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Phys. Rev. Lett. **107**, 230405 — Published 2 December 2011

DOI: 10.1103/PhysRevLett.107.230405

Exact three-body local correlations for excited states of the 1D Bose gas

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We derive an exact analytic expression for the three-body local correlations in the Lieb–Liniger model of 1D Bose gas with contact repulsion. The local three-body correlations control the thermalization and particle loss rates in the presence of terms which break integrability, as is realized in the case of 1D ultracold bosons. Our result is valid not only at finite temperature but also for a large class of non-thermal excited states in the thermodynamic limit. We present finite temperature calculations in the presence of external harmonic confinement within local density approximation, and for a highly excited state that resembles an experimentally realized configuration.

PACS numbers: 67.85.-d,03.75.Hh,02.30.Ik,68.65.-k

When ultracold bosons are confined to move in only one dimension (1D), they provide a very clean realization [1–3] of a seminal exactly solvable model introduced by Lieb and Liniger (LL) [4]. Being an integrable model, it has a very special dynamics showing almost no relaxation in experiments [3]. This fact stimulated lots of theoretical interest in understanding of the thermalization of isolated 1D systems and the role of integrability and its breaking in this process [5–9]. In particular, it has been shown [8, 10], that virtual excitations of bosons to higher transverse modes of a confining potential result in a weak three-body *local* interaction that violates integrability of the many-body problem. Thus it is important to understand three-body local correlations in the absence of integrability breaking terms first. Such correlations have also been measured recently using analysis of particle losses [11, 12], density fluctuation statistics [13], time-of-flight correlation statistics [14], and scanning electron microscopy [15]. They provide a very sensitive test of coherence, and e.g. for Bose–Einstein condensates they increase by a factor of $6 = 3!$ if the temperature is raised to be much larger than the condensation temperature [16, 17]. In spite of the LL model being integrable, analytical calculation of its correlation functions is notoriously hard [18]. Two-body local correlations in equilibrium can be simply obtained using the Hellmann–Feynman theorem and knowledge of exact thermodynamics and show excellent agreement with experiments [19], while three-body local correlations were analytically calculated only at zero temperature in a remarkable tour de force [20], as well as numerically in Ref. [21].

In this Letter, we exactly evaluate three-body local correlations in the thermodynamic limit for a large class of excited states which can be described by density matrices diagonal in the energy representation. In particular, we apply our method at finite temperatures and for highly excited states similar to the ones created in experiments [3], and we take into account external harmonic confinement within local density approximation (LDA). We note that local two-body correlations in 1D play the role of the "contact" introduced by S. Tan [22, 23]. Similarly, three-body local correlations correspond to a three-body contact which is being actively explored [24]. Our exact results provide an important benchmark for such theories, as well as for numerical methods for simulating field theories in 1D [25].

The model.— The LL model describes a system of identical bosons in 1D interacting via a Dirac-delta potential. The Hamiltonian in second quantized formulation is given by

$$H = \int_0^L \mathrm{d}x \, \frac{\hbar^2}{2m} \left(\partial_x \psi^\dagger \partial_x \psi + c\, \psi^\dagger \psi^\dagger \psi \psi \right) , \qquad (1)$$

where $c > 0$ in the repulsive regime we wish to study, and m is the atomic mass. The dimensionless coupling constant is given by $\gamma = c/n$, where $n = N/L$ is the density of the gas. We will express temperature T in dimensionless units $\tau = T/T_\mathrm{D}$, where $T_\mathrm{D} = \hbar^2 n^2/(2mk_\mathrm{B})$ is the quantum degeneracy temperature.

The exact thermodynamics of the model can be obtained via Bethe Ansatz [4, 18]. Each eigenstate of the system with N particles on a ring of circumference L is characterized by a distinct set of quantum numbers $\{I_j\}$ that are integers (half-integers) for N odd (even). The wave function can be expressed in terms of N quasimomenta $\{p_j\}$ that satisfy a set of algebraic equations

$$Lp_j + \sum_{k=1}^{N} \theta(p_j - p_k) = 2\pi I_j \, , \qquad (2)$$

where $\theta(p) = 2\arctan(p/c)$. The wave function is identically zero if any two of the $\{I_j\}$ coincide, which is reminiscent of the Pauli principle for fermions. In the Tonks–Girardeau (TG) limit $c \to \infty$, $\{I_j\}$ correspond to the quantum numbers of occupied single-particle states of free fermions.

In the thermodynamic limit, if one wants to consider a mixed state diagonal in the energy basis, this is achieved by introducing a filling fraction $0 < f_I < 1$ in the space of quantum numbers, which plays a role similar to the occupation number of free fermions. All results of the present letter are valid for f_I which have a finite thermodynamic limit at constant I/N; the limiting function should be piecewise continuous and normalized. For calculations, it is more convenient to define a function $f(p)$ in terms of the quasimomenta: denoting by $\rho(p)$ the maximal allowed density of quasimomenta in the vicinity of p, the quasimomenta density for a mixed state is given by $f(p)\rho(p)$.

Since all quasimomenta are coupled to each other by Eq. (2), the density $\rho(p)$ is not independent of $f(p)$: it satisfies the integral equation and normalization condition

$$\rho(p) = \frac{1}{2\pi} + \int \frac{\mathrm{d}p'}{2\pi}\, f(p')\, \varphi(p-p')\, \rho(p')\,, \tag{3a}$$

$$n = \int \mathrm{d}p\, f(p)\, \rho(p)\,, \tag{3b}$$

with the kernel $\varphi(p) = 2c/(p^2+c^2)$. In thermal equilibrium, $f(p)$ has to satisfy a set of nonlinear integral equations [26, 27], but our results will be valid for more general $f(p)$.

Local correlations.— The local k-body correlation functions are defined as

$$g_k(\gamma,\tau) = \frac{\left\langle \psi^{\dagger k}(x)\psi^k(x)\right\rangle}{n^k}\,. \tag{4}$$

The first two of them are relatively easy to calculate: $g_1 = 1$, while g_2 in equilibrium is given by the Hellmann–Feynman theorem [19, 27].

Here we report the results for $k = 2$ and $k = 3$ for general $f(p)$, which can be written in terms of functions $h_m(p)$ ($m = 1, 2$) satisfying the following integral equations:

$$h_m(p) = p^m + \int \frac{\mathrm{d}p'}{2\pi}\, f(p')\varphi(p-p')h_m(p')\,. \tag{5}$$

In the case of g_2 the final formula is

$$g_2(\gamma,\tau) = \frac{2\gamma^2}{c^3}\int \frac{\mathrm{d}p}{2\pi}\, f(p)\left[2\pi\rho(p)\, p^2 - h_1(p)\, p\right]\,, \tag{6}$$

which agrees with the result of the Hellmann–Feynman theorem for thermal equilibrium [27], but is more general. Similarly, for $k = 3$ the final expression is given by

$$g_3(\gamma,\tau) = \frac{\gamma^3}{c^5}\int \frac{\mathrm{d}p}{2\pi}\, f(p)\Big[(p^4 + c^2p^2)2\pi\rho(p) - \left(4p^2 + (1+2/\gamma)c^2\right) p\, h_1(p) + 3p^2h_2(p)\Big] + \frac{2\gamma^3}{c^4}\left(\int \mathrm{d}p\, f(p)\rho(p)p\right)^2. \tag{7}$$

In the case when $f(p)$ is even, in equilibrium for example, the last term in Eq. (7) is zero because the integrand is odd in p. Both Eq. (6) and Eq. (7) are Galilean invariant expressions [27]. In the following we will first consider an equilibrium case and then will proceed to highly excited states.

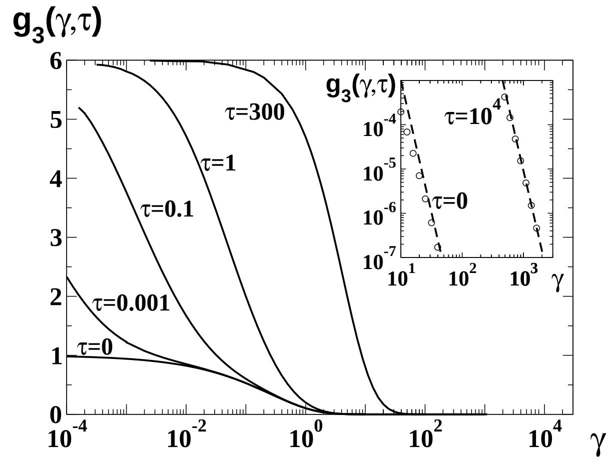

FIG. 1: Local three-body correlator $g_3(\gamma,\tau)$ as a function of dimensionless coupling $\gamma = c/n$ for the uniform system at fixed dimensionless temperature $\tau = T/T_{\mathrm{D}}$, where $T_{\mathrm{D}} = \hbar^2 n^2/(2mk_{\mathrm{B}})$ is the quantum degeneracy temperature. The inset shows the large γ asymptotic behavior on a log-log scale.

In Fig. 1 we plot the result in thermal equilibrium for fixed τ as a function of the coupling γ. In particular, at zero temperature our result agrees with that of Ref. [20], up to the precision of the numerical evaluation of both expressions, $\approx 10^{-3}$. The behavior of g_3 is qualitatively similar to that of g_2 analyzed in Ref. [19] and it distinguishes three different physical regimes: (a) $\gamma \gtrsim \max(1, \sqrt{\tau})$, strong coupling (TG) regime, $g_3 \ll 1$; (b) $\tau^2 \lesssim \gamma \lesssim 1$, quasicondensate regime, $g_3 \approx 1$; (c) $\gamma \lesssim \min(\tau^2, \sqrt{\tau})$, decoherent regime, $g_3 \approx 6$. In the inset of Fig. 1 the large γ asymptotics are plotted together with the analytic forms of Ref. [19]: $g_3 \sim 16\pi^6/(15\gamma^6)$ for $\tau = 0$ and $g_3 \sim 9\tau^3/\gamma^6$ for $\gamma^2 \gg \tau \gg 1$.

Harmonic traps.— Next we turn to the experimentally more realistic case of atoms confined in a waveguide with a harmonic longitudinal potential. The 1D regime is reached if $\mu, k_{\mathrm{B}}T \ll \hbar\omega_\perp$, where μ is the chemical potential and $\omega_\perp$ is the transverse oscillator frequency [28]. If the density profile in the trap varies smoothly, the correlations can be calculated by combining our exact results with LDA [29]. The relevant properties of the gas can be characterized by the LL coupling γ_0 and the temperature parameter τ_0 at the center of the trap. In Fig. 2 we plot the three-body correlator $g_3(\gamma_0,\tau_0)$ at the trap center and the normalized average, $\overline{g_3}(\gamma_0,\tau_0) = \int \mathrm{d}x \left\langle \psi^{\dagger 3}(x)\psi^3(x)\right\rangle / \left(\int \mathrm{d}x\, n^3(x)\right)$, against the dimensionless temperature τ_0 for different fixed values of γ_0. Similarly to the results of Ref. [29] for the case of g_2, we find that unless the coupling γ_0 is very small, $g_3(\gamma_0,\tau_0) \approx \overline{g_3}(\gamma_0,\tau_0)$ at any temperature.

The curves in Fig. 2 are related to the observed change in time of the particle loss rate in Ref. [12]. With increasing temperature, the three-body correlations grow according to our result, which leads to a higher proba-

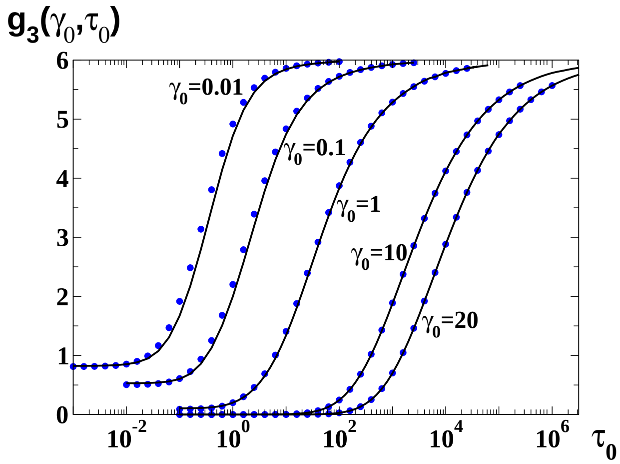

FIG. 2: Local three-body correlators $\overline{g_3}(\gamma_0, \tau_0)$ averaged over the trap (dots) and $g_3(\gamma_0, \tau_0)$ in the center (solid lines), as a function of the dimensionless temperature τ_0 for fixed dimensionless coupling γ_0 in the center of the trap. At high temperature, g_3 approaches the value $6 = 3!$, reflecting Bose statistics.

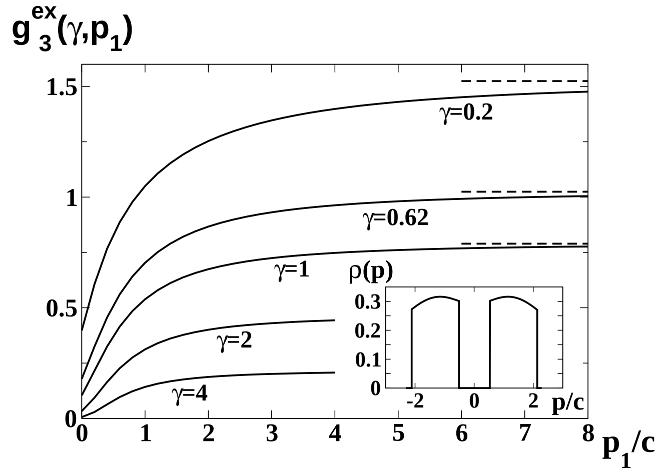

FIG. 3: Local three-body correlator $g_3^{\rm ex}(\gamma, p_1)$ as a function of p_1 for different values of γ. The excited state is characterized by the inner "Fermi quasimomentum" p_1. The horizontal dashed lines correspond to $g_3^{ex}(\gamma, \infty) = [g_3(2\gamma) + 9g_2(2\gamma)]/4$. The inset illustrates a typical quasimomentum density for $\gamma = 1$, $p_1 = 0.5c$.

bility of inelastic three-particle processes which in turn raises further the temperature of the gas. This positive feedback causes a non-trivial dependence of the particle loss on time, and a detailed analysis of heating mechanisms is needed to describe the time dependences of the loss rates.

Three-body correlations for highly excited states.— Since Eq. (8) is valid for general distributions $f(p)$ [30], we can use our results (6),(7) in situations where the system is neither in equilibrium nor is in its ground state. We will illustrate this by considering a state which is motivated by the experiment of Kinoshita *et al.* [3], where each atom was put in a momentum superposition state, after which the two clouds performed many oscillations without observable thermalization. The state created in the experiment is not an eigenstate, and the harmonic trap might play an important role. However, let us consider here a simple "caricature" eigenstate which might capture the behavior of g_3, and hence the role of integrability breaking, in these experiments. This state is characterized by an $f(p)$ consisting of two disjoint rectangular "Fermi steps" symmetric with respect to $p = 0$ at zero temperature: $f(p) = \theta(p^2 - p_1^2) - \theta(p^2 - p_2^2)$ with $p_2 > p_1 > 0$ (see inset of Fig. 3). We are interested in the dependence of $g_3^{\rm ex}(\gamma, p_1)$ on the "inner Fermi quasimomentum" p_1. If p_1 is fixed then the "outer Fermi quasimomentum", p_2, is determined from the normalization (3b). The momentum kick in Ref. [3] corresponds to p_1/c of order one. In Fig. 3 we plot $g_3^{\rm ex}(\gamma, p_1)$ for fixed values of γ as a function of p_1. We find that the correlations grow with the momentum of the kick and they can become greater than 1. For large p_1, the quasimomentum distributions of left and right goers become approximately independent of each other. However, to obtain the correct limit as $p_1 \to \infty$ one needs to take into account deviations of $\theta(2p_1/c \gg 1)$ in Eq. (3) from π. This results in $g_3^{ex}(\gamma, \infty) = [g_3(2\gamma) + 9g_2(2\gamma)]/4$; in particular, $g_3^{ex}(\gamma \to 0, \infty) = 5/2$. Similarly, $g_2^{ex}(\gamma, \infty) = [g_2(2\gamma) + 2]/2$, and $g_2^{ex}(\gamma \to 0, \infty) = 3/2$ [27].

Derivation of Eqs. (6) *and* (7).— In Ref. [31] a novel method was proposed to calculate the g_k correlators based on the observation that the LL model can be viewed as the combined non-relativistic, weak coupling limit of the sinh–Gordon model. The resulting formula reads as [30, 31]

$$g_k = \sum_{s=k}^{\infty} \frac{1}{s!} \int \prod_{j=1}^{s} \frac{\mathrm{d}p_j}{2\pi}\, f(p_j)\, \gamma^k F_s^{(k)}(p_1, \ldots, p_s)\,, \qquad (8)$$

where the form factors $F_s^{(k)}(p_1, \ldots, p_s)$ are the infinite volume s-particle diagonal matrix elements of the operator $\psi^{\dagger k}\psi^k$, which can be obtained from known sinh–Gordon form factors [32–34]. These series were investigated previously by truncating them after the first few terms [31]. Here we resum these series to all orders obtaining closed analytical expressions for the local correlations.

It has been proven in Ref. [30] that

$$F_s^{(1)} = \frac{1}{c} \sum_P \varphi(p_{12})\varphi(p_{23}) \ldots \varphi(p_{s-1,s})\,, \qquad (9a)$$

$$F_s^{(2)} = \frac{1}{c^3} \sum_P \varphi(p_{12})\varphi(p_{23}) \ldots \varphi(p_{s-1,s})\; p_{1,s}^2\,, \qquad (9b)$$

and based on evaluations performed in Mathematica for the first few $F_s^{(3)}$ we conjecture

$$F_s^{(3)} = \frac{1}{c^5}\sum_P \varphi(p_{12})\varphi(p_{23})\dots\varphi(p_{s-1,s})\times \frac{1}{2}p_{1,s}\left[p_{1,s}^3 - (p_{12}^3 + p_{23}^3 \dots + p_{s-1,s}^3)\right], \quad (9c)$$

where $p_{ij} = p_i - p_j$ and $\sum_P$ denotes a sum over all permutations of $\{p_j\}$. Below we will illustrate how series (8) can be analytically resummed for g_2, and details of similar calculations for g_3 are presented in EPAPS [27].

We will use abbreviations $\tilde{\mathrm{d}}p = \mathrm{d}p/(2\pi)f(p)$ and $\varphi_{ij} = \varphi(p_{ij})$. Using the symmetries of the integrand in Eq. (8), we have for $c^3 g_2(\gamma,\tau)/(2\gamma^2)$

$$\frac{1}{2}\sum_{s=2}^{\infty}\int\tilde{\mathrm{d}}p_1\dots\int\tilde{\mathrm{d}}p_s\,\varphi_{12}\dots\varphi_{s-1,s}(p_1-p_s)^2 = \int\tilde{\mathrm{d}}p_1\,p_1^2\left[\int\tilde{\mathrm{d}}p_2\,\varphi_{12}+\int\tilde{\mathrm{d}}p_2\int\tilde{\mathrm{d}}p_3\,\varphi_{12}\varphi_{23}+\dots\right] - \int\tilde{\mathrm{d}}p_1 p_1\left[\int\tilde{\mathrm{d}}p_1\,\varphi_{12}\,p_2+\int\tilde{\mathrm{d}}p_2\int\tilde{\mathrm{d}}p_3\,\varphi_{12}\varphi_{23}\,p_3+\dots\right] = \int\tilde{\mathrm{d}}p_1\,p_1^2\left[2\pi\rho(p_1)-1\right] - \int\tilde{\mathrm{d}}p_1\,p_1\left[h_1(p_1)-p_1\right], \quad (10)$$

where the terms in the first square bracket coincide with the iterative solution of the integral equation (3a). Similarly, comparison of the terms in the second bracket with the iterative solution of Eq. (5) leads to $h_1(p_1)-p_1$. Now the second terms in the parentheses cancel each other and we obtain Eq. (6).

In summary, we derived an *exact* formula for the local three-body correlation in a paradigmatic system, the 1D Lieb–Liniger Bose gas. Given that exact expression for correlation functions are scarce even in integrable models, we emphasize the analytic nature of our result. Our non-perturbative formula is valid at any temperature for arbitrary value of the coupling γ, and for a large class of excited states of the system. The result can open the window to an analytic treatment of integrability breaking perturbations and thermalization in nearly integrable systems.

We acknowledge funding from The Welch Foundation, grant C-1739, from the Sloan Foundation and from the NSF Career Award DMR-1049082.

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