

Connection between nonlocal one-body and local three-body correlations of the Lieb-Liniger model

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We derive a connection between the fourth coefficient of the short-distance Taylor expansion of the one-body correlation function, and the local three-body correlation function of the Lieb-Liniger model of δ -interacting spinless bosons in one dimension. This connection, valid at arbitrary interaction strength, involves the fourth moment of the density of quasimomenta. Generalizing recent conjectures, we propose approximate analytical expressions for the fourth coefficient covering the whole range of repulsive interactions, validated by comparison with accurate numerics. In particular, we find that the fourth coefficient changes sign at interaction strength $\gamma_c \simeq 3.816$, while the first three coefficients of the Taylor expansion of the one-body correlation function retain the same sign throughout the whole range of interaction strengths.

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I. INTRODUCTION

One-dimensional quantum systems are generically more strongly correlated than their higher-dimensional counterparts, due to the inevitability of collisions when particles cross each other. The one-dimensional Bose gas with contact interactions, known as the Lieb-Liniger model, is the paradigm of such systems [1]. This model well describes experiments with ultracold atoms in tight waveguides and some of its correlation functions have been experimentally probed in all interaction regimes [2–9]. From a theoretical point of view, since the model is integrable, its k -body correlations can in principle be obtained explicitly at all orders k , since they are linked to the (infinite) set of integrals of motion. In practice, however, the exact analytical calculation at arbitrary interaction strength is tremendously difficult for two reasons: the coefficients of their Taylor expansion at small distance are related to each other in a nontrivial way, and the defining system of equations, in turn derived using the Bethe ansatz, is technically very challenging. In the thermodynamic limit, finding an explicit expression for the various spatially nonlocal, equal time correlations from Bethe ansatz techniques actually requires to link them to the moments of the density of quasimomenta, and thus to solve a type II homogeneous Fredholm integral equation with Lorentzian kernel, whose exact analytic solution is yet unknown.

In this work, we focus on the link between nonlocal correlation functions of the Lieb-Liniger model and its integrals of motion, thus elucidating a special structure of the ground state for this integrable model. In particular, we derive a relation, first proposed in Ref. [10], that links the fourth coefficient of the Taylor expansion of the one-body correlation function at short distances with various moments of the quasimomentum distribution and their derivatives with respect to the coupling constant. Then, we use a recently developed method [11,12], and generalize recent conjectures [12–14], to evaluate these quantities with excellent accuracy in a wide range of interaction strengths.

The paper is organized as follows: In Sec. II we introduce the Hamiltonian of the system and the relevant notations. We also define the notion of connection, which is the key concept in this work, and illustrate it in simple cases. Then, in Sec. III we derive a connection between the fourth coefficient of the Taylor expansion of the one-body correlation function at short distances, c_4 , the local three-body correlation function, and the fourth moment of the density of pseudomomenta, which is one of the main results of this work. In Sec. IV, we provide conjectures about the moments of the density of pseudomomenta, and we illustrate them in Sec. V where we find, in particular, that c_4 changes sign at interaction strength $\gamma \simeq 3.8$. In Sec. VI, we summarize our main results and give an outlook to our work.

II. HAMILTONIAN AND DEFINITIONS

In this work, we consider a one-dimensional system of N indistinguishable pointlike bosons of mass m subject to contact interactions, known as the Lieb-Liniger model. We choose periodic boundary conditions, possibly realized by using a ring geometry. The Hamiltonian of the system reads

$$\hat{\mathcal{H}} = \frac{\hbar^2}{2m} \left[\sum_{i=1}^N -\frac{\partial^2}{\partial x_i^2} + 2c \sum_{i=1}^{N-1} \sum_{j=i+1}^N \delta(x_i - x_j) \right], \quad (1)$$

where the first term of the right-hand side stands for the kinetic energy, $\{x_i\}$ label the positions of the atoms, δ is the Dirac delta function, $c = 2/a$ is related to the coupling constant, with $a = -a_{1D} > 0$ for repulsive interactions, and a_{1D} is the one-dimensional scattering length related to the many-body wave function by $\Psi(\dots, x_i, \dots, x_j, \dots) \propto |x_i - x_j| - a_{1D} + \dots$. The usual one-dimensional coupling constant of the model is $g_{1D} = -2\hbar^2/(ma_{1D}) = (\hbar^2/m)c$ [15].

The action of the Hamiltonian on the Bethe ground state $|\chi_N\rangle$ of the many-body system reads

$$\hat{\mathcal{H}}|\chi_N\rangle = \sum_{i=1}^N \lambda_i^2 |\chi_N\rangle, \quad (2)$$

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the eigenvalue is the sum of Bethe rapidities λ_i squared, and the ground state in coordinate representation reads [16,17]

$$\chi_N(x_1, \dots, x_N) = \text{const} \times \sum_{\sigma \in S_N} (-1)^{\mathcal{P}[\sigma]} \prod_{i=1}^{N-1} \prod_{j=i+1}^N \left[\lambda_{\sigma_i} - \lambda_{\sigma_j} - \frac{2i}{a} \text{sgn}(x_i - x_j) \right] \exp \left[i \sum_{k=1}^N \lambda_{\sigma_k} x_k \right]. \quad (3)$$

In Eq. (3), σ are elements of the symmetry group S_N , i.e., permutations of N elements, $\mathcal{P}[\sigma]$ is their parity, and σ_i denotes the image of i by σ . These eigenstates are also eigenfunctions of all conservation laws, as required by the integrability of the model.

The correlation functions we are interested in are the k -body density matrices normalized to unity by choice of the constant in Eq. (3), and such that

$$\begin{aligned} \rho_k(x_1, \dots, x_k; x'_1, \dots, x'_k) & \\ \equiv \int dx_{k+1} \cdots dx_N \chi_N^*(x'_1, \dots, x'_k, x_{k+1}, \dots, x_N) & \\ \times \chi_N(x_1, \dots, x_N) & \\ = \rho_k(x_1 - x'_1, \dots, x_k - x'_k; 0, \dots, 0), & \end{aligned} \quad (4)$$

due to Galilean invariance. In particular, in this work we consider the one-body density matrix, whose series expansion at short distance can be written as

$$\rho_1(x; x') = \frac{1}{L} \sum_{l=0}^{+\infty} c_l (n|x-x'|)^l. \quad (5)$$

In what follows we also make use of the notation

$$g_k \equiv \frac{N!}{(N-k)!} \frac{\rho_k(0, \dots, 0; 0, \dots, 0)}{n^k}, \quad (6)$$

where $n = N/L$ is the mean linear density, the system being of size L . Correlations g_k are referred to as k -body local correlations; they represent the probability to find k atoms at the same place and time. It is quite intuitive that the combined effect of geometry and interactions enforces $g_{k+1} < g_k$ at finite interaction strengths, and that g_k are decreasing functions of the interaction strength.

The first aim of this work is to illustrate the fact that, due to the integrability of the model, those correlations are related to each other via the moments e_{2k} of the dimensionless density of quasimomenta $g(z; \alpha)$, defined as the solutions of the set of Bethe equations derived by Lieb and Liniger [1] in the thermodynamic limit $N \rightarrow \infty$, $L \rightarrow \infty$, at fixed N/L and at zero temperature:

$$g(z; \alpha) - \frac{1}{2\pi} \int_{-1}^1 dy \frac{2\alpha g(y; \alpha)}{\alpha^2 + (y-z)^2} = \frac{1}{2\pi}, \quad (7)$$

$$\gamma \int_{-1}^1 dy g(y; \alpha) = \alpha, \quad (8)$$

and

$$e_{2k}(\gamma) = \frac{\int_{-1}^1 dy g(y; \alpha(\gamma)) y^{2k}}{\left[\int_{-1}^1 dy g(y; \alpha(\gamma)) \right]^{2k+1}}, \quad (9)$$

where α is a positive coefficient and $\gamma \equiv 2/(na)$ is the Lieb parameter, representing the natural dimensionless coupling constant of the model. The quantities e_{2k} are integrals of motions of the model: for example, e_2 corresponds to the thermodynamic limit of the ground-state energy $E_2 = \sum_i \lambda_i^2$, through $E_2 = Nn^2 e_2$. More generally, we define $E_{2k} = Nn^{2k} e_{2k}$, and $e_{2k+1} = 0$ from parity arguments.

To finish with, we define connections as functionals \mathcal{F} such that

$$\mathcal{F}(c_l(\gamma), g_k(\gamma), \{e_n(\gamma), e'_n(\gamma), \dots\}, \gamma) = 0, \quad (10)$$

where $'$ denotes differentiation with respect to γ . We denote each connection by a pair of indices (l, k) , where by convention an index is 0 if the corresponding quantity in the notation above does not appear in the functional. This compact notation helps in classifying the connections. To illustrate this concept, we derive the first few connections from conservation laws.

The first conserved quantity is

$$\hat{H}_0 = \sum_{i=0}^N \frac{\partial^0}{\partial x_i^0} = N, \quad (11)$$

the number of atoms. Trivially,

$$\langle \chi_N | \hat{H}_0 | \chi_N \rangle = N \langle \chi_N | \chi_N \rangle = N \quad (12)$$

since the Bethe eigenstate is normalized to unity. On the other hand,

$$\begin{aligned} \langle \chi_N | \hat{H}_0 | \chi_N \rangle &= N \int dx_1 \cdots dx_N \chi_N^*(x_1, \dots, x_N) \chi_N(x_1, \dots, x_N) \\ &= N \int dx_1 \int dx'_1 \delta(x_1 - x'_1) \int dx_2 \cdots dx_N \\ &\quad \times \chi_N^*(x'_1, \dots, x_N) \chi_N(x_1, \dots, x_N) \\ &= NL \rho_1(x; 0)|_{x=0} = Nc_0 = Ng_1, \end{aligned} \quad (13)$$

hence

$$c_0 = g_1 = e_0 = 1, \quad (14)$$

yielding the connections (0,0) and (0,1).

The second conserved quantity is

$$\hat{H}_1 = \sum_{i=0}^N \frac{\partial}{\partial x_i} \quad (15)$$

and, proceeding as before, we find

$$c_1 = e_1 = 0, \quad (16)$$

the connection of type (1,0), in agreement with Ref. [18].

Then, from the Hamiltonian we obtain

$$\langle \chi_N | \hat{\mathcal{H}} | \chi_N \rangle = Nn^2 e_2. \quad (17)$$

We also evaluate

$$\begin{aligned} \langle \chi_N | \sum_{i=1}^N -\frac{\partial^2}{\partial x_i^2} | \chi_N \rangle &= NL \frac{\partial^2}{\partial x^2} \rho_1(x; 0)|_{x=0} \\ &= 2Nn^2 c_2, \end{aligned} \quad (18)$$

and

$$\langle \chi_N | \sum_{i=1}^{N-1} \sum_{j=i+1}^N \delta(x_i - x_j) | \chi_N \rangle = \frac{N}{2} n g_2, \quad (19)$$

hence the connection of order (2,2),

$$-2c_2 + \gamma g_2 = e_2. \quad (20)$$

The connection of type (0,2) is obtained by applying the Hellmann-Feynman theorem to the Hamiltonian and reads [19]

$$g_2 = e'_2. \quad (21)$$

Combining the connections of orders (2,2) and (0,2) yields order (2,0), i.e. [18],

$$c_2 = \frac{1}{2}(\gamma e'_2 - e_2). \quad (22)$$

III. DERIVATION OF THE CONNECTION OF ORDER (4,3)

In this section, we derive a new connection, namely,

$$24c_4 - 2\gamma^2 g_3 = e_4 - \gamma e'_4. \quad (23)$$

It is the connection of type (4,3) according to our nomenclature.

First, we introduce an operator \hat{H}_4 that yields, when applied to an eigenstate (3), the fourth integral of motion, E_4 ,

$$\hat{H}_4 | \chi_N \rangle = E_4 | \chi_N \rangle, \quad (24)$$

with

$$E_4 = \sum_{i=1}^N \lambda_i^4. \quad (25)$$

From these definitions, by construction the higher Hamiltonian \hat{H}_4 can be written explicitly as [20–22]

$$\begin{aligned} \hat{H}_4 &= \sum_{i=1}^N \frac{\partial^4}{\partial x_i^4} + \frac{48}{a^2} \sum_{i=1}^{N-2} \sum_{j=i+1}^{N-1} \sum_{k=j+1}^N \delta(x_i - x_j) \delta(x_j - x_k) \\ &\quad - \frac{4}{a} \sum_{i=1}^{N-1} \sum_{j=i+1}^N \left\{ \left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial x_j^2} + \frac{\partial^2}{\partial x_i \partial x_j} \right) \delta(x_i - x_j) \right. \\ &\quad \left. + \delta(x_i - x_j) \left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial x_j^2} + \frac{\partial^2}{\partial x_i \partial x_j} \right) \right\} \\ &\quad + \frac{8}{a^2} \sum_{i=1}^{N-1} \sum_{j=i+1}^N \delta^2(x_i - x_j) \\ &= \hat{h}_4^{(1)} + 48\kappa^2 \hat{h}_4^{(2)} - 4\kappa \hat{h}_4^{(3)} + 8\kappa^2 \hat{h}_4^{(4)}, \end{aligned} \quad (26)$$

where $\kappa = \frac{1}{a}$.

For convenience, we introduce the auxiliary operator

$$\hat{Q}_4 = \frac{1}{\kappa} \hat{H}_4, \quad (27)$$

and apply the Hellmann-Feynman theorem to it:

$$\langle \chi_N | \left(\frac{d}{d\kappa} \hat{Q}_4(\kappa) \right) | \chi_N \rangle = \frac{d}{d\kappa} \left(\frac{1}{\kappa} E_4(\kappa) \right). \quad (28)$$

The left-hand side is related to operator \hat{H}_4 introduced above by

$$\begin{aligned} \langle \chi_N | \left(\frac{d}{d\kappa} \hat{Q}_4(\kappa) \right) | \chi_N \rangle &= -\frac{1}{\kappa^2} \langle \chi_N | \hat{h}_4^{(1)} | \chi_N \rangle + 48 \langle \chi_N | \hat{h}_4^{(2)} | \chi_N \rangle \\ &\quad + 8 \langle \chi_N | \hat{h}_4^{(4)} | \chi_N \rangle. \end{aligned} \quad (29)$$

We evaluate the terms of the right-hand side separately. First, we find

$$\begin{aligned} \langle \chi_N | \hat{h}_4^{(1)} | \chi_N \rangle &= NL \frac{\partial^4}{\partial x^4} \rho_1(x; 0) \Big|_{x=0} \\ &= 12Ln^4 c_3 \delta(0) + 24Ln^5 c_4. \end{aligned} \quad (30)$$

Actually, the infinity in the form of $\delta(0)$ is canceled by the analogous divergence produced by

$$\langle \chi_N | \hat{h}_4^{(4)} | \chi_N \rangle = \frac{1}{2} Ln^2 g_2 \delta(0) \quad (31)$$

as can be shown using the connection of order (3,2),

$$c_3 = \frac{1}{3} \frac{1}{(na)^2} g_2. \quad (32)$$

The latter is deduced from (0,2) above, Eq. (21), and (3,0) that reads [18]

$$c_3 = \frac{\gamma^2}{12} e'_2. \quad (33)$$

We remark that conversely, starting from the sole requirement that \hat{H}_4 is divergence free, Eq. (32) naturally follows from our derivation, which can thus be seen as a new and independent proof of this connection. Then, (3,0) is derived by combination with (0,2).

Another way to derive (3,2) is as follows: due to the contact condition, one can write

$$\begin{aligned} \rho_k(x_1, \dots, x_k; x'_1, \dots, x'_k) \\ = \sum_{m=0}^{+\infty} \rho_k^{(m)} \left(\frac{x_1 + x'_1}{2}, x_2, \dots, x_k; x'_2, \dots, x'_k \right) |x_1 - x'_1|^m. \end{aligned} \quad (34)$$

Since

$$\rho_1 = \int dx_2 \rho_2(x_1, x_2; x'_1, x_2) \quad (35)$$

and

$$\int dx_2 |x_1 - x_2| |x'_1 - x_2| =_{x_1 \rightarrow x'_1} \frac{1}{3} |x_1 - x'_1|^3 + \dots, \quad (36)$$

where the dots represent a regular function, one finds the general result

$$\rho_k^{(3)}(0, \dots; 0, \dots) = \frac{N-k}{3a^2} \rho_{k+1}(0, \dots; 0, \dots) \quad (37)$$

or, written another way,

$$c_3^{(k)} = \frac{\gamma^2}{12} g_{k+1}, \quad (38)$$

a higher-order connection from which (3,2) follows as a corollary.

To finish with, we evaluate

$$\langle \chi_N | \hat{h}_4^{(2)} | \chi_N \rangle = \frac{1}{6} L n^3 g_3. \quad (39)$$

Inserting Eqs. (30), (31), and (39) into Eqs. (28) and (29) ends the derivation. We now comment on the physical meaning of Eq. (23). The fact that g_3 appears stems from $\hat{h}_4^{(2)}$ in Eq. (26), that involves three-body processes provided $N \geq 3$. The coefficient c_4 , that stems from $\hat{h}_4^{(1)}$, is related to the higher kinetic energy in that the momentum operator applied to the density matrix generates the coefficients of its Taylor expansion when taken at zero distance.

One can even go further, combining the connection (0,3) [23,24],

$$g_3(\gamma) = \frac{3}{2} \frac{e'_4}{\gamma} - 5 \frac{e_4}{\gamma^2} + \left(1 + \frac{\gamma}{2}\right) e'_2 - 2 \frac{e_2}{\gamma} - 3 \frac{e_2 e'_2}{\gamma} + 9 \frac{e_2^2}{\gamma^2}, \quad (40)$$

with the connection (4,3), Eq. (23), to obtain the connection (4,0),

$$c_4(\gamma) = \frac{\gamma e'_4}{12} - \frac{3}{8} e_4 + \frac{2\gamma^2 + \gamma^3}{24} e'_2 - \frac{\gamma e_2}{6} - \frac{\gamma e_2 e'_2}{4} + \frac{3}{4} e_2^2, \quad (41)$$

given in Ref. [10] without proof. The right-hand sides of these last two equalities involve moments of the pseudomomentum distribution only, and it is a general fact that all correlations of the model are defined through connections of type $(l,0)$ and $(0,k)$, as a consequence of integrability.

IV. CONJECTURES ABOUT THE EXACT MOMENTS OF THE DENSITY OF PSEUDOMOMENTA

As illustrated above, local correlation functions are linked to the even-order moments e_{2k} of the density of pseudomomenta (we recall that odd ones are trivially null by parity). Their exact and explicit analytical expression is not known to date, only the first few terms of their exact asymptotic expansions in the weakly and strongly interacting regimes have been computed exactly. To go further and cover the full range of repulsive interaction strengths $\gamma \in [0, +\infty[$, we generalize to arbitrary moments recent conjectures about the ground-state energy.

A. Conjecture in the weakly interacting regime

The first conjecture concerns the Taylor expansion of e_{2k} in the weakly interacting regime, and reads

$$e_{2k}(\gamma) = \sum_{i=0}^{+\infty} \frac{a_{2k,i}}{\pi^i} \gamma^{k+i/2}, \quad (42)$$

where $\{a_{2k,i}\}$ are real coefficients. This is a generalization to arbitrary k of the conjecture proposed in Ref. [13] for e_2 .

According to Eq. (9), a trivial necessary condition is $a_{0,i} = \delta_{i,0}$, where $\delta_{..}$ is the Kronecker symbol. The exact nontrivial coefficients unambiguously found so far are $a_{2,0} = 1$, $a_{2,1} = -4/3$ [1], $a_{2,2} = \zeta(2) - 1$ [13], where ζ is

the Riemann zeta function, $a_{4,0} = 2$, and $a_{4,1} = -88/15$ [23]. Based on accurate numerics by Prolhac, Lang conjectured $a_{2,3} = 3\zeta(3)/8 - 1/2$. Prolhac also proposed $a_{2,4} = a_{2,3}/3$ and $a_{2,5} = -45\zeta(5)/1024 + 15\zeta(3)/256 - 1/32$ [14]. Higher-order coefficients $a_{2,i}$ are numerically known with high accuracy up to order $i = 10$ [14].

Using the conjecture (42) together with the known expansion at low α , heuristically introduced in Ref. [25] and proven in Ref. [26] (we refer to Appendix A for a derivation of the first part),

$$g(z; \alpha) \simeq_{\alpha \ll 1} \frac{\sqrt{1-z^2}}{2\pi\alpha} + \frac{1}{4\pi^2\sqrt{1-z^2}} \left[z \ln \left(\frac{1-z}{1+z} \right) + \ln \left(\frac{16\pi}{\alpha} \right) + 1 \right], \quad (43)$$

combined with Eqs. (7)–(9), we find the general form of the first two coefficients at fixed order k ,

$$a_{2k,0} = \frac{1}{k+1} \binom{2k}{k} = C_k, \quad (44)$$

where $\{C_k\}$ denote the Catalan numbers, and

$$a_{2k,1} = \binom{2k}{k} - \frac{2^{2k}}{\binom{2k+1}{k}} \frac{1}{k+1} \sum_{i=0}^k \left[\frac{1}{2^{2i}} \binom{2i}{i} \right]^2. \quad (45)$$

B. Conjecture in the strongly interacting regime

In the strongly interacting regime, we generalize a recent conjecture on e_2 [12] by stating that the asymptotic expansion in $1/\gamma$ is partially resummed in a natural way as

$$e_{2k}(\gamma) = \left(\frac{\gamma}{2+\gamma} \right)^{2k} \sum_{i=0}^{+\infty} \frac{\pi^{2(k+i)}}{(2+\gamma)^{3i}} \mathcal{L}_{2k,i}(\gamma), \quad (46)$$

where $\mathcal{L}_{2k,i}$ are polynomials with rational coefficients, such that $\mathcal{L}_{2k,0} = 1/(2k+1)$ and $\mathcal{L}_{2k,i \geq 1}$ is of degree $i-1$. Using a basis of orthogonal polynomials to systematically find a $1/\gamma$ expansion of the moments as explained in Refs. [11,12], together with the conjecture Eq. (46), we find the following by identification:

$$\begin{aligned} \mathcal{L}_{4,1}(X) &= \frac{32}{35}, \\ \mathcal{L}_{4,2}(X) &= -\frac{1984}{1575} X + \frac{3424}{1575}, \\ \mathcal{L}_{4,3}(X) &= \frac{8192}{3465} X^2 - \frac{37376}{5775} X + \frac{169728}{45045}, \\ \mathcal{L}_{4,4}(X) &= -\frac{47104}{9009} X^3 + \frac{59337728}{3378375} X^2 \\ &\quad - \frac{61582336}{3378375} X + \frac{137573632}{23648625}, \\ \mathcal{L}_{4,5}(X) &= \frac{192512}{15015} X^4 - \frac{765952}{15925} X^3 + \frac{80326709248}{1206079875} X^2 \\ &\quad - \frac{594448384}{14189175} X + \frac{295196160000}{38192529375}, \end{aligned}$$

$$\mathcal{L}_{4,6}(X) = -\frac{335872}{9945}X^5 + \frac{132872192}{984555}X^4 - \frac{2316542492672}{10416144375}X^3 + \frac{3689660465152}{18091198125}X^2 - \frac{184095784026112}{2406129350625}X + \frac{12238234443776}{1260353469375}. \quad (47)$$

V. ILLUSTRATIONS

In this section, we illustrate the various results obtained above. Within our approach, in order to evaluate g_3 and c_4 with good accuracy from Eqs. (40) and (41), it is crucial to correctly evaluate not only e_2 and e_4 , but also their derivatives. For e_2 , we refer to previous studies [12,14], where it was found that the combination of the weakly interacting expansion of Ref. [14] and the conjectural partial resummation in the strongly interacting regime of Ref. [12] yields excellent agreement with accurate numerics. In this work, we checked that e_2' obtained from the conjectures in their respective ranges is also numerically exact for all interaction strengths, as shown in Appendix B.

More important, we benchmark the conjectures on the fourth moment. In Fig. 1 we plot e_4 from the conjectures Eq. (42) and Eq. (46) over the experimentally relevant range $\gamma \in [0,10]$ and find excellent agreement with the numerical integration of the Bethe ansatz equations (6)–(8). The coefficients used in the weakly interacting regime are found by fitting data at $\gamma \ll 1$ and the whole curve thereby obtained closely follows numerical solution of the Bethe equations for interaction strengths $\gamma > 1$, validating the conjecture. However, our numerical data are not accurate enough to guess the analytical exact value of the unknown coefficients $a_{4,i}$ for $i \geq 2$.

While no discrepancy between the conjecture from the strongly interacting regime, Eq. (46), and numerical solution of

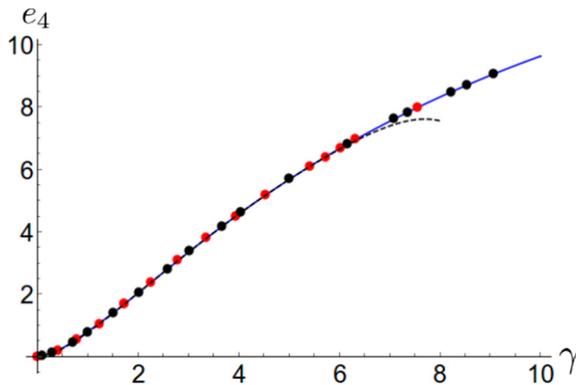


FIG. 1. Dimensionless fourth moment of the distribution of quasimomenta e_4 as a function of the dimensionless interaction strength γ . Analytical result from the conjecture (47) (solid blue line) is in excellent agreement with independent accurate numerics from the authors (red and black dots) for all interaction strengths. The conjecture in the weakly interacting regime, Eq. (42), with appropriate coefficients (black dashed line) reproduces numerical calculations with excellent accuracy up to intermediate interactions.

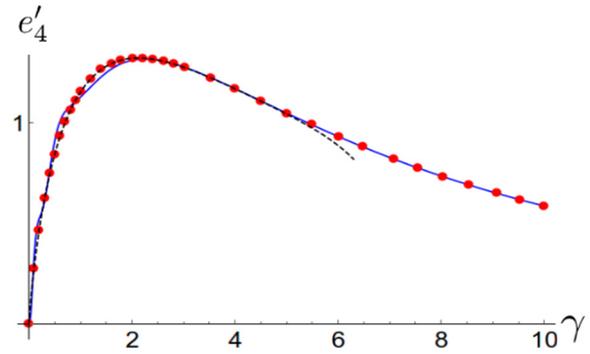


FIG. 2. Derivative of the dimensionless fourth moment of the distribution of quasimomenta e_4 with respect to the dimensionless interaction strength γ as a function of the latter. Using the analytical results either from the conjectures (47) (solid blue line) at strong interactions or Eq. (42) (dashed black line) at weak interactions, one finds an excellent agreement with accurate numerics (black dots) for all interaction strengths.

the Bethe ansatz equations is seen on this graph, by looking at e_4' shown in Fig. 2, one sees that the large- γ expansion displays spurious oscillations at intermediate interactions; hence an appropriate combination of both conjectures at weak and strong coupling is needed to recover agreement with numerical calculations over the whole range of interaction strengths.

We have also checked that our numerical data for e_2 and e_4 , when used in Eq. (40), yield $g_3(\gamma)$ in close agreement with accurate approximate expressions obtained in Ref. [23] by fitting on the numerical solution of Eqs. (7)–(9), and (40), as illustrated in Appendix C. Having performed all these verifications, we plot in Fig. 3 the coefficient c_4 as a function of γ from numerical calculations and the conjectures on e_2 and e_4 . We find that c_4 changes sign at $\gamma = \gamma_c \simeq 3.8$. We evaluated the value with more accuracy as $\gamma_c = 3.8160616255908\dots$ by comparing two independent numerical solutions of the Bethe ansatz equations, with agreement of all digits up to this order. This change of sign had already been predicted, based on numerical analysis in Ref. [27], that suggested $1 < \gamma_c < 8$. In Fig. 4 we plot the known coefficients c_2 , c_3 , and c_4 as

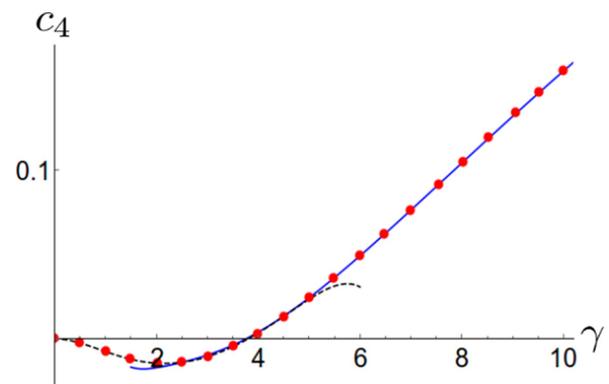


FIG. 3. Dimensionless coefficient c_4 as a function of the dimensionless interaction strength γ , as predicted from the conjectures (solid blue and dashed black lines), compared to accurate numerics (red dots). A sign inversion occurs around $\gamma = 3.8$.

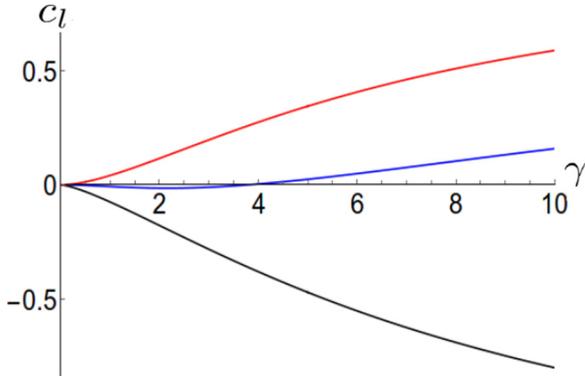


FIG. 4. Dimensionless coefficients c_2 , c_4 , and c_3 (black, blue, and red lines, from bottom to top, respectively) as predicted from conjectures, as functions of the dimensionless interaction strength γ .

functions of γ . They are also known by direct calculation in the Tonks-Girardeau regime of infinite interaction strength, where their values are $c_2 = -\pi^2/6$, $c_3 = \pi^2/9$, and $c_4 = \pi^4/120$, respectively, in agreement with our results in the limit $\gamma \rightarrow +\infty$, but higher-order terms are known as well in this regime, such as $c_5 = -11\pi^4/1350 \dots$ [28–30]. Note that very high interaction strengths are needed to approach the value in the Tonks-Girardeau regime up to a few percent; thus it is quite difficult, for the observable ρ_1 , to reach this regime experimentally.

VI. CONCLUSIONS AND OUTLOOK

In conclusion, in this work we have derived an exact relation linking the fourth coefficient of the Taylor expansion of the one-body correlation function at short distances and the local three-body correlation function of the Lieb-Liniger model. This connection can be recast in a form where c_4 is expressed in terms of moments of the density of pseudomomenta. We have investigated the fourth moment e_4 in detail and provided conjectural expressions that are extremely accurate in the whole range of interaction strengths. Both analytically and numerically, we find that c_4 changes sign around $\gamma = 3.8$.

In outlook, it would be interesting to investigate the link between c_5 and the coefficient of the first subleading, high-momentum $1/p^6$ term of the momentum distribution $n(p)$ of the gas, beyond the well-known Tan contact (i.e., the coefficient of the leading $1/p^4$ term). Knowing more terms of the Taylor expansion of g_1 and $n(p)$ also allows one to probe in a finer way the validity of the renormalization group–Luttinger liquid approach by comparing their predictions at large distances or short momenta [10]. In the perspective of taking a harmonic trapping into account, it also allows one to discuss the validity of the local density approximation [18] by comparison with exact numerics [31]. To this aim, the equation of state from the $1/\gamma$ expansion is accurate in the strongly interacting regime, while the conjecture thereby deduced is also accurate at intermediate γ [32]. The attractive regime of the super-Tonks-Girardeau gas may also provide new insights [33,34]. To finish with, the equivalence between Eq. (40) and another one derived in Refs. [35,36], that does not

involve the momenta e_{2k} but requires solving other Fredholm integral equations instead, checked numerically so far, still awaits rigorous proof. It will provide an interesting alternative way to tackle connections, especially in out-of-equilibrium situations. Another approach from field theory, based on an appropriate nonrelativistic limit of the sinh-Gordon model, has also shown remarkable efficiency already [37,38] as compared with previous Bethe ansatz results [19,39,40]. The full characterization of the local correlations g_k seems, however, especially challenging and insightful. Even the connection (0,3) has not been derived yet based on Bethe ansatz techniques only.

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APPENDIX A: DERIVATION OF THE SEMICIRCULAR LAW

In this Appendix, we provide a derivation of the semicircular law verified by the density of pseudomomenta at very small interactions, i.e., the dominant term of the solution to Eq. (7) in the limit $\alpha \rightarrow 0$, that reads

$$g(z; \alpha) \simeq_{\alpha \ll 1} \frac{\sqrt{1-z^2}}{2\pi\alpha}. \quad (\text{A1})$$

This derivation is based on the methods of Ref. [41]. First, the kernel of the integral equation is rewritten as

$$\frac{2\alpha}{\alpha^2 + (y-z)^2} = \int_{-\infty}^{+\infty} dp e^{-\alpha|p|} \cos[p(y-z)]. \quad (\text{A2})$$

Then the Fourier integral theorem, stating that

$$f(z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy f(y) \int_{-\infty}^{+\infty} dp \cos[p(y-z)], \quad (\text{A3})$$

is applied to g to transform Eq. (7) into

$$2 \int_0^{+\infty} dp (1 - e^{-\alpha p}) \int_{-1}^1 dy g(y; \alpha) \cos(py) = 1 \quad (\text{A4})$$

after a few simplifications.

To go further, $g(y; \alpha)$ is expanded over the basis of Gegenbauer polynomials $\{U_n\}$, that are orthogonal on $[-1, 1]$, as

$$g(y; \alpha) = \sqrt{1-y^2} \sum_{n=0}^{+\infty} A_n(\alpha) U_{2n}(y). \quad (\text{A5})$$

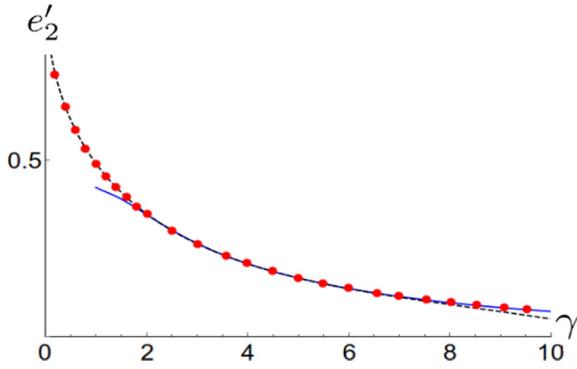


FIG. 5. Derivative e'_2 of the dimensionless energy as a function of the dimensionless interaction strength γ , as predicted from the conjectures (solid blue and dashed black lines), compared to accurate numerics (red dots).

Thus, to lowest order in α , Eq. (A4) becomes

$$2\alpha \int_0^{+\infty} dp p \int_{-1}^1 dy \sqrt{1-y^2} A_0 \cos(py) = 1, \quad (\text{A6})$$

and using the property

$$\int_{-1}^1 dy \sqrt{1-y^2} \cos(py) = \pi \frac{J_1(p)}{p}, \quad (\text{A7})$$

where J_1 is the first Bessel function, Eq. (A6) becomes

$$2\pi A_0 \alpha \int_0^{+\infty} dp J_1(p) = 2\pi A_0 = 1, \quad (\text{A8})$$

and one obtains Eq. (A1) as announced.

APPENDIX B: TEST OF THE CONJECTURES FOR e'_2

In Fig. 5, we plot e'_2 from the conjectures with known coefficients from Refs. [12,14] and compare with accurate numerics. The agreement is pretty satisfying over the whole range of interactions.

APPENDIX C: TEST OF OUR NUMERICAL DATA FOR g_3

In Fig. 6, we compare the local three-body operator g_3 obtained numerically and accurate expressions from Ref. [23]. The agreement is excellent.

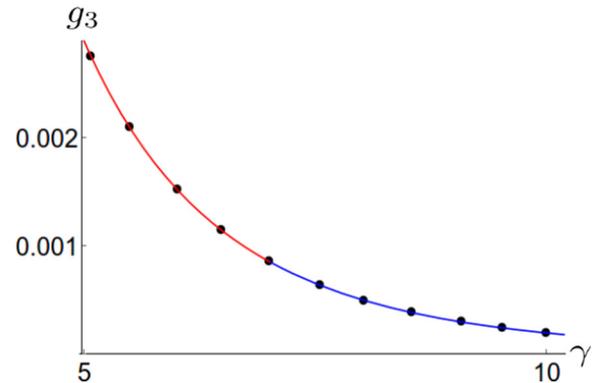
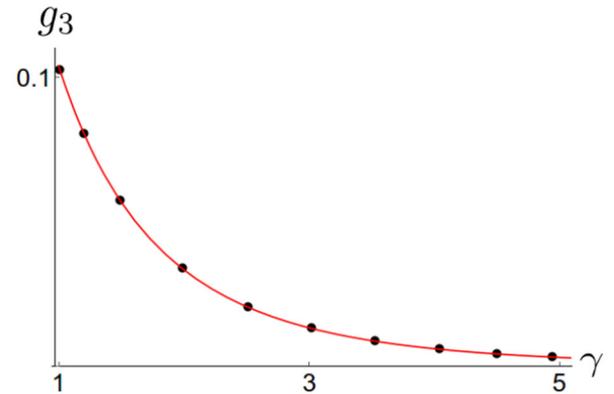
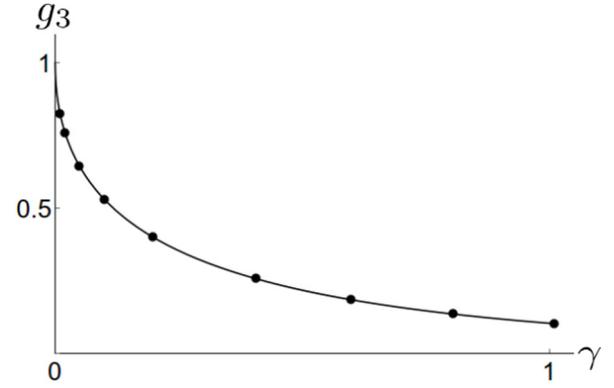


FIG. 6. Dimensionless three-body local correlation function g_3 , as a function of the dimensionless interaction strength γ obtained numerically (dots) compared to the three accurate expressions in Ref. [23] (solid black, red, and blue lines) in a wide range of interaction strengths.

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