

## Temperature-driven crossover in the Lieb-Liniger model

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The large-distance behavior of the density-density correlation function in the Lieb-Liniger model at finite temperature is investigated by means of the recently derived nonlinear integral equations characterizing the correlation lengths. We present extensive numerical results covering all the physical regimes from weak to strong interaction and all temperatures. We find that the leading term of the asymptotic expansion becomes oscillatory at a critical temperature which decreases with the strength of the interaction. As we approach the Tonks-Girardeau limit the asymptotic behavior becomes more complex with a double crossover of the largest and next-largest correlation lengths. The crossovers exist only for intermediate couplings and vanish for  $\gamma = 0$  and  $\infty$ .

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### I. INTRODUCTION

Correlation functions play a fundamental role in our understanding of low-dimensional strongly correlated systems. As a result of the remarkable progress in the field of ultracold gases atomic correlations can now be accessed through a variety of techniques (see [1,2] and references therein) highlighting the necessity of high-quality experimental phenomenology. In one dimension the class of exactly solvable models represents a particular type of strongly correlated systems for which the powerful techniques associated with the Bethe ansatz allows us to go beyond the mean-field Bogoliubov approximation. The paradigmatic example is the Lieb-Liniger (LL) model [3], which is experimentally realizable [4–9] and has been the subject of various theoretical investigations for more than fifty years [10].

In this article we investigate the large distance of the static density-density correlation function at finite temperature in the LL model. Even though the model is integrable the complicated form of the wave functions means that the analytical derivation or numerical analysis of the correlators is still an extremely challenging task. While important progress has been made in recent years [11–25] a complete characterization of the temperature-dependent correlators is still lacking. At zero temperature there are two distinct phases in the LL model: for chemical potential  $\mu < 0$  the particle density is zero, whereas  $\mu > 0$  is characterized by a finite density and realizes a Tomonaga Luttinger liquid (TLL) with algebraically decaying correlation functions that are described by conformal field theory (CFT). At low but finite temperature the TLL phase is still present with exponentially decaying correlation functions and correlation lengths determined by CFT. The phase  $\mu < 0$  may be denoted “gas phase” as at low temperatures it has a nonzero but small density of particles and the ideal gas law holds. The main interest of this article lies on the finite density phase at finite especially intermediate and high temperatures, where the correlation functions are not described by TLL-CFT and which has not been thoroughly investigated until now. Our analysis is based on the use of the so-called quantum transfer matrix  $T_q$ , which describes the evolution of correlators in the spatial direction. The eigenvalue equations [24,25] enjoy a symmetry property, which is equivalent to saying that  $T_q$  is a normal operator, i.e.,  $[T_q^+, T_q] = 0$ , from which follows that all eigenvalues are real or occur in complex conjugate pairs.

We calculated the leading and next-leading eigenvalues of  $T_q$  for various densities and temperatures and found results which cannot be captured by the TLL-CFT [26] approach or other approximation or numerical methods. There is a complex crossover scenario with a counterintuitive change of symmetry and dimensionality of the involved states. In the spectral decomposition of the density-density correlator the leading state is symmetric at low temperatures, but has broken symmetry at *higher* temperatures, where it is two-dimensional with complex conjugate eigenvalues.

### II. THE MODEL

The Lieb-Liniger model describes one-dimensional bosons interacting via a  $\delta$ -function potential. The second-quantized Hamiltonian is

$$H = \int dx \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x), \quad (1)$$

where  $c > 0$  is the coupling constant and we consider  $\hbar = 2m = k_B = 1$ , with  $m$  the mass of the particles. In Eq. (1)  $\Psi^\dagger(x)$  and  $\Psi(x)$  are Bose fields satisfying the canonical commutation relations  $[\Psi(x), \Psi^\dagger(x')] = \delta(x - x')$ ,  $[\Psi(x), \Psi(x')] = [\Psi^\dagger(x), \Psi^\dagger(x')] = 0$ . The LL model is exactly solvable [3,10,27] and, at finite temperature, is completely characterized by two parameters: the coupling strength  $\gamma = c/n$  with  $n$  the linear density and the temperature  $T$ .

The density-density correlation function is defined by

$$\langle \rho(x) \rho(0) \rangle_T = \frac{\text{Tr}[e^{-H/T} \rho(x) \rho(0)]}{\text{Tr} e^{-H/T}},$$

where  $\rho(x) = \Psi^\dagger(x) \Psi(x)$ . Due to translational invariance and invariance under spatial reflection,  $\langle \rho(x) \rho(0) \rangle_T = \langle \rho(0) \rho(x) \rangle_T$ , which means that it is sufficient to consider  $x > 0$ . The density-density correlator is closely related to the (un-normalized) second-order correlation function  $g_T^2(x) = \langle : \rho(x) \rho(0) : \rangle_T$  via  $\langle \rho(x) \rho(0) \rangle_T = g_T^2(x) + \delta(x)n$ , where  $:$  denotes normal ordering. The large-distance asymptotic expansion of  $\langle \rho(x) \rho(0) \rangle_T$  valid for any value of the coupling strength and temperature has been derived only recently [24,25]:

$$\langle \rho(x) \rho(0) \rangle_T = n^2 + \sum_i A_i e^{-\frac{x}{\xi_{|w_i|}}}, \quad x \rightarrow \infty, \quad (2)$$

with the correlation lengths given by

$$\frac{1}{\xi[u_i]} = \frac{1}{2\pi} \int_{\mathbb{R}} \ln \left( \frac{1 + e^{-\varepsilon(k)/T}}{1 + e^{-u_i(k)/T}} \right) dk - i \sum_{j=1}^r k_j^+ + i \sum_{j=1}^r k_j^-, \quad (3)$$

and  $\varepsilon(k)$  the excitation energy satisfying the Yang-Yang equation:

$$\varepsilon(k) = k^2 - \mu - \frac{T}{2\pi} \int_{\mathbb{R}} K(k - k') \ln \left( 1 + e^{-\varepsilon(k')/T} \right) dk'. \quad (4)$$

In Eq. (2),  $u_i(k)$  is a set of functions satisfying the nonlinear integral equations (NLIEs):

$$u_i(k) = k^2 - \mu + iT \sum_{j=1}^r \theta(k - k_j^+) - iT \sum_{j=1}^r \theta(k - k_j^-) - \frac{T}{2\pi} \int_{\mathbb{R}} K(k - k') \ln \left( 1 + e^{-u_i(k')/T} \right) dk', \quad (5)$$

where  $\theta(k) = i \ln \left( \frac{ic+k}{ic-k} \right)$ ,  $\lim_{k \rightarrow \pm\infty} \theta(k) = \pm\pi$ , and  $K(k - k') = \frac{d}{dk} \theta(k - k') = 2c / [(k - k')^2 + c^2]$ . Equation (5) depends on  $2r$  parameters,  $\{k_j^+\}_{j=1}^r$ ,  $\{k_j^-\}_{j=1}^r$ , located in the upper (lower) half of the complex plane, which are subject to the constraint

$$1 + e^{-u_i(k_j^\pm)/T} = 0. \quad (6)$$

For a given  $r$  there are more than one set of  $\{k_j^\pm\}_{j=1}^r$  that satisfy the previous constraint and each one defines a distinct  $u$  function. The subscript  $i$  labels all these functions for all  $r = 1, 2, \dots, \infty$ .

It should be noted that the correlation lengths  $\xi[u_i]$  can be complex, but then appear in conjugate pairs. In this case the two appropriate terms in the expansion (2) oscillate and may be combined into  $\text{Re} [A_i e^{-x/\xi[u_i]}]$ . We should also make an observation regarding the prefactors  $A_i$  appearing in Eq. (2). While analytical expressions were derived in [24] they are too cumbersome to allow for an efficient numerical investigation. For this reason in the following we are going to consider these prefactors as unknowns. Equation (2) can be understood as the generalization for all nonzero temperatures of the TLL-CFT asymptotic expansion [26] (valid for low  $T$  and  $x \gg n^{-1}$ ):

$$\langle \rho(x)\rho(0) \rangle_T - n^2 = - \frac{(TZ/v_F)^2}{2 \sinh^2(\pi T x/v_F)} + \sum_{l \in \mathbb{Z}^*} A_l e^{2ixlk_F} \left( \frac{\pi T/v_F}{\sinh(\pi T x/v_F)} \right)^{2l^2 Z^2}. \quad (7)$$

In Eq. (7),  $v_F$  and  $k_F$  are the Fermi velocity and wave vector,  $A_l$  are unknown prefactors, and  $Z = Z(q)$  with the dressed charge  $Z(k)$  satisfying the integral equation  $Z(k) - \frac{1}{2\pi} \int_{-q}^q K(k - k') Z(k') dk' = 1$ . In [24,25] it was shown that in the low-temperature limit the correlation lengths obtained using Eq. (3) reproduce the TLL-CFT predictions in Eq. (7). We should stress that even though the TLL-CFT expansion (7) is valid for  $0 < \gamma < \infty$  it does not show any crossovers in  $T$

as the correlation lengths are reciprocal to the temperature in the conformal regime.

### III. TONKS-GIRARDEAU LIMIT

We can perform an additional check of Eq. (3) in the limit of impenetrable particles. This will also allow us to understand the distribution in the complex plane of the discrete parameters that characterize the leading correlation lengths. In the Tonks-Girardeau limit the second-order correlation function can be calculated analytically [10] with the result

$$\langle : \rho(x)\rho(0) : \rangle_T = n^2 - \frac{1}{4\pi^2} \left( \int_{-\infty}^{+\infty} e^{ikx} \vartheta(k) dk \right)^2, \quad (8)$$

where  $\vartheta(k) = 1/(1 + e^{(k^2 - \mu)/T})$  is the Fermi function and  $n = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \vartheta(k) dk$ . As we will show below, even though Eq. (8) is valid for all temperatures, in the limit of impenetrable particles no crossover is present.

The large-distance behavior of Eq. (8) (note that the density-density correlation function has the same large-distance asymptotic behavior as  $\langle : \rho(x)\rho(0) : \rangle_T$  because they differ only by a delta function, which is zero for large  $x$ ) can be derived deforming the contour of integration in the upper-half plane (for  $x > 0$ ) with the leading terms being the residues closest to the real axis (see the Appendix). The poles of the integrand are given by the solutions of the equation  $k^2 - \mu = i\pi(2s + 1)T$ ,  $s = 0, \pm 1, \pm 2, \dots, \pm \infty$ . Explicitly, the solutions closest to the real axis ( $s = 0$ ) are

$$k_r^\pm = [(\alpha + \mu)^{1/2} \pm i(\alpha - \mu)^{1/2}]/\sqrt{2}, \quad (9)$$

$$k_l^\pm = [-\alpha - \mu)^{1/2} \pm i(\alpha - \mu)^{1/2}]/\sqrt{2},$$

with  $\alpha = \sqrt{\mu^2 + \pi^2 T^2}$  implying the asymptotic expansion:

$$\langle \rho(x)\rho(0) \rangle_T = n^2 + \frac{T^2}{2k_l^+ k_r^+} e^{i(k_l^+ + k_r^+)x} + \frac{T^2}{4(k_l^+)^2} e^{2ik_l^+ x} + \frac{T^2}{4(k_r^+)^2} e^{2ik_r^+ x} + o(e^{2i\text{Re}(k_j^+)x}). \quad (10)$$

We note that the leading term of the expansion is oscillatory at all temperatures and no crossover is present. We can show that the correlation lengths appearing in Eq. (10) can also be derived using Eq. (3). For this, we need to notice that in the Tonks-Girardeau limit Eq. (5) reduces to  $u_i(k) = k^2 - \mu = i\pi(2s + 1)T$ ,  $s = 0, \pm 1, \pm 2, \dots, \pm \infty$ , and the expression for the correlation lengths takes the simple form  $1/\xi[u_i] = -i \sum_{j=1}^r k_j^+ + i \sum_{j=1}^r k_j^-$ . Then, the leading correlation lengths ( $r = 1$ ) are  $1/\xi_0 = -ik_l^+ + ik_l^- = -ik_r^+ + ik_r^- = -i(k_l^+ + k_r^+)$  and  $1/\xi_{-1} = -ik_l^+ + ik_r^- = -2ik_l^+$ ;  $1/\xi_1 = -ik_r^+ + ik_l^- = -2ik_r^+$ , proving our previous assertion. In the low- $T$  limit the expansion (10) reduces to the  $l = 0, \pm 1$  terms of the TLL-CFT expression in Eq. (7). This can be easily seen using  $k_r^+ = \sqrt{\mu} + i \frac{\pi T}{2\sqrt{\mu}} + O(T^2)$ ,  $k_l^+ = -\sqrt{\mu} + i \frac{\pi T}{2\sqrt{\mu}} + O(T^2)$ , and the fact that for the impenetrable gas  $Z = 1, k_F = \sqrt{\mu}, v_F = 2\sqrt{\mu}$ .

#### IV. NUMERICAL RESULTS

From the numerical point of view the relevant NLIEs and the subsidiary equations for the discrete parameters are solved using an iterative algorithm which is quickly convergent. The efficiency of the algorithm is enhanced by the calculation of convolution type integrals in “momentum space,” where they are reduced to products of Fourier transforms of the involved functions. For all the functions investigated  $\text{Re}(1/\xi[u_i]) \geq 0$  (a nonzero imaginary part of the correlation length means that the corresponding term in the expansion is oscillatory).

The leading correlation length, denoted by  $\xi_0$ , is obtained considering  $r = 1$  in Eq. (5) and  $k_1^\pm$  the pair of parameters which are closest to the real axis with  $k_1^+$  located in the first quadrant of the complex plane ( $\text{Re} k_1^+ \geq 0, \text{Im} k_1^+ \geq 0$ ) and  $k_1^-$  located in the fourth quadrant ( $\text{Re} k_1^- \geq 0, \text{Im} k_1^- \leq 0$ ). Similar to the impenetrable case there is another correlation length with the same magnitude which can be obtained considering  $k_1^+$  located in the second quadrant of the complex plane ( $\text{Re} k_1^+ \leq 0, \text{Im} k_1^+ \geq 0$ ) and  $k_1^-$  located in the third quadrant ( $\text{Re} k_1^- \leq 0, \text{Im} k_1^- \leq 0$ ). In Fig. 1 we plot  $1/\xi_0$  as a function of temperature for several values of  $\gamma$ . At low  $T$ ,  $k_1^+$  and  $k_1^-$  are complex conjugate ( $k_1^+ = \overline{k_1^-}$ ), which also means that  $\xi_0$  is real. In this regime  $1/\xi_0$  reproduces the exponential decay predicted by the first term on the right-hand side of the TLL-CFT expansion (7). However, there is a critical temperature, which depends on  $\gamma$ , at which the discrete parameters are no longer complex conjugates and  $\text{Im}[1/\xi_0]$  is no longer zero. Above this temperature, which we will denote  $T_o(\gamma)$ , the leading term of the asymptotic expansion becomes oscillatory with a wave vector  $2k_{nF}$ , which is incommensurate with  $2k_F$ . In addition, at  $T_o$  the derivative of the correlation length is discontinuous. From Fig. 1 we can infer that  $T_o(0) = \infty$  and  $T_o(\infty) = 0$  with the best fit given by  $T_o(\gamma) \sim \gamma^{-0.55}$ . Regarding this last statement it is instructive to look at the asymptotic expansion [Eq. (10)] of  $\langle \rho(x)\rho(0) \rangle_T$  in the  $\gamma = \infty$  limit, from which it is easy to see that in this case

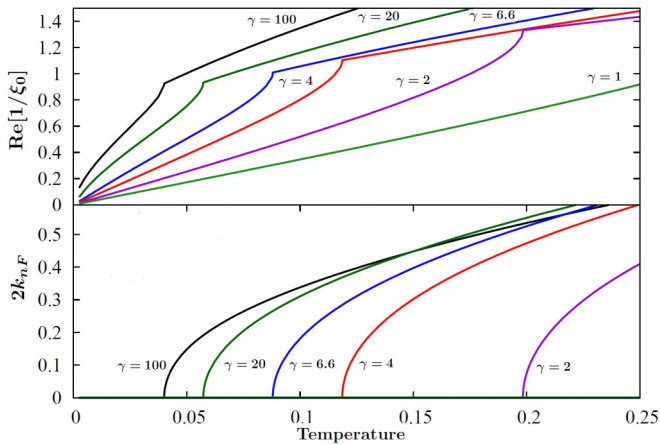


FIG. 1. (Color online) Upper panel:  $\text{Re}[1/\xi_0]$  with  $\xi_0$  the leading correlation length as a function of temperature for various values of  $\gamma$ . Lower panel:  $2k_{nF} = \text{Im}[1/\xi_0]$  for the same parameters. The critical temperature  $T_o(\gamma)$  is the value for which  $2k_{nF}$  becomes nonzero. Note the kinks of  $\text{Re}[1/\xi_0]$  at  $T_o$ . (All quantities are in units of  $1/l_0$  and  $T_0$  [28].)

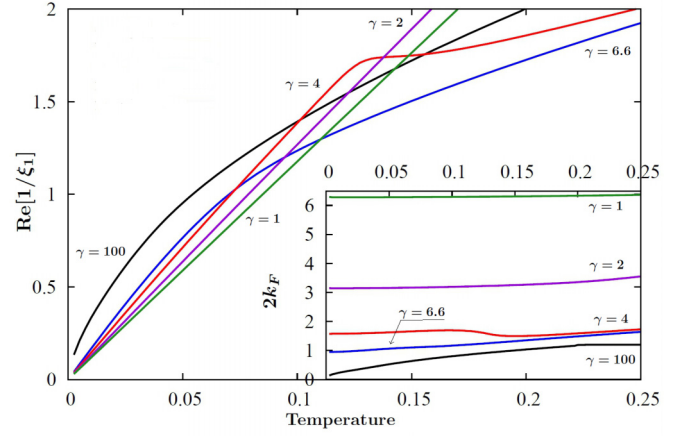


FIG. 2. (Color online)  $\text{Re}[1/\xi_1]$  with  $\xi_1$  the next-leading correlation length as a function of temperature for various values of  $\gamma$ . Inset:  $2k_F = \text{Im}[1/\xi_1]$  for the same parameters. (All quantities are in units of  $1/l_0$  and  $T_0$ .)

the leading term of the correlator is oscillatory at all nonzero temperatures. We would like to emphasize the peculiar nature of this oscillatory crossover, which contrasts with the more common case in which the next leading correlation length becomes dominant (see below). In the case at hand  $\xi_0$  still remains dominant but acquires an imaginary part which gives incommensurate oscillations.

The next-leading correlation lengths are obtained considering  $k_1^+$  in the second quadrant and  $k_1^-$  in the fourth quadrant (denoted by  $\xi_1$ ) or  $k_1^+$  in the first quadrant and  $k_1^-$  in the third quadrant (denoted by  $\xi_{-1}$ ). At low  $T$  these correlation lengths reproduce the asymptotic behavior of the  $l = \pm 1$  terms in the TLL-CFT expansion (7). In Fig. 2 we show graphs of  $1/\xi_1$  for some relevant values of  $\gamma$ . We notice that the region of validity for the TLL-CFT predictions (linear dependence on temperature of the correlation lengths and constancy of the wave vector) decreases with  $\gamma$ . Also we can clearly see that, for  $\gamma = 4$ ,  $\text{Re}[1/\xi_1]$  develops a “shoulder” in the region of temperatures for which the conformal predictions break down. However, it should be stressed that the derivative remains continuous unlike the case of the leading correlation length.

Plotting  $1/\xi_0$  and  $1/\xi_1$  in the same graph as in Fig. 3 (see also Fig. 4) reveals an extremely interesting phenomenon. For weak interactions we have  $\text{Re}[1/\xi_0] < \text{Re}[1/\xi_1]$  for all temperatures, but for stronger interactions a complex crossover scenario emerges. We find that for large  $\gamma$  we can distinguish three distinct intervals of temperature for which the asymptotic behavior of  $\langle \rho(x)\rho(0) \rangle_T$  is different. For  $T \in (0, T_{lc}(\gamma))$ , where  $T_{lc}(\gamma)$  is the lower crossover temperature, the leading correlation length is  $\xi_0$ , which is real for all temperatures in this interval.  $\xi_1$  becomes dominant for the  $T \in (T_{lc}(\gamma), T_{hc}(\gamma))$  interval, in which also lies  $T_o$ , the temperature for which  $\xi_0$  acquires a nonzero imaginary part. Here  $\langle \rho(x)\rho(0) \rangle_T$  is oscillatory and exponentially decreasing with leading correlation length  $\xi_1$ . Finally, for  $T > T_{hc}(\gamma)$  we have another crossover with  $\xi_0$  (for which  $\text{Im}[1/\xi_0] \neq 0$ ) characterizing the leading term of the expansion. It should be emphasized that the description of this crossover scenario is out of the reach of the TLL-CFT approach or other approximation methods.

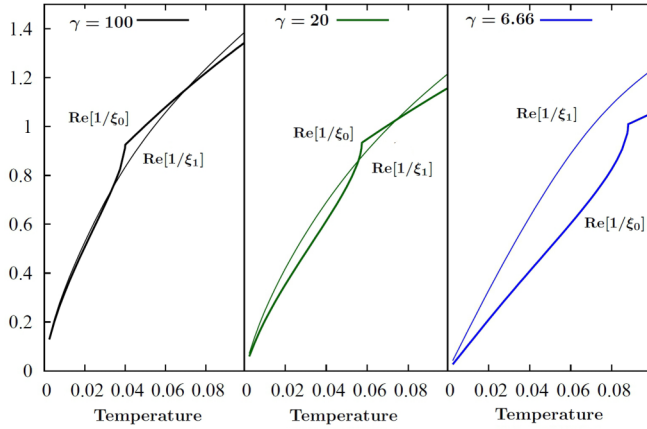


FIG. 3. (Color online)  $\text{Re}[1/\xi_0]$  (thick line) and  $\text{Re}[1/\xi_1]$  (thin line) as functions of temperature for various values of  $\gamma$ . For  $\gamma = 20$  and 100 a complex crossover scenario can be seen. (All quantities are in units of  $1/l_0$  and  $T_0$ .)

## V. CONCLUSIONS

We have performed an extensive numerical investigation of the large-distance asymptotic behavior of the second-order correlation function in the Lieb-Liniger model, discovering an extremely complex crossover phenomenon. Our findings can be summarized as follows. For all strengths of interactions the leading correlation length develops a nonzero imaginary part for temperatures larger than a critical temperature  $T_o(\gamma)$ , with  $T_o(0) = \infty$  and  $T_o(\infty) = 0$ . As we approach the Tonks-Girardeau limit we find two additional crossovers in which  $\xi_0$  and  $\xi_1$  successively change places as the dominant one. Interestingly, the crossover phenomena happen when leaving the low-temperature dense phase either by increasing the temperature or by decreasing the density. The incommensurate oscillations stay deep into the gaseous phase, which appears more complex than a true ideal gas. In the gaseous phase Eq. (5) simplifies as the contribution by the integral vanishes, but the function  $u_i$  is still more complicated than in the ideal gas case.

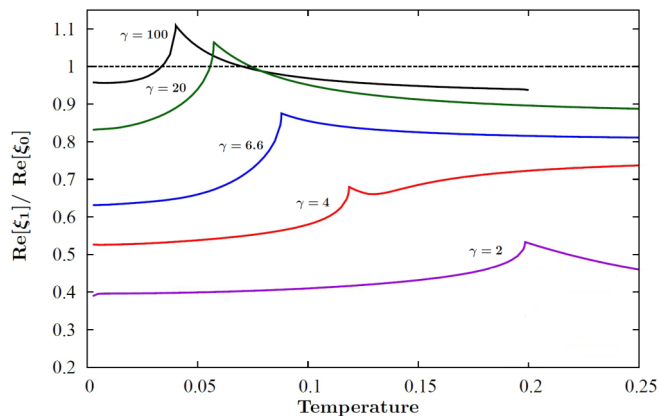


FIG. 4. (Color online)  $\text{Re}[\xi_1]/\text{Re}[\xi_0]$  as a function of temperature for various values of  $\gamma$ . For  $\gamma = 20$  and 100 in the region of temperatures where this ratio is greater than 1,  $\xi_1$  becomes the leading correlation length. (Temperature is in units of  $T_0$ .)

The crossover to oscillatory behavior of the leading correlation length is reminiscent of the one observed in the XXZ spin chain [29] in the ferromagnetic region ( $-1 < \Delta < 0$ ) and zero magnetization. This may somewhat be expected if we take into account that the Bose gas is a continuum limit of the XXZ spin chain at  $\Delta = -1$ , but this holds close to the fully polarized state. Naturally, the full temperature scenarios are different for the two systems. However, for cold gases the prospects of finding experimental signatures of the crossovers are much better than for crystals as a result of the continuous improvement in the creation and manipulation of such systems.

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## APPENDIX: ASYMPTOTIC BEHAVIOR IN THE TONKS-GIRARDEAU LIMIT

Deriving the large-distance asymptotic behavior of the density correlator in the Tonks-Girardeau limit,

$$\langle : \rho(x)\rho(0) : \rangle_T = n^2 - \frac{1}{4\pi^2} \left( \int_{-\infty}^{+\infty} e^{ikx} \vartheta(k) dk \right)^2, \quad (\text{A1})$$

reduces to the asymptotic investigation of the Fourier transform of the Fermi distribution:

$$\int_{-\infty}^{+\infty} \frac{e^{ikx}}{1 + e^{(k^2 - \mu)/T}} dk. \quad (\text{A2})$$

We introduce the notation  $f(k|x) = e^{ikx}/(1 + e^{(k^2 - \mu)/T})$ .  $f(k|x)$  is a meromorphic function on the complex plane with poles given by the solutions of the equation  $k^2 - \mu = i\pi(2s + 1)T$ ,  $s = 0, \pm 1, \pm 2, \dots, \pm \infty$ . The solutions of this equation are

$$k_r^\pm(s) = \{[\alpha(s) + \mu]^{1/2} \pm i[\alpha(s) - \mu]^{1/2}\}/\sqrt{2}, \quad (\text{A3})$$

$$k_l^\pm(s) = \{-[\alpha(s) + \mu]^{1/2} \pm i[\alpha(s) - \mu]^{1/2}\}/\sqrt{2},$$

with  $\alpha(s) = \sqrt{\mu^2 + (2s + 1)^2\pi^2 T^2}$ . For  $x > 0$  (it is sufficient to consider only this case because  $\langle \rho(x)\rho(0) \rangle_T = \langle \rho(0)\rho(x) \rangle_T$ ),  $f(k|x)$  vanishes at infinity in the upper half plane, which means that

$$\int_{-\infty}^{+\infty} f(k|x) dk = \int_{\mathcal{C}} f(k|x) dk,$$

with  $\mathcal{C}$  a complex contour which contains the real axis and a semicircle extending at infinity in the upper half plane. Using this identity and Cauchy's residue theorem we find

$$\int_{-\infty}^{+\infty} f(k|x) dk = 2\pi i \sum_{s=0}^{\infty} \text{Res}[f(k_l^+(s)|x) + f(k_r^+(s)|x)],$$

where we have used the fact that the poles in the upper half plane of the function  $f(k|x)$  are  $k_l^+(s)$  and  $k_r^+(s)$  with  $s = 0, 1, 2, \dots, \infty$  and residues  $\text{Res}f(k_{l,r}^+(s)|x) = -T e^{ik_{l,r}^+ x} / (2k_{l,r}^+)$ . Taking only the  $s = 0$  terms and squaring we obtain Eq. (10).

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