Universal Tan relations for quantum gases in one dimension

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We investigate universal properties of one-dimensional multi-component systems comprised of fermions, bosons, or an arbitrary mixture, with contact interactions and subjected to an external potential. The masses and the coupling strengths between different types of particles are allowed to be different and we also take into account the presence of an arbitrary magnetic field. We show that the momentum distribution of these systems exhibits a universal $n_{\sigma}(k) \sim C_{\sigma}/k^4$ decay with $C_{\sigma}$ the contact of species $\sigma$ which can be computed from the derivatives of an appropriate thermodynamic potential with respect to the scattering lengths. In the case of integrable fermionic systems we argue that at fixed density and repulsive interactions the total contact reaches its maximum in the balanced system and monotonically decreases to zero as we increase the magnetic field. The converse effect is present in integrable bosonic systems: the contact is largest in the fully polarized state and reaches its minimum when all states are equally populated. We obtain short distance expansions for the Green’s function and pair distribution function and show that the coefficients of these expansions can be expressed in terms of the density, kinetic energy and contact. In addition we derive universal thermodynamic identities relating the total energy of the system, pressure, trapping energy and contact. Our results are valid at zero and finite temperature, for homogeneous or trapped systems and for few-body or many-body states.

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I. INTRODUCTION

Many current experiments with ultracold atomic gases investigate the so-called zero range regime in which the thermal de Broglie wavelength and the average interparticle distance is much larger than the effective range of the interaction potential. In this regime the thermodynamic properties of the gas are universal and depend on the interaction potential through the s-wave scattering length which characterizes the low-energy scattering of two atoms. In the case of 3D spin-1/2 fermions in the zero range regime Tan has shown [1–3] that the large momentum distribution exhibits a universal decay $n_{+\downarrow}(k) \sim C/k^4$ with $C$ an extensive quantity called contact which is the same for spin-up and -down particles. In 1D a similar decay of the momentum distribution for the Lieb-Liniger model [4] (bosons with delta-function interaction) was derived earlier for any value of the interaction strength by Olshanii and Dunjko in [5]. The contact, which in the case of spin-1/2 fermions quantifies the probability that two particles of opposite spin to be found in the same region of space, appears in a series of relations, known also as Tan relations, connecting the short distance expansions of the one- and two-particle reduced density matrices and thermodynamic properties such as the energy and pressure. While initial theoretical investigations were focused on 3D spin-1/2 fermions [1–3] and 1D spin-1/2 fermions [4] they were soon extended in the case of 2D systems [10–12], 3D bosonic systems [13], general 2D and 3D mixtures [14] and 1D spin-1/2 fermions [15]. These powerful universal relations are important and interesting not only because they relate a microscopic quantity to macroscopic quantities like the energy, but also due to their wide range of applicability being valid both in the superfluid and normal phase, at zero or finite temperature in the case of few-body or many-body states. The contact is also experimentally accessible through a variety of methods that measure: a) the molecular fraction from photo-association experiments [14–16], b) the tail of the momentum distribution [17], c) the RF spectroscopy signal at large frequencies [17–19], d) the equation of state [20] e) and the static structure factor at large momenta using Bragg spectroscopy [21–24]. In addition to the measurement of the contact several Tan relations were also checked experimentally [17–21,23].

In 1D the $1/k^4$ decay of the momentum distribution and the contact were investigated numerically and analytically for the Lieb-Liniger model [25–35], attractive and repulsive spin-1/2 fermions [36–50], the fermionic polaron problem [43–51,53], spin-1/2 bosons [39–42,54], spin-1 bosons [54–57], $\kappa$-component ($\kappa > 2$) fermions and mixtures [58–62], and impenetrable anyons [63–65]. Despite this intense activity a comprehensive set of Tan relations or an analytical derivation of the tail of the momentum distribution can be found in the literature only for the case of single-component bosons [5,33,38] and balanced spin-1/2 fermions [14]. Further motivated by the recent experimental realization [66] of 1D multi-component repulsive fermions (with $\kappa = 2, \cdots , 6$), in this article we derive Tan relations for the most general multi-component 1D system with contact interactions in an external potential. In [1–3] Tan used a new type
of generalized functions to prove the universal relations involving the contact. Subsequently, it was shown that they can be rederived using the Operator Product Expansion of local operators \([6, 7]\). Here, we use what we consider to be the most powerful and transparent technique which uses the fact that the derivative of the wave-function of a system with contact interactions is discontinuous when the coordinates of two particles coincide \([67, 68]\). This is the same method employed by Olshanii and Dunjko \([5]\) in their study of the short distance, large momentum distribution of the Lieb-Liniger model and by Werner and Castin in their comprehensive papers on Ton relations for 2D and 3D mixtures \([10, 13]\).

First, we establish that the derivative of the wave-function has a discontinuity which is a direct consequence of the delta function interaction. This discontinuity produces a \(1/k^2\) large wave-number asymptotics of the wave-function in the momentum representation which implies that the momentum distribution (which is bilinear in the momentum representation of the wave-function) presents a \(1/k^4\) tail. Then, the short-distance expansion of the Green’s function can be obtained from the inverse Fourier transform of the momentum distribution and identification of certain terms with known quantities.

The plan of the paper is as follows. In Sect. II we introduce the model and the definition of the relevant quantities. In Sect. III we study the large momentum distribution and we determine the contact. Short distance expansion of the correlation functions and thermodynamic identities are derived in Sects. IV and V. The particular case of integrable models is analyzed in Sect. VI. We conclude in Sect. VII.

II. MODEL AND CORRELATION FUNCTIONS

We consider a one-dimensional system comprised of \(\kappa\)-types of particles interacting via a delta-function potential in an external potential. The particles can be bosons, fermions or an arbitrary mixture. Different types of particles will be labeled by an integer \(\sigma \in \{1, \cdots, \kappa\}\) and the number of particles of each species will be denoted by \(N_\sigma\) with the total number of particles being \(N = \sum_\sigma N_\sigma\). In second quantization the Hamiltonian is \(H = \int \mathcal{H}(x) \, dx\) with the Hamiltonian density

\[
\mathcal{H}(x) = \sum_\sigma \frac{\hbar^2}{2m_\sigma} \left( \frac{\partial}{\partial x} \bar{\Psi}_\sigma^\dagger(x) \frac{\partial}{\partial x} \Psi_\sigma(x) + \sum_{\sigma' \leq \sigma} \frac{g_{\sigma\sigma'}}{1 + \delta_{\sigma\sigma'}} \bar{\Psi}_\sigma^\dagger(x) \Psi_{\sigma'}^\dagger(x) \Psi_{\sigma'}(x) \Psi_\sigma(x) \right) + \sum_\sigma \left( V(x) - \mu_\sigma \right) \bar{\Psi}_\sigma^\dagger(x) \Psi_\sigma(x). \tag{1}
\]

Here, \(\Psi_\sigma^\dagger(x)\) and \(\Psi_\sigma(x)\) are bosonic and/or fermionic fields which obey canonical commutation or anticommutation relations, \(m_\sigma\) and \(\mu_\sigma\) are the mass and the chemical potentials of particles of type \(\sigma\) and \(V(x) = m_\sigma \alpha_\nu x^\nu\) is the external trapping potential with \(\nu = 2, 4, \cdots\). The presence of an external magnetic field is taken into account by the presence of a magnetic field \(\alpha_\nu\). The coupling strengths can be expressed in terms of the 1D scattering length \(a_{\sigma\sigma'}\) via \(g_{\sigma\sigma'} = -\hbar^2/(m_\sigma m_{\sigma'})\) where \(m_{\sigma\sigma'} = m_\sigma m_{\sigma'}/(m_\sigma + m_{\sigma'})\) is the reduced mass. We will consider attractive and repulsive values of the coupling strength in the case of fermionic particles and only repulsive interactions between bosonic particles. Due to the fact that \(a_{\sigma\sigma'} = a_{\sigma'\sigma}\) there are only \(\kappa(\kappa+1)/2\) distinct scattering lengths.

In order to study correlation functions we need to introduce some notations. We will say that particle \(i\) is of type \(\sigma\) if \(i \in I_\sigma\) where \(I_\sigma\) is a partition of \(\{1, \cdots, N\}\) in \(\kappa\) subsets with cardinalities \(N_\sigma\). The most obvious choice, which will be used throughout this paper, is \(I_1 = \{1, \cdots, N_1\}\), \(I_2 = \{N_1 + 1, \cdots, N_1 + N_2\}\), \cdots which means that the first \(N_1\) particles are of type 1 the next \(N_2\) particles are of type 2, etc. We will denote by \(P_{\sigma\sigma'}\) the set of all pairs of particles with one particle in \(\sigma\) and the other one in \(\sigma'\) counted only once i.e., \(P_{\sigma\sigma'} \equiv \{(i, j) \in (I_\sigma \times I_{\sigma'}) / i < j\}\). For example, if \(\kappa = 2\) \(N = 5\), \(I_1 = \{1, 2, 3\}\) and \(I_2 = \{4, 5\}\) then \(P_{1,2} = \{(1, 4), (1, 5), (2, 4), (2, 5), (3, 4), (3, 5)\}\). Using these notations the Hamiltonian (1) in first quantized form can be written as

\[
H = -\sum_\sigma \sum_{i \in I_\sigma} \frac{\hbar^2}{2m_\sigma} \frac{\partial^2}{\partial x_i^2} + \sum_{\sigma' \leq \sigma} \sum_{(i,j) \in P_{\sigma\sigma'}} g_{\sigma\sigma'} \delta(x_i - x_j) + \sum_\sigma \sum_{i \in I_\sigma} V(x_i) - \sum_\sigma \mu_\sigma N_\sigma. \tag{2}
\]

A consequence of the delta function appearing in Hamiltonian (2) is that the derivative of the wave-function is discontinuous when the coordinates of any two particles coincide and regular elsewhere. More precisely, if we consider the limit when the relative distance between two particles of species \(\sigma\) and \(\sigma'\) becomes zero and all the other coordinates are kept fixed we have (see Appendix A)

\[
\lim_{x_i \to x_j} \psi_N(x_1, \cdots, x_i, \cdots, x_j, \cdots, x_N) \sim \psi_N(x_1, \cdots, X_{ij}, \cdots, X_{ij}, \cdots, x_N) \left[1 - |x_{ij}|/a_{\sigma\sigma'} + O(x_{ij}^2)\right], \tag{3}
\]

where \(X_{ij} = (m_\sigma x_i + m_{\sigma'} x_j)/(m_\sigma + m_{\sigma'})\) and \(x_{ij} = x_i - x_j\) are the center of mass and relative coordinates of the two particles. Due to the discontinuity the Fourier transform of the wave-functions at large momenta will have an \(1/k^2\)
asymptotic behavior [67, 68]. This fundamental observation will be used extensively throughout this paper and will constitute our main tool in deriving the Tan relations.

The Green’s function or the one-body density matrix is defined as

$$g^{(1)}_{\sigma}(x,x') \equiv \langle \Psi \sigma(1)(x) \Psi_{\sigma}(x') \rangle = \sum_{i \in I_\sigma} \int \prod_{j=1, j \neq i}^N dx_j \psi^*_N(x_1, \ldots, x_i, \ldots, x_N) \psi_N(x_1, \ldots, x_i, \ldots, x_N),$$  \tag{4}

with the arrows showing that $x$ and $x'$ appear on the $i$-th position. If we assume that the wave-functions are normalized to one $\int \prod_{i=1}^N dx_j |\psi_N(x_1, \ldots, x_N)|^2 = 1$ then we have $\int g^{(1)}_{\sigma}(x,x) dx = N_\sigma$. The momentum distribution is the Fourier transform of the one-body density matrix

$$n_\sigma(k) = \int \int e^{-ik(x-x')} g^{(1)}_{\sigma}(x,x') dx dx' = \sum_{i \in I_\sigma} \int \prod_{j=1, j \neq i}^N dx_j \left| \int e^{-ikx} \psi_N(x_1, \ldots, x_i, \ldots, x_N) dx \right|^2,$$  \tag{5}

where in the last relation we have used the definition (4) and interchanged the order of integration. Using the integral representation of the delta function, $\int e^{-ikx} dx = 2\pi \delta(x)$ we obtain the normalization of the momentum distribution $\int n_\sigma(k) dk = 2\pi \int g^{(1)}_{\sigma}(x,x) dx = 2\pi N_\sigma$.

The pair distribution function is defined as $g^{(2)}_{\sigma\sigma'}(x,x') \equiv \langle \Psi \sigma(2)(x') \Psi_{\sigma'}(x') \Psi (x) \rangle$ and has the following expression in terms of the wave-function

$$g^{(2)}_{\sigma\sigma'}(x,x') = \int \prod_{i=1}^N dx_1 |\psi_N(x_1, \ldots, x_N)|^2 \sum_{i \in I_\sigma, j \in I_{\sigma'}, i \neq j} \delta(x-x_i)\delta(x'-x_j).$$  \tag{6}

It is important to note that $g^{(2)}_{\sigma\sigma'}(x,x') = g^{(2)}_{\sigma\sigma'}(x',x)$. Under the assumption of normalization of the wave-functions we have $\int g^{(2)}_{\sigma\sigma'}(x,x') dx dx' = N_\sigma(N_\sigma - 1)$ and $\int g^{(2)}_{\sigma\sigma'}(x,x') dx dx' = N_\sigma N_{\sigma'}$.

III. TAIL OF THE MOMENTUM DISTRIBUTION AND EXPRESSION FOR THE CONTACT

We start our investigation by showing that for all systems described by the Hamiltonians [11] the large momentum distribution has an $n_\sigma(k) \sim C_\sigma/k^4$ decay with $C_\sigma$ an extensive quantity called contact. The contact can be expressed in terms of the pair distribution functions $g^{(2)}_{\sigma\sigma'}(x,x)$ and can be computed from the thermodynamic properties of the system via the Helmann-Feynman theorem. Our proof will follow the original idea of Oshahni and Dunjko [8] first employed in the case of the Lieb-Liniger model and subsequently generalized by Werner and Castin [10, 13] for 2D and 3D systems. For reasons of clarity we will first remind of the calculations for single component bosons and then show how the same method can be used in the case of two-component systems. As we will see the general result can be easily inferred form these particular cases.

A. Warm up. The Lieb-Liniger model

The simplest realization of the Hamiltonian [11] is in terms of single component bosons which is also known as the Lieb-Liniger model (single component fermions are equivalent with free fermions because spin polarized fermions do not “feel” the contact interaction). The homogeneous Lieb-Liniger model is integrable and for the last 60 years its correlation functions have been the subject of extensive theoretical and numerical investigations. The Hamiltonian density has the following simple form

$$\mathcal{H}(x) = \frac{\hbar^2}{2m} \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + \frac{\hbar^2}{2} \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) + (V(x) - \mu) \Psi^\dagger(x) \Psi(x),$$  \tag{7}

where $\Psi^\dagger(x), \Psi(x)$ are canonical bosonic fields, $m$ is the mass of the particles and $g = -2\hbar^2/m a$. The short distance expansion of the one-body density matrix of impenetrable bosons was first obtained by Lenard [25] (see also [26, 28]) who showed that the first nonanalytic contribution appears in the $|x|^3$ term (we will show below that this implies a $1/k^4$ decay of the momentum distribution). In the case of trapped impenetrable bosons the $1/k^4$ decay was investigated in
and for any finite interaction it was derived in [5] (numerical results for various finite couplings can be found in [32]). Below, we follow [4].

We are interested in computing the decay of the momentum distribution at large momenta. Eq. (5) shows that this task is accomplished by investigating the large-$k$ asymptotic behavior of the Fourier transform of the wavefunction. In this limit the main contributions will be given by the points where the derivative of the wavefunction is discontinuous (3) or, more precisely, when the coordinates of two particles are equal. We should stress that $\psi_N(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N)$ is regular if all the other variables except $x_i$ are different. Our analysis will use the following result:

Lemma III.1. [32] Consider a function absolutely integrable, vanishing at infinity which has a singularity of the type $f(x) = |x - x_0|^{\alpha} F(x)$ at $x_0$ with $F(x)$ analytic and $\alpha > -1$, $\alpha \neq 0, 2, 4, \ldots$. Then, we have

$$\lim_{k \to \infty} \int_{-\infty}^{+\infty} e^{-ikx} f(x) \, dx \sim 2 \cos \frac{\pi}{2} (\alpha + 1) \Gamma(\alpha + 1) \frac{e^{-ikx_0}}{|k|^{\alpha+1}} F(x_0) + O(1/|k|^\alpha).$$

In the case of multiple singular points of the same type the asymptotic behavior of the integral is given by the sum of all the corresponding contributions given by the r.h.s of (8).

Now, we have all the tools to complete our analysis. First, we notice that as a result of the bosonic symmetry Eq. (5) can be rewritten as (in this case $I_k = \{1, \ldots, N\}$), $n(k) = N \int \prod_{j=2}^{N} dx_j |\int e^{-ikx_1} \psi_N(x_1, x_2, \ldots, x_N) \, dx_1|^2$, which shows that we can focus our analysis on the Fourier transform with respect to the first particle. Taking into account (3) and employing Lemma III.1 at the points $x_1 = \{x_2, \ldots, x_N\}$ we find

$$\lim_{k \to \infty} \int e^{-ikx_1} \psi_N(x_1, x_2, \ldots, x_N) \, dx_1 \sim \int e^{-ikx_1} \sum_{j=2}^{N} \psi_N(X_j, \ldots, X_j, \ldots, x_N) \left[ 1 - \frac{|x_{1j}|}{a} + O(|x_{1j}|^2) \right] \, dx_1,$n(k) \sim N \int \prod_{m=2}^{N} dx_m \left[ \sum_{j=2}^{N} \frac{4 e^{-ik(x_j-x_1)}}{k^4 a^2} \psi_N(x_j, \ldots, x_j, \ldots, x_N) \psi_N^*(x_1, \ldots, x_1, \ldots, x_N) \right],$$

$$\sim \frac{4N}{k^4 a^2} \sum_{j=2}^{N} \int \prod_{i=2}^{N} dx_i |\psi_N(x_j, \ldots, x_j, \ldots, x_N)|^2 = \frac{4}{k^4 a^2} \int g^{(2)}(x, x) \, dx.$$

Here, the second line is obtained by neglecting the off-diagonal terms which vanish faster than $1/k^4$ due to the Riemann-Lebesgue lemma and using the definition (6) of the pair distribution function. [4] This result shows that the momentum distribution presents a $1/k^4$ decay with extensive contact $C = (4/a^2) \int g^{(2)}(x, x) \, dx$. We see that the contact is expressed in terms of the local pair distribution function a feature which is also present in the multi-component case. Eq. (9) (which was first derived in [5]) is valid not only for an arbitrary pure state but also for any statistical mixture (see Sect. III C) if we replace $g^{(2)}(x, x)$ by its thermal expectation value $g_T^{(2)}(x, x)$.

B. Two-component systems

Two-component systems already present all the features that will allow us to easily identify the general structure of the contact for the $\kappa$-component case. There are three possibilities: two types of bosons, two types of fermions and

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1 Assumption that the wave-function and derivatives are regular when two coordinates do not coincide and that they are zero at infinity, an estimate of the rate of decay for the off-diagonal terms can be obtained by performing integration by parts (on the intervals of continuous differentiability), which shows that they are of the order $O(1/k^6)$. The same type of reasoning can be applied in the case of periodic boundary conditions (no trapping potential) in a box of length $L$ by considering periodic wave-functions and derivatives and discrete momentum $k = 2\pi s/L$ with $s$ an integer, see [4].
the Bose-Fermi mixture. If we assume that in the case of the Bose-Fermi mixture particles of type 1 are bosons and particles of type 2 are fermions the Hamiltonian density is

\[ \mathcal{H}(x) = \sum_{\sigma=\{1,2\}} \frac{\hbar^2}{2m_\sigma} \partial_x \Psi^\dagger_{\sigma}(x) \partial_x \Psi_{\sigma}(x) + V_i(x) + \sum_{\sigma=\{1,2\}} (V_\sigma(x) - \mu_\sigma) \Psi^\dagger_{\sigma}(x) \Psi_{\sigma}(x), \]  

(10)

with \( V_i(x) \) the interacting potential

\[ V_i(x) = \begin{cases} \frac{g_{11}}{a_{11}} \Psi^\dagger_{1}(x) \Psi^\dagger_{1}(x) \Psi_{1}(x) \Psi_{1}(x) + \frac{g_{12}}{a_{12}} \Psi^\dagger_{1}(x) \Psi^\dagger_{2}(x) \Psi_{2}(x) \Psi_{1}(x) + g_{12} \Psi^\dagger_{1}(x) \Psi^\dagger_{1}(x) \Psi_{2}(x) \Psi_{1}(x) & \text{BB case} \\ g_{12} \Psi^\dagger_{1}(x) \Psi^\dagger_{1}(x) \Psi_{1}(x) \Psi_{1}(x) + g_{12} \Psi^\dagger_{1}(x) \Psi^\dagger_{2}(x) \Psi_{2}(x) \Psi_{1}(x) & \text{FF case} \\ \frac{g_{12}}{a_{12}} \Psi^\dagger_{1}(x) \Psi^\dagger_{1}(x) \Psi_{2}(x) \Psi_{1}(x) & \text{BF case} \end{cases} \]

(11)

The case of balanced fermions (\( \mu_1 = \mu_2 \)) at zero temperature was investigated by Barth and Zwerg [14] using operator product expansion techniques and constitutes the only 1D multi-component system for which a comprehensive set of Tan relations was derived. The \( 1/k^4 \) tail of the momentum distribution for two-component impenetrable bosons and fermions was analytically derived from the Fredholm determinant representation of the Green’s function in [39].

We will also assume that in the wave-function the coordinates of the particles of type 1 are \( x_1, \ldots, x_{N_1} \) and the coordinates of particles of type 2 are \( x_{N_1+1}, \ldots, x_{N_1+N_2} \). This also implies that \( I_1 = \{1, \ldots, N_1\} \) and \( I_2 = \{N_1+1, \ldots, N_1+N_2\} \) with the total number of particles \( N = N_1 + N_2 \). Remembering that for fermionic particles \( g_{\sigma\sigma}^{(2)}(x,x) = 0 \) we can treat all cases simultaneously. We will compute first the large momentum distribution of type 1 particles i.e., \( n_1(k) \). As in the Lieb-Liniger case we will focus on the large-\( k \) limit of the Fourier transform of the wave-function. We introduce the following notation for the Fourier transform (\( i \in I_1 \))

\[ \tilde{\psi}_N(x_1, \ldots, k, \ldots, x_N) = \int e^{-ikx} \psi_N(x_1, \ldots, x_i, \ldots, x_N) \, dx. \]

(12)

The main difference in analysing the Fourier transform of the two-component system compared with the single component case is given by the fact that the discontinuity of the derivative is different depending on the type of particles that collide. Using Lemma [11] and [13] we obtain (\( \lim_{x_i \to x_j} X_{ij} = x_j \))

\[ \lim_{k \to \infty} \tilde{\psi}_N = \sum_{j=1}^{N_1} \frac{2e^{-ikx_j}}{a_{11} k^2} \psi_N(x_1, \ldots, x_j, \ldots, x_N) \]

where the first sum represents the contribution of the coinciding points \( x = x_j \) with \( x_j \in I_1 \) and the second sum gives the contributions of \( x = x_j \) with \( x_j \in I_2 \). Using this last result we find

\[ \lim_{k \to \infty} \int \frac{dx_j}{dx} \left| \tilde{\psi}_N(x_1, \ldots, k, \ldots, x_N) \right|^2 \]

\[ = \int \frac{dx_j}{dx} \left( \sum_{j=1}^{N_1} \frac{4}{a_{11}^2 k^4} |\psi_N(\ldots, x_j, \ldots)|^2 + \sum_{j=N_1+1}^{N_2} \frac{4}{a_{12}^2 k^4} |\psi_N(\ldots, x_j, \ldots)|^2 \right). \]

(14)

where again the off-diagonal terms vanish faster than \( 1/k^4 \) due to the Riemann-Lebesgue lemma. The momentum distribution [5] requires the summation of all terms of this type with \( i \in I_1 \) with the result

\[ \lim_{k \to \infty} n_1(k) \sim \int \frac{dx}{k^4} \left( \frac{4}{a_{11}^2} \int g_{11}^{(2)}(x,x) \, dx + \frac{4}{a_{12}^2} \int g_{12}^{(2)}(x,x) \, dx \right). \]

(15)

In a similar fashion we obtain for \( n_2(k) \)

\[ \lim_{k \to \infty} n_2(k) \sim \int \frac{dx}{k^4} \left( \frac{4}{a_{22}^2} \int g_{22}^{(2)}(x,x) \, dx + \frac{4}{a_{12}^2} \int g_{12}^{(2)}(x,x) \, dx \right). \]

(16)

From these results we infer that \( C_1 = (4/a_{11}^2) \int g_{11}^{(2)}(x,x) \, dx + (4/a_{12}^2) \int g_{12}^{(2)}(x,x) \, dx \) and \( C_2 = (4/a_{22}^2) \int g_{22}^{(2)}(x,x) \, dx + (4/a_{12}^2) \int g_{12}^{(2)}(x,x) \, dx \). In the case of the two-component fermionic gas \( g_{11}^{(2)}(x,x) = g_{22}^{(2)}(x,x) = 0 \) and therefore the
contacts are equal $C_1 = C_2$ even in the case of an unbalanced system ($\mu_1 \neq \mu_2$ or, equivalently, we can say that the magnetic field is nonzero). In the case of the two-component bosonic gas the contacts for an arbitrary pure state which is not the groundstate are equal only in the balanced system ($\mu_1 = \mu_2$) when $g_{11}^{(2)}(x, x) = g_{22}^{(2)}(x, x)$. The groundstate of two-component bosons is fully polarized [71,72] which means that at zero temperature $C_1 = (4/a_1^2) \int g_{11}^{(2)}(x, x) \, dx$ and $C_2 = 0$.

C. General case

Guided by the results of Sect. 111,13 we can now present the general results for a $\kappa$-component system. For all systems described by the Hamiltonians (1) the momentum distribution of each type of particles has the asymptotic behavior $\lim_{k \to \infty} n_\sigma(k) \sim C_\sigma/k^4$ with the contact given by

$$C_\sigma = \frac{\kappa}{\kappa} \int \frac{g_{\sigma\sigma'}^{(2)}(x, x)}{a_{\sigma\sigma'}^2} \, dx = \frac{\kappa}{\kappa} \int \langle \Psi^{\dagger}_\sigma(x) \Psi^{\dagger}_{\sigma'}(x) \Psi_{\sigma}(x) \rangle \, dx.$$  \hspace{1cm} (17)

An alternative form of the previous expression involving derivatives of the energy with respect to the scattering lengths can be derived using the Helmann-Feynman theorem. We obtain $\partial E/\partial a_{\sigma\sigma'} = \hbar^2 \int g_{\sigma\sigma'}^{(2)}(x, x) \, dx/m_{\sigma'}^2 a_{\sigma\sigma'}^2 (1 + \delta_{\sigma\sigma'})$ which shows that (17) can be also written as

$$C_\sigma = \frac{4}{\hbar^2} \sum_{\sigma = 1}^{\kappa} m_{\sigma}(1 + \delta_{\sigma\sigma'}) \frac{\partial E}{\partial a_{\sigma\sigma'}}.$$  \hspace{1cm} (18)

where $\partial E/\partial a_{\sigma\sigma'} = 0$ if particles of type $\sigma$ are fermions. In the particular case of two-component fermions this last relation takes the form $\partial E/\partial a_{12} = \hbar^2 C_{12}/4m_{12}$ which is also known as the adiabatic Tan theorem [11,14].

Eqs. (17) and (18) are valid for any pure state. In the case of an arbitrary statistical mixture defined by $\langle \cdot \rangle = \sum p_\sigma \langle \psi_\sigma | \cdot | \psi_\sigma \rangle$ the contact is $C_\sigma = \sum p_\sigma C_\sigma^{(n)}$ with $C_\sigma^{(n)} = \sum_{\sigma' = 1}^{\kappa} (4/a_{\sigma\sigma'}^2) \int g_{\sigma\sigma'}^{(2)}(x, x) \, dx$ and $g_{\sigma\sigma'}^{(2)}(x, x) = \langle \psi_\sigma | \Psi^{\dagger}_{\sigma'}(x) \Psi_{\sigma'}(x) \Psi_{\sigma}(x) | \psi_\sigma \rangle$. In the particular case of the grand-canonical ensemble Eq. (18) takes the form

$$C_\sigma = \frac{4}{\hbar^2} \sum_{\sigma = 1}^{\kappa} m_{\sigma}(1 + \delta_{\sigma\sigma'}) \left( \frac{\partial \Phi}{\partial a_{\sigma\sigma'}} \right)_{\mu, T},$$  \hspace{1cm} (19)

with $\Phi(\mu_\sigma, T, a_{\sigma\sigma'})$ the grand-canonical potential.

Let us consider the particular case of systems which are characterized by $m_\sigma = m_\sigma' = m$ and $a_{\sigma\sigma'} = a$ for all $\sigma, \sigma' \in \{1, \cdots, \kappa\}$ and repulsive interactions $a < 0$ (if $V_\sigma(x) = 0$ these systems would be integrable but all the consideration below hold also in the presence of an external potential). The total contact is now given by $C_{\text{tot}} = (4/a^2) \sum_\sigma \sum_{\sigma'} \int g_{\sigma\sigma'}^{(2)}(x, x) \, dx$. The pair distribution function $g_{\sigma\sigma'}^{(2)}(x, x)$ quantifies the probability that two particles of type $\sigma$ and $\sigma'$ to be found in the same region of space. If we consider a system comprised of only fermionic particles then the pair distribution functions and the total contact will be largest when the system is balanced i.e., when the number of particles of each type is equal $N_\sigma = N_{\sigma'} = N/\kappa$. Switching a magnetic field and keeping the total number of particles constant the resulting imbalance will cause the pair distribution functions and total contact to decrease. Therefore, for fixed density in a fermionic system the total contact is largest in the balanced system and is a monotonously decreasing function of the magnetic field vanishing when only one type of particles survive. This behavior was numerically confirmed in the case of two-component fermions at zero and finite temperature in [50] and for finite numbers of particles in two- and three-component systems in [61]. If in the case of fermionic systems the ground-state is antiferromagnetic as a consequence of the Lieb-Mattis theorem [73] in purely bosonic systems the ground-state is ferromagnetic [71,72]. The wave-function of the ground-state is real and positive $\Psi^0_{J=NS}(x_1, \cdots, x_N) \geq 0$ for all $x_1, \cdots, x_N$ (the wave-function can be zero at coinciding points only in the case of infinite repulsive interactions) with total spin $J = NS$ where $S$ is each boson’s spin. An eigenstate with total spin $J < NS$ denoted by $\Psi^0_{J < NS}$ is no longer positive [72] and numerical data for two-component bosons reveals that $\langle \Psi^0_{J=J_{\chi}/2} | V_{\text{int}} | \Psi^0_{J=J_{\chi}/2} \rangle > \langle \Psi^0_{J < J_{\chi}/2} | V_{\text{int}} | \Psi^0_{J=J_{\chi}/2} \rangle$ with $V_{\text{int}}$ the interaction term of the Hamiltonian (11). The last relation also implies that (subscripts identify the state) $g_{11}^{(2)}(x, x)_{J=J_{\chi}/2} > \sum_{\sigma, \sigma'}=1 g_{\sigma\sigma'}^{(2)}(x, x)_{J < J_{\chi}/2}$ which shows that the total contact of the two-component bosonic system is largest in the ferromagnetic state. The minimum (which is nonzero) is reached for the balanced system in contrast with the fermionic case. It is sensible to assume that this behavior of the total contact is also present in the case of $\kappa$-component systems with $\kappa > 2$. 

IV. SHORT DISTANCE EXPANSION OF CORRELATORS

The behavior of the wave-functions in the vicinity of the coinciding points can be used to derive short distance expansions of the pair distribution functions and one-body density matrices. In both cases the first terms of these expansions can be expressed in terms of quantities that can be obtained from the thermodynamic properties of the system.

A. The pair distribution function

We start with the short distance expansion of the pair distribution function $g^{(2)}_{\sigma\sigma'}(X + m_{\sigma'}x/m_{\sigma}, X - m_{\sigma'}x/m_{\sigma'})$ defined in [19]. Using Eq. (13) and the definition we find

$$g^{(2)}_{\sigma\sigma'}(X + m_{\sigma'}x/m_{\sigma}, X - m_{\sigma'}x/m_{\sigma'}) = \sum_{i\in I_{\sigma}, j\in I_{\sigma'}} \sum_{k\notin\{i,j\}} \int dk |\psi_N(x_1, \cdots, X_\uparrow, x_2, \cdots, x_N)|^2 \left[ 1 - \frac{2|x|}{a_{\sigma\sigma'}} + O(|x|^2) \right],$$

$$= g^{(2)}_{\sigma\sigma'}(X, X) \left[ 1 - \frac{2|x|}{a_{\sigma\sigma'}} + O(|x|^2) \right].$$

A simple application of the Helmann-Feynman theorem (see the remark before Eq. (18)) allows us to express the expansion of the spatially integrated distribution function as

$$\int g^{(2)}_{\sigma\sigma'}(X + m_{\sigma'}x/m_{\sigma}, X - m_{\sigma'}x/m_{\sigma'}) dX = a^2_{\sigma\sigma'}(1 + \delta_{\sigma\sigma'}) \frac{m_{\sigma'}}{k^2} \frac{\partial E}{\partial a_{\sigma\sigma'}} \left[ 1 - \frac{2|x|}{a_{\sigma\sigma'}} + O(|x|^2) \right].$$

Previous expressions simplify considerably in the case of homogeneous systems with particles of equal mass. In the case of two-component fermions it was first shown in [13] that the $|x|$ non-analyticity at short distances imply that the static structure factor $S(k) \sim 1 + n \int dx e^{-ikx} [g^{(2)}_{12}(X + x/2, X - x/2) - 1]$ will decay at large momenta like $S(k \to \infty) \sim 1 - \text{const} \, C_1/k^2$ with $C_1$ the contact. In 3D the tail of the static structure factor of spin-$\frac{1}{2}$ fermions is proportional to $C_1/k$ from which the contact was measured using Bragg spectroscopy [21, 22].

B. The one-body density matrix

Here, we derive the short distance asymptotics of the spatially integrated one-body density matrix i.e., $G^{(1)}_{\sigma\sigma}(x) = \int g^{(1)}_{\sigma\sigma}(X + x/2, X - x/2) dX$, which can also be understood as the Fourier transform of the momentum distribution $G^{(1)}_{\sigma\sigma}(x) = \int e^{ikx} n_{\sigma}(k) dk/2\pi$. We will assume a short distance expansion of the type

$$g^{(1)}_{\sigma\sigma}(X + x/2, X - x/2) = N_{\sigma}(x) + a^2_{\uparrow}(X) x + a^2_{\downarrow}(X)x^2 + a^3_{\sigma}(x) |x|^3 + O(x^4).$$

In the previous expansion we have not considered an $|x|$ term because we already know that $n_{\sigma}(k) \sim C_{\sigma}/k^4$ which together with Lemma [13] means that the first nonanalytic term is $|x|^3$ from which we can compute $\int a^3_{\sigma}(X) dX = C_{\sigma}/12$. We still need to determine $a^2_{\uparrow}(X)$ and $a^2_{\downarrow}(X)$. Expanding $e^{ikx}$ to second order we obtain

$$G^{(1)}_{\sigma\sigma}(x) \sim \int \left( 1 + ikx + \frac{(ikx)^2}{2!} \right) \frac{n_{\sigma}(k)}{2\pi} \frac{k^2}{4\pi} dk + O(x^3),$$

which allows to make the identifications $\int N_{\sigma}(x) dX = N_{\sigma}$, $\int a^2_{\uparrow}(X) dX = i \int k n_{\sigma}(k)/2\pi dk$ and $\int a^2_{\downarrow}(X) dX = -i \int k^2 n_{\sigma}(k)/4\pi dk$. If we consider a system with symmetric momentum distribution $n(k) = n(-k)$ then $a^2_{\uparrow}(X) = 0$. Also it is easy to see that $\int a^3_{\sigma}(X) dX = -m_{\sigma} T_{\sigma}/k^2$ with $T_{\sigma}$ the kinetic energy of the $\sigma$ type particles. Therefore, we obtain

$$G^{(1)}_{\sigma\sigma}(x) \equiv \int g^{(1)}_{\sigma\sigma}(X + x/2, X - x/2) dX = N_{\sigma} - \frac{m_{\sigma} T_{\sigma}}{h^2} x^2 + \frac{C_{\sigma}}{12} |x|^3 + O(x^4).$$

Similar short distance expansions of the Green’s function were obtained in [5] for the Lieb-Liniger model and in [14] for two-component fermions.
V. THERMODYNAMIC IDENTITIES

In this Section we are going to derive several universal thermodynamic identities connecting the total energy, trapping energy, momentum distribution and derivatives of thermodynamic potentials with respect to the scattering lengths.

The total energy of the system \( E = \langle H \rangle \) can be expressed as the sum of the kinetic energy \( T \), interaction energy \( I \) and trapping energy \( V \) i.e., \( E = T + I + V \). Rewriting the kinetic energy of the Hamiltonian (11) in momentum space and employing the Helmann-Feynman theorem we obtain

\[
E = \sum_{\sigma} \int \frac{dk}{2\pi} \frac{\hbar^2 k^2}{2m_\sigma} n_\sigma(k) - \sum_{\sigma \leq \sigma'} \frac{\partial E}{\partial a_{\sigma\sigma'}} a_{\sigma\sigma'} + V
\]  

(24)

where \( \partial E/\partial a_{\sigma\sigma} = 0 \) if the particles of type \( \sigma \) are fermions. Eq. (24) also holds in the case of an arbitrary statistical mixture (see the discussion in Sect. III C). In the case of the grand-canonical ensemble we only need to replace \( \partial E/\partial a_{\sigma\sigma} \) by \( \partial \Phi/\partial a_{\sigma\sigma} \).

We will also derive two more universal relations known as the pressure and energy identities. As a preliminary step we need to investigate certain scaling relations. The Hamiltonian in the first quantization for the general case is given by (2) with coupling strengths \( g_{\sigma\sigma'} = -\hbar^2/(m_\sigma a_{\sigma\sigma'}) \) and external potentials of the type \( V_\sigma(x) = m_\sigma \alpha_\nu(x) \) with \( \nu = 2, 4, 6, \ldots \). In the case of the harmonic trapping potential \( \nu = 2 \) and \( \alpha_2 = \omega^2 \) with \( \omega \) the trapping frequency. We want to find what is the behaviour of the Hamiltonian (2) under a scaling transformation \( x = x'/\lambda \) with \( \lambda \in \mathbb{R}_+^* \). Under this transformation we have \( d^2/dx^2 \rightarrow \lambda^2 d^2/dx'^2 \), \( \delta(x) \rightarrow \delta(x'/\lambda) = \lambda \delta(x') \) and \( V_\sigma(x) \rightarrow m_\sigma \alpha_\nu(x'/\lambda) \). Therefore,

\[
H_{\lambda}/\lambda \left( \{ \lambda^{-1} a_{\sigma\sigma'} \}, \lambda^{2+n} \alpha_\nu, \{ \lambda^2 \mu_\nu \} \right) = \lambda^2 H_L \left( \{ a_{\sigma\sigma'} \}, \alpha_\nu, \{ \mu_\nu \} \right),
\]  

(25)

where we have introduced the notations \( \{ \lambda^{-1} a_{\sigma\sigma'} \} = \{ \lambda^{-1} a_{11}, \lambda^{-1} a_{12}, \ldots, \lambda^{-1} a_{\nu\nu} \} \), \( \{ \lambda^2 \mu_\nu \} = \{ \lambda^2 \mu_1, \ldots, \lambda^2 \mu_\nu \} \) and the subscripts \( L/\lambda \) and \( L \) denote the size of the finite systems. An obvious consequence of Eq. (25) is that a similar relation exists between the energy eigenvalues of the two Hamiltonians. Using the definition of the grand-canonical potential we obtain

\[
\Phi_{\lambda}/\lambda \left( \{ \lambda^{-1} a_{\sigma\sigma'} \}, \lambda^{2} \alpha_\nu, \{ \lambda^2 \mu_\nu \}, \lambda^2 T \right) = \lambda^3 \Phi_L \left( \{ a_{\sigma\sigma'} \}, \alpha_\nu, \{ \mu_\nu \}, T \right).
\]  

(26)

In the case of an homogeneous system \( \alpha_\nu = 0 \) introducing the grandcanonical potential per length \( \phi = \Phi/L \) we have

\[
\phi \left( \{ \lambda^{-1} a_{\sigma\sigma'} \}, \{ \lambda^2 \mu_\nu \}, \lambda^2 T \right) = \lambda^3 \phi \left( \{ a_{\sigma\sigma'} \}, \{ \mu_\nu \}, T \right).
\]  

(27)

A. Pressure identity for the homogeneous system

Taking the thermodynamic limit and differentiating (27) with respect to \( \lambda \) and then setting \( \lambda = 1 \) we obtain

\[
-\sum_{\sigma \leq \sigma'} \frac{\partial \phi}{\partial a_{\sigma\sigma'}} a_{\sigma\sigma'} + 2 \sum_{\sigma} \frac{\partial \phi}{\partial \mu_\sigma} \mu_\sigma + 2 \frac{\partial \phi}{\partial T} T = 3\phi.
\]

From thermodynamics we have \( \phi = -p = \dot{E} - TS - \sum_\sigma \mu_\sigma n_\sigma \) where \( p \) is the pressure, \( \dot{E} \) is the energy density, \( S \) the entropy density and \( n_\sigma \) the particles densities. Also we have \( \frac{\partial \phi}{\partial \mu_\sigma} = -S \) and \( \frac{\partial \phi}{\partial T} = -n_\sigma \). Collecting everything we obtain the pressure relation

\[
p = 2\dot{E} + \sum_{\sigma \leq \sigma'} \frac{\partial \phi}{\partial a_{\sigma\sigma'}} a_{\sigma\sigma'} = 2\dot{E} - I,
\]  

(28)

with \( I \) the interaction energy density.

B. Energy identity for the inhomogeneous system

Similarly as in the homogeneous case by taking the thermodynamic limit and differentiating (26) with respect to \( \lambda \) and then setting \( \lambda = 1 \) we obtain

\[
-\sum_{\sigma \leq \sigma'} \frac{\partial \phi}{\partial a_{\sigma\sigma'}} a_{\sigma\sigma'} + (2 + \nu) \frac{\partial \phi}{\partial a_\nu} a_\nu + 2 \sum_{\sigma} \frac{\partial \phi}{\partial \mu_\sigma} \mu_\sigma + 2 \frac{\partial \phi}{\partial T} T = 2\phi.
\]

Using \( \Phi = \dot{E} - TS - \sum_\sigma \mu_\sigma N_\sigma \) and \( \frac{\partial \phi}{\partial \mu_\sigma} a_\nu = \langle \sum_\sigma m_\sigma \alpha_\nu(x) \rangle \equiv V \) with \( V \) the trapping energy, we obtain the energy identity

\[
E = \frac{2 + \nu}{2} V - \frac{1}{2} \sum_{\sigma \leq \sigma'} \frac{\partial \phi}{\partial a_{\sigma\sigma'}} a_{\sigma\sigma'} = \frac{2 + \nu}{2} V + \frac{1}{2} I.
\]  

(29)

The universal identities (24), (28), and (29) were first derived in the case of two-component fermions in [14] and in the case of the Lieb-Liniger model in [33].
VI. THE INTEGRABLE CASE

The Hamiltonian (11) is integrable when \( V(x) = 0 \) and all masses and scattering lengths are independently equal \([73, 77]\). In order to make contact with the relevant literature in this section we are going to use units of \( \hbar = 2m = k_B = 1 \) and introduce \( c = -2/a \). In this case the systems are homogeneous and it is useful to introduce the contact density denoted by \( C_\sigma = C_\sigma / L \), energy density \( \mathcal{E} = E / L \), etc. Unfortunately, compared with the nonintegrable case, from the thermodynamics of the systems we can only obtain the total contact

\[
C_{\text{tot}} \equiv \sum_{\sigma=1}^{\kappa} C_\sigma = c^2 \frac{\partial \phi}{\partial c},
\]

with \( \phi \) the grandcanonical potential per length. If we would have considered the ground state or any other pure state \( C_{\text{tot}} = c^2 \frac{\partial \phi}{\partial c} \) with \( \mathcal{E} \) the energy density of the state. In the case of a balanced pure fermionic or bosonic system we can derive the individual contacts using \( C_\sigma = c^2 \frac{\partial \phi}{\partial c} / \kappa \). The short distance expansions of the correlators become

\[
g^{(2)}_{\sigma \sigma}(X + x/2, X - x/2) = g^{(2)}_{\sigma \sigma}(X, X) \left( 1 + c|x| + \mathcal{O}(|x|^2) \right)
\]

and

\[
\sum_{\sigma=1}^{\kappa} g^{(1)}_{\sigma \sigma}(X + x/2, X - x/2) = n - \frac{T_{\text{tot}}}{2} x^2 + \frac{C_{\text{tot}}}{12} |x|^3 + \mathcal{O}(x^4).
\]

with \( n \) the total density and \( T_{\text{tot}} \) the total kinetic energy density. Again, in a balanced pure fermionic or bosonic system we have \( g^{(1)}_{\sigma \sigma}(X + x/2, X - x/2) = \left( n - \frac{T_{\text{tot}}}{2} x^2 + \frac{C_{\text{tot}}}{12} |x|^3 \right) / \kappa \). The thermodynamic identities take the form

\[
p = 2\mathcal{E} - \frac{C_{\text{tot}}}{c}, \quad E = \frac{2 + \nu}{2} V + \frac{1}{2} \frac{C_{\text{tot}}}{c},
\]

where for the last relation we have considered the integrable system in the presence of the external potential \( V(x) = mA_\nu x^\nu \) with \( V = \langle mA_\nu x^\nu \rangle \) the trapping energy.

VII. CONCLUSIONS

In this paper we derived Tan relations for multi-component 1D models with contact interactions. We considered the most general case in which the masses and the inter- and intra-couplings can be different and also took into account the presence of an external potential and magnetic field. We showed that the tail of the momentum distribution presents a universal \( 1/k^4 \) decay with the amplitude given by the contact which can be expressed in terms of the local pair distribution functions. In addition we obtained short distance expansions of the correlation functions and several thermodynamic identities. We have also argued that in the case of purely fermionic systems at fixed density the total contact is a decreasing function of the imbalance while in a purely bosonic system the converse is true. The case of systems with mixed symmetry was numerically investigated by Decamp et al. \([62] \) (see also \([61, 78, 79]\)) and it was found that the ground-state has the most symmetric wave-function allowed by the mixture which can be understood as a generalization of the Lieb-Mattis theorem \([73]\).

The dependence of the contact on the temperature is an issue that needs further exploration. In the case of integrable systems at high-temperatures it is expected that it is monotonously increasing as a function of the temperature for all values of the coupling strengths \([50, 55, 61, 62]\). However, at low-temperatures and strong coupling in the case of two-component models the total component exhibits a local minimum which signals a significant momentum reconstruction. This phenomenon is present for all integrable models with two-components \([50, 55]\) and is due to the transition from the low-temperature phase to the spin-incoherent regime \([39]\). We expect that this behavior is also present in the case of systems with more than two-components. This is left for further investigation.

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Appendix A: Discontinuity of the derivative of the wave-function

Here we prove Eq. (3). Because we consider all the other coordinates kept fixed it will be sufficient to investigate the nonanalyticity of the wave-function for a system with the Hamiltonian

\[ H = -\frac{\hbar^2}{2m_\sigma} \frac{\partial^2}{\partial x_i^2} - \frac{\hbar^2}{2m_{\sigma'}} \frac{\partial^2}{\partial x_j^2} + g_{\sigma\sigma'} \delta(x_i - x_j), \tag{A1} \]

where we have neglected the external potential and chemical potential terms which are irrelevant for the present discussion. Introducing the center of mass and relative coordinates of the two particles i.e., \( X_{ij} = (m_\sigma x_i + m_{\sigma'} x_j) / (m_\sigma + m_{\sigma'}) \) and \( x_{ij} = x_i - x_j \), the eigenvalue problem of the Hamiltonian (A1) becomes

\[ \left( -\frac{\hbar^2}{2(m_\sigma + m_{\sigma'})} \frac{\partial^2}{\partial X_{ij}^2} - \frac{\hbar^2}{2m_{\sigma'}} \frac{\partial^2}{\partial x_{ij}^2} + g_{\sigma\sigma'} \delta(x_{ij}) \right) \psi(X_{ij}, x_{ij}) = E \psi(X_{ij}, x_{ij}), \]

with \( m_{\sigma\sigma'} = m_\sigma m_{\sigma'}/(m_\sigma + m_{\sigma'}) \) the reduced mass of the two particles. Integrating over \( x_{ij} \) in a small vicinity of 0 we obtain

\[- \frac{\hbar^2}{2m_{\sigma'}} \int_{-\epsilon}^{+\epsilon} \frac{\partial^2 \psi(R_{ij}, x_{ij})}{\partial x_{ij}^2} \, dx_{ij} + g_{\sigma\sigma'} \int_{-\epsilon}^{+\epsilon} \delta(x_{ij}) \psi(R_{ij}, x_{ij}) \, dx_{ij} = 0.\]

implying \( \partial_{x_{ij}} \psi(R_{ij}, 0_+) - \partial_{x_{ij}} \psi(R_{ij}, 0_-) = 2g_{\sigma\sigma'} m_\sigma m_{\sigma'} \psi(R_{ij}, 0)/\hbar^2 \) which shows that the derivative of the wave-function is discontinuous. We can write \( \Psi(X_{ij}, x_{ij}) = \psi(X_{ij}, 0) \left( 1 - |x_{ij}|/a_{\sigma\sigma'} + O(x_{ij}^2) \right) \) where we have used \( g_{\sigma\sigma'} = -\hbar^2/(m_{\sigma\sigma'} a_{\sigma\sigma'}). \) Using \( x_i = X_{ij} + m_{\sigma\sigma'} x_{ij}/m_\sigma \) and \( x_j = X_{ij} - m_{\sigma\sigma'} x_{ij}/m_{\sigma'} \) the generalization to the case of \( N \) particles is given by Eq. (3).

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