Omega) = \frac{m}{4\pi a} + \sum_{\mathbf{k}'}\left[T\sum_m G_{0\uparrow}(\mathbf{k}',i\omega_m)G_{0\downarrow} \times(\mathbf{K}-\mathbf{k}',\Omega - i\omega_m) - \frac{1}{2\epsilon_{k'}}\right]. \tag{B2}$$

Deforming contour $\mathcal{C}$ as we have done in Sec. V A, we will from Eq. (B1) express $\Sigma(\mathbf{k},\omega)$ in terms of the singularities of $\Gamma(\mathbf{K},\Omega)$ and of $G_0(\mathbf{k},\omega)$, which are on the real-frequency axis. On one hand $G_0(\mathbf{k},\omega)$ has a simple pole at $\omega+\mu=\epsilon_k$. On the other hand the singularities of $\Gamma(\mathbf{K},\Omega)$ correspond first to the continuum of scattering states with energy $\Omega+2\mu=\epsilon_{\mathbf{k}'}+\epsilon_{\mathbf{K}-\mathbf{k}'}\geq K^2/4m$, arising from the product of the two G_0 in Eq. (B2). In addition there is the possibility of a bound state of the two particles, corresponding to a zero of the right-hand side of Eq. (B2). As a result the spectrum of these singularities has some lower bound $\Omega_{\min}$. On the other hand for large K their frequencies are bounded from below by $\Omega\approx K^2/4m$, corresponding to the kinetic energy of the mass center.

Now let us first consider the contribution from the pole of $G_0(\mathbf{K}-\mathbf{k},\Omega-i\omega_n)$ in Eq. (B1), located at $\Omega=i\omega_n+\epsilon_{\mathbf{K}-\mathbf{k}}-\mu$. The Bose factor $b(\Omega/T)$ will produce a factor $f(\epsilon_{\mathbf{K}-\mathbf{k}}/T)$, which for large k implies an exponentially small factor of $e^{-k^2/2mT}$. This makes the corresponding contribution to the self-energy irrelevant for the algebraic tail of n_k. The only way to avoid this is to have also a large $\mathbf{K}\approx\mathbf{k}$, so $\epsilon_{\mathbf{K}-\mathbf{k}}$ is not large. However in this case we will obtain a factor $\Gamma(\mathbf{K},i\omega_n+\epsilon_{\mathbf{K}-\mathbf{k}}-\mu)$. The singularities of $\Sigma(\mathbf{k},\omega)$ we are looking for are obtained from this factor by continuing the imaginary frequency $i\omega_n$ to the real-ω axis. However we know that when K is large, the singularities of $\Gamma(\mathbf{K},\Omega)$ are located at large frequencies on the order of $K^2/4m$. This implies that the corresponding singularities of $\Sigma(\mathbf{k},\omega)$ will be for $\omega+\epsilon_{\mathbf{K}-\mathbf{k}}-\mu\approx K^2/4m\approx k^2/4m$, that is, $\omega\approx k^2/4m$ since $\epsilon_{\mathbf{K}-\mathbf{k}}$ is not large. As explained below Eq. (37) these large-ω singularities in $\Sigma(\mathbf{k},\omega)$ give only exponentially small contributions to n_k and again do not come in the k^{-4} tail we are looking for. Hence we conclude that the pole of G_0 in Eq. (B1) gives no contribution to this tail, which comes accordingly only from the contribution of $\Gamma(\mathbf{K},\Omega)$.

For this contribution the dependence of $\Sigma(\mathbf{k},\omega)$ on frequency comes explicitly from the G_0 term, and it has poles for $\omega=\Omega-\epsilon_{\mathbf{K}-\mathbf{k}}+\mu$. Here Ω runs over the frequencies of the singularities of $\Gamma(\mathbf{K},\Omega)$, but in practice the Bose factor limits them to some finite range $\Omega\lesssim T$. This implies in particular that K is bounded (just as above the terms produced by the tail of the Bose factor will necessarily have an exponential factor and do not contribute to the algebraic tail of n_k). Hence, for large $k\to\infty$, we obtain from the G_0 term a single pole located at $\omega\approx -k^2/2m$. The corresponding residue is, from Eq. (B1),

$$R_\Sigma = -\frac{1}{2i\pi}\sum_{\mathbf{K}}\int_{\mathcal{C}_\Gamma} d\Omega b\left(\frac{\Omega}{T}\right)\Gamma(\mathbf{K},\Omega)$$
$$= -\frac{1}{\pi}\sum_{\mathbf{K}}\int_{\Omega_{\min}}^\infty d\Omega b\left(\frac{\Omega}{T}\right)\mathrm{Im}\,\Gamma(\mathbf{K},\Omega+i\epsilon), \tag{B3}$$

where $\mathcal{C}_\Gamma$ is a clockwise contour enclosing only the singularities of $\Gamma(\mathbf{K},\Omega)$ and the last expression (with $\epsilon\to 0_+$) is the real-axis integral obtained by calculating the contour integral from the jump of the imaginary part of Γ across the real-frequency axis.

Let us consider now the general situation where no approximation is made. Actually, provided we replace the bare propagator G_0 with the full propagator G, Eq. (B1) remains valid. We have

$$\Sigma(\mathbf{k},i\omega_n) = T\sum_{\mathbf{K},\nu}\gamma(\mathbf{K},i\omega_\nu;\mathbf{k},i\omega_n)G(\mathbf{K}-\mathbf{k},i\omega_\nu - i\omega_n)$$
$$= \frac{1}{2i\pi}\int_{\mathcal{C}} d\Omega b\left(\frac{\Omega}{T}\right)\sum_{\mathbf{K}}\gamma(\mathbf{K},\Omega;\mathbf{k},i\omega_n) \times G(\mathbf{K}-\mathbf{k},\Omega - i\omega_n). \tag{B4}$$

Indeed, considering the self-energy of, say, the $\uparrow$ particle, there will be in any diagram a first interaction with a $\downarrow$ particle, hence correspondingly a $G_\downarrow$ factor. Merely isolating this factor and gathering the rest into γ produces Eq. (B4). We may express γ in terms of the standard [12] full vertex $\tilde{\Gamma}$ by isolating the Hartree term in the self-energy. This gives, for a contact interaction,

$$\gamma(K;k) = g - gT\sum_{k'} G_\uparrow(k')G_\downarrow(K-k')\tilde{\Gamma}(k',K-k';k,K-k), \tag{B5}$$

where we have used a four-vector notation $k \equiv (\mathbf{k}, i\omega_n)$. Here the coupling constant g is related to the scattering length a and to the cutoff k_c, related to the contact interaction, by $g^{-1} = m_r/(2\pi a) - \Sigma^{k_c} 2m_r/k^2$.

Physically $\gamma(\mathbf{K}, i\omega_\nu; \mathbf{k}, i\omega_n)$ describes the scattering of two particles k and $K-k$, and accordingly it will have the same qualitative properties as we have discussed above for $\Gamma(\mathbf{K}, \Omega)$ (where we have been quite general for purpose). We consider the contributions in Eq. (B4) from the singularities of G. Either $\mathbf{K}$ is small compared to $\mathbf{k}$, so $\mathbf{K}-\mathbf{k}$ is large and we can replace G with G_0, and as above we will have an exponential factor coming from the Bose factor, or $\mathbf{K}$ is comparable to $\mathbf{k}$, in which case the corresponding singularities of γ will start around $K^2/4m$ and the resulting singularities for $\Sigma(\mathbf{k}, \omega)$ will be at least $\omega \approx k^2/4m$, which makes them irrelevant for the algebraic tail of n_k.

Hence we have only to consider the contributions of the singularities of γ in the calculation of Eq. (B4). Again those with large $\mathbf{K}$ (i.e., with small $\mathbf{K}-\mathbf{k}$) will be located at high frequency Ω, and the Bose factor produces an exponential factor which makes them irrelevant. We are left only with contributions arising for $\mathbf{K}$ small compared to $\mathbf{k}$, in which case G can again be replaced by G_0. This produces for $\Sigma(\mathbf{k}, \omega)$ an explicit pole at $\omega \approx -k^2/2m$, with a residue

$$R_\Sigma = -\frac{1}{2i\pi}\sum_{\mathbf{K}} \int_{\mathcal{C}_\Gamma} d\Omega b\left(\frac{\Omega}{T}\right)\gamma\left(\mathbf{K}, \Omega; \mathbf{k}, -\frac{k^2}{2m}\right). \tag{B6}$$

Actually it seems physically reasonable that in the large-$\mathbf{k}$ limit, $\gamma(\mathbf{K}, \Omega; \mathbf{k}, -k^2/2m)$ depends only on $(\mathbf{K}, \Omega)$. Indeed this limit corresponds to a short-range scattering between two $\uparrow$ and $\downarrow$ particles. In this case, in a way analogous to the one discussed in Sec. II for the energy formula, this scattering should be essentially described by two-body physics. The situation is then similar to the one found in the ladder approximation. The k dependence is just the one which is already explicit, and we are left with a constant for the residue, given by a formula such as Eq. (B3) with a modified $\Gamma(\mathbf{K}, \Omega)$.

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