PHYSICAL REVIEW A **94**, 051606(R) (2016)

Few-body route to one-dimensional quantum liquids

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(Received 3 August 2016; revised manuscript received 12 September 2016; published 29 November 2016)

Gapless many-body quantum systems in one spatial dimension are universally described by the Luttinger liquid effective theory at low energies. Essentially, only two parameters enter the effective low-energy description, namely, the speed of sound and the Luttinger parameter. These are highly system dependent and their calculation requires accurate nonperturbative solutions of the many-body problem. Here we present a simple theoretical method that only uses collisional information to extract the low-energy properties of spinless one-dimensional systems. Our results are in remarkable agreement with available results for integrable models and from large-scale Monte Carlo simulations of one-dimensional helium and hydrogen isotopes. Moreover, we estimate theoretically the critical point for spinodal decomposition in one-dimensional ^{4}He and show that the exponent governing the divergence of the Luttinger parameter near the critical point is exactly $1/2$, in excellent agreement with Monte Carlo simulations.

DOI: 10.1103/PhysRevA.94.051606

I. INTRODUCTION

Interacting quantum systems in one spatial dimension, long ago considered toy models far away from the three-dimensional reality, now hold the status of physically relevant theories. Advances in the transversal confinement of trapped ultracold atomic gases [1,2], the realization of carbon nanotubes by rolling up sheets of graphene [3,4], or helium isotopes adsorbed in nanopores [5–7] make it possible to investigate many-body quantum physics in wire geometries with unprecedented level of control. Most one-dimensional systems, whether weakly or strongly interacting, are universally described by the Luttinger liquid effective field theory at low energies [8] and by its recently developed nonlinear counterpart at higher energies [9]. Essentially, many correlation functions, and the excitation spectrum, have universal behaviors and the nonuniversal parameters, i.e., the Luttinger parameter and speed of sound, are the only system-dependent quantities of interest. To extract these, however, one needs to either invoke perturbation theory, only valid for weak interactions, or numerically solve the many-body problem "exactly" using Monte Carlo [6,10–12] for continuous or density-matrix renormalization-group methods [13] for lattice models or quasianalytically for integrable models via the Bethe ansatz [9,14]. In this Rapid Communication, we develop a simple yet highly nonperturbative method that uses only two-body scattering information to extract the speed of sound and the Luttinger parameter of strongly interacting many-body quantum systems in one dimension. To show the reliability of our theory, we study all the stable isotopes of helium and spin-polarized hydrogen, and tritium, when tightly confined to one dimension, using realistic molecular potentials, which are strongly interacting and intractable with perturbative methods, and compare our results to the Monte Carlo data of Refs. [10–12]. Using similar methods, we also study the liquid phase of ^{4}He, which is not a Luttinger liquid.

The excitations of gapless one-dimensional many-body systems are characterized, at low energy, by the speed of sound v, corresponding to an excitation spectrum $\hbar\omega(q) = \hbar v q + O(q^2)$, with q the momentum of the excitation. For bosons, in the weak- and strong-coupling limits, corresponding to the quasicondensate and fermionized (or Tonks-Girardeau) regimes, respectively, Bogoliubov and many-body (fermionic) perturbation theory can be used to extract approximations to the speed of sound [14–16] in these limits. A weak-coupling approximation to the speed of sound can also be obtained by fitting the Tomonaga-Luttinger model's coupling constant to reproduce the correct reaction matrix of the original model in the fermionized situation [17]. Unfortunately, no simple and reliable nonperturbative approximation is currently available.

One-dimensional spin-polarized Fermi gases (or strongly coupled spinless Bose gases) owe much of their special phenomenology to the fact that the Fermi surface is composed of only two (Fermi) points $\pm k_F$. It is reasonable to assume that one can go beyond first-order (Born) approximation in the speed of sound by using only two particles that, in the case of no interactions, have momenta $\pm k_F$, based on the fact that Nth-order perturbation theory only needs processes involving N "active" particles close to the Fermi points. The complexity of many-body perturbation theory, as opposed to few-body physics, is much increased by the presence of the Fermi sea. Here we strive to obtain a nonperturbative method that uses two-body physics only, without the extra complications of the Fermi sea. Our method works best in the repulsive to intermediately attractive fermionic (or fermionized) regime of these systems. Beyond this regime, bosonic methods, such as mean-field theory, must be used to describe the low-energy physics.

II. TWO FERMIONS ON A RING

Consider two spin-polarized fermions whose dynamics is governed by the Hamiltonian

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1 - x_2). \tag{1}$$

If the interaction $V(x)$, with $x \equiv x_1 - x_2$, falls off faster than $1/|x|$ at long distances, then the stationary scattering states $\psi_k(x)$, after separation of center of mass and relative coordinates, of the Hamiltonian (1), behave asymptotically as

$$\psi_k(x) \to \mathrm{sgn}(x)\sin[k|x| + \theta(k)], \quad x \to \pm\infty. \tag{2}$$

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Above, we assume $k > 0$, $\mathrm{sgn}(x)$ is the signum function, and $\theta(k)$ is the scattering phase shift. We place the two fermions on a ring of length L (periodic boundary conditions). It is easy to see that, for total momentum $K = 0$, the energies of the two-body states are given by $\hbar^2 k^2/m$, where k must satisfy the equation

$$k = \frac{2\pi n}{L} - \frac{2}{L}\theta(k), \tag{3}$$

with $n \in \mathbb{Z}^+$. From now on, we particularize to $n = 1$ in Eq. (3) and identify $k_F = 2\pi/L$.

III. UNIVERSALITY HYPOTHESIS

In a many-body system, the thermodynamic limit is attained by taking the length of the ring to infinity while keeping the density constant. This, in a few-particle system, is not possible. To remedy this inherent deficiency, we invoke a universality hypothesis, stating that two thermodynamically large one-dimensional gapless quantum systems at zero temperature but at different densities have the same dimensionless low-energy properties if all their dimensionless coupling constants at energies near the Fermi points are identical. Clearly, this hypothesis is very reasonable and is verified in well-known integrable models, such as the Lieb-Liniger model [15], or its fermionic dual [18–20], whose ratio of speed of sound to Fermi velocity, and its Luttinger parameter only depend on the coupling constant γ (see Supplemental Material [21]), regardless of the density of the system. For generic, nonintegrable models, with two-body forces only, the universality hypothesis implies that the two-body T matrices, on and off shell, of the two target models must be the same. The theory we present below is a pure two-particle theory and therefore we can only invoke universality on the on-shell (i.e., phase shift) scattering. Note that universality in this case implies that the speed of sound, when $\theta(k_F) = 0$, must be given by the Fermi velocity $v = v_F$. This last condition, which is not exact, is a very good approximation nevertheless, as we will see below (see also [10–12]), and coincides with the result obtained by weak-coupling theory from the Tomonaga-Luttinger model [9,17,22].

IV. CALCULATION OF THE SPEED OF SOUND

In order to excite the system, we need to add more incident relative momentum in Eq. (3). The lowest excitation is obtained by setting $n = 2$, corresponding to $2k_F$, which is too large to extract low-momentum expansions of the excitation energies. Instead, we can shorten the ring, $L \to L - \delta$, with $0 < \delta \ll L$. Identifying, to leading order, the incident momentum in Eq. (3) with $k_F + q/2$, we obtain $\delta = L^2 q/4\pi$. Since in this way not only the incident momentum ($\equiv k_F$) but also the density is increased, we need to ensure that the coupling constants of the theory remain fixed, in order to guarantee that the universality hypothesis stated in the previous paragraph holds at the two-body level. We find that the speed of sound is given by

$$\hbar v = \frac{\hbar^2 L^2}{4\pi m}\frac{dk_\delta^2}{d\delta}\bigg|_{\delta=0}, \tag{4}$$

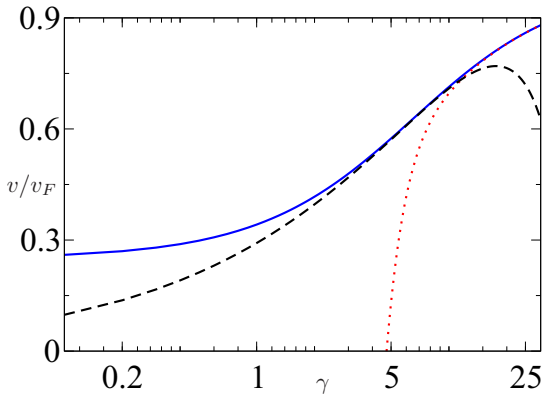

FIG. 1. Speed of sound vs Lieb-Liniger constant γ. We plot the theoretical results from Eqs. (4) and (3) (blue solid line), fourth-order perturbation theory in $1/\gamma$ (red dotted line), and Bogoliubov theory (black dashed line).

while leaving the dimensionless coupling constants of the particular problem fixed, where k_δ is the solution to Eq. (3) with L substituted by $L - \delta$.

To show how good an approximation one can achieve with Eq. (4), we calculate the speed of sound for the hard-rod (HR) (with diameter a)[1] and the Lieb-Liniger (LL) model to third order. The two models are defined as follows. The interaction potential $V(x)$ for the HR model, whether spinless bosonic or fermionic, is given by $V(x) = \infty$ for $|x| < a$ and $V(x) = 0$ otherwise. The only dimensionless interaction parameter in the HR model is the gas parameter ρa, with ρ the density. The phase shifts for the HR model read $\theta(k) = -ka$. The Lieb-Liniger model consists of a system of spinless bosons interacting via Dirac delta interactions, that is, $V(x) = g\delta(x)$. The Lieb-Liniger parameter γ for a gas of density ρ is defined as $\gamma = mg/\hbar^2\rho$ and plays the role of dimensionless interaction parameter in this case. The phase shifts for the LL model read $\theta(k) = \arctan(2\hbar^2 k/mg)$. Using Eq. (4) for the HR and LL models, we obtain

$$\frac{v_{\mathrm{HR}}}{v_F} = (1 - \rho a)^{-2}, \tag{5}$$

$$\frac{v_{\mathrm{LL}}}{v_F} = 1 - \frac{4}{\gamma} + \frac{12}{\gamma^2} + \frac{16}{3\gamma^3}(\pi^2 - 6) + O(\gamma^{-4}). \tag{6}$$

Above, and as one could expect for the very simple HR model, we see that its speed of sound is exact [9,10], while for the Lieb-Liniger model it is correct to third order in perturbation theory [16,24]. In Fig. 1 we plot the numerically calculated speed of sound for the LL model and compare it with fourth-order perturbation theory [16,24] in $1/\gamma$ and the Bogoliubov approximation [14,15]. There we observe that the results are highly nonperturbative and are valid beyond the perturbative regime and down to $\gamma \approx 5$ and that our results interpolate between the Bogoliubov and the Tonks-Girardeau regimes.

[1]Or the extended HR model [23] with scattering length a.

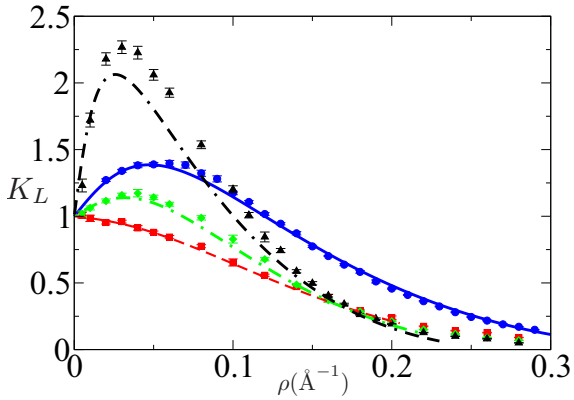

FIG. 2. Luttinger parameter vs density for ^{3}He (blue solid line), ^{3}H (black double-dash–dotted line), ^{2}H (green dash-dotted line), and ^{1}H (red dashed line). Blue dots (^{3}He), black triangles (^{3}H), green diamonds (^{2}H), and red squares (^{1}H) are the Monte Carlo data from Refs. [11,12].

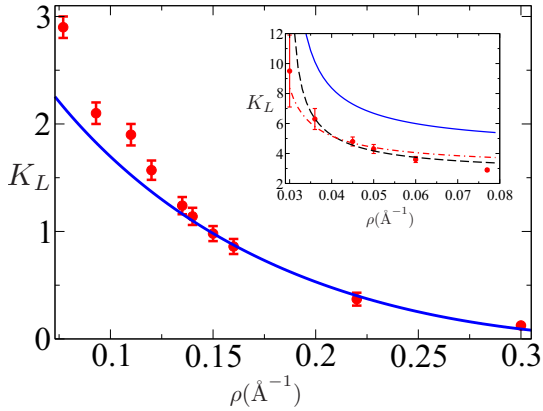

FIG. 3. Luttinger parameter vs density for ^{4}He (solid blue line). Red dots are Monte Carlo data of Ref. [10]. The inset shows the Luttinger parameter from Eq. (9) (blue solid line) and the renormalized Luttinger parameter (see the text) with $\rho_* = 0.0296$ Å^{-1} (black dashed line) and with $\rho_* = 0.026$ Å^{-1} (red dash-dotted line). Red dots are the Monte Carlo data of Ref. [10].

V. LIGHT ATOMIC GASES

We now move on to discuss more realistic, nonintegrable systems in one dimension. We study ^{4}He, ^{3}He, and spin-polarized ^{3}H, ^{2}H, and ^{1}H. For all the above atoms there are extensive Monte Carlo data [10–12] for the Luttinger parameter K_L. This, in the case of Galilean-relativistic systems, is related to the speed of sound as $K_L = v_F/v$ [22]. These systems are very different from the LL and HR models, for which, once the only dimensionless parameter γ is fixed, we have a density-independent v/v_F. For H and He, the use of γ as a parameter is only valid in the low-density regime [11,12]. We calculate the phase shifts $\theta(k)$ using the Aziz HFDHF2 potential for ^{4}He [25], the Aziz II potential for ^{3}He [26,27], and a cubic-spline interpolation of the Jamieson-Dalgarno-Wolniewicz (JDW) potential [28], readjusted to match the $1/|x|^6$ tails [29] as in Ref. [12], for hydrogen.[2] Since all these interactions have short-distance hard cores, the distinction between fermion and boson is void and we will treat all these atoms as fermions. The phase shifts (see [21]) can be locally approximated by linear functions as

$$\theta(k) \approx \theta_0 - a(k - k_F), \tag{7}$$

where θ_0 is the phase shift at $k = k_F$. We have verified that adding higher-order terms in Eq. (7) does not change the results below in a significant way. The manipulations in Eq. (4) are done by keeping the dimensionless coupling constants θ_0 and $k_F a$ fixed. The results are shown in Figs. 2 and 3 and are in excellent agreement with the Monte Carlo results of Refs. [10–12]. As noted above, the universality hypothesis at the two-body level implies $K_L = 1$ whenever $\theta(k_F) = 0$, which, as seen in Figs. 2 and 3, is nearly true in most cases. This constraint may be lifted by nonintegrability effects beyond two-body physics.

VI. LIQUID ^{4}He

Of all the helium and hydrogen isotopes, the most difficult to describe is ^{4}He, as is seen in Fig. 3. This is due to the existence of a very weakly bound s-wave state in three dimensions, with a binding energy $E_B = 1.1^{+0.3}_{-0.2}$ mK [31].[3] In strict one dimension, the binding energy is identical to the three-dimensional case due to the short-distance hard core of the He-He interaction. For the Aziz HFDHF2 potential, the scattering length and effective range are $a = 124.65$ Å and $r = 7.39$ Å, respectively, yielding $E_B \approx 0.83$ mK. The liquid phase of ^{4}He [10] exists at low densities ρ below a critical point ρ_*, which was calculated to be $\rho_* = 0.026 \pm 0.002$ Å^{-1} in Ref. [10]. To estimate the critical point theoretically, we use the well-established energy-dependent scattering length $a(k)$ [32], given by $-1/a(k) = -1/a + rk^2/2$, where $k = \sqrt{mE/\hbar^2}$, and E the relative energy, giving an effective interaction strength $g(k) = -2m/\hbar^2 a(k)$, with $V \sim g(k)\delta(x)$. We place two particles in a ring of length L and find the critical k,k_*, by setting $g(k_*) = 0$, which yields $k_* = 0.0466$ Å^{-1}. This is in very good agreement with the resonance found numerically, located at $k_* = 0.0465$ Å^{-1}. Identifying $\rho = 2/L$, we obtain $\rho_* = 2k_*/\pi = 0.0296$ Å^{-1}, in good agreement with Ref. [10]. At low densities $\rho \ll \rho_*$, we expect the effective range to contribute minimally and we can use the attractive mean-field (Gross-Pitaevskii) theory with the Lieb-Liniger parameter $\gamma = -2/\rho a$. At higher densities, the effective range will play a role, but effective-range mean-field theory with a homogeneous ground state shows no effect of r [33]. We therefore use a Hammer-Furnstahl field redefinition [34,35] to trade the effective range for a three-body force of strength λ_3 and avoid its microscopic calculation [36–38]

[2]These interactions are used for the sake of comparison with the data of Refs. [10–12]. In reality [6], the phase shifts should be calculated including the external confinement [30].

[3]Note that the binding energy of ^{4}He$_2$ is seven orders of magnitude smaller than for H_2, for instance.

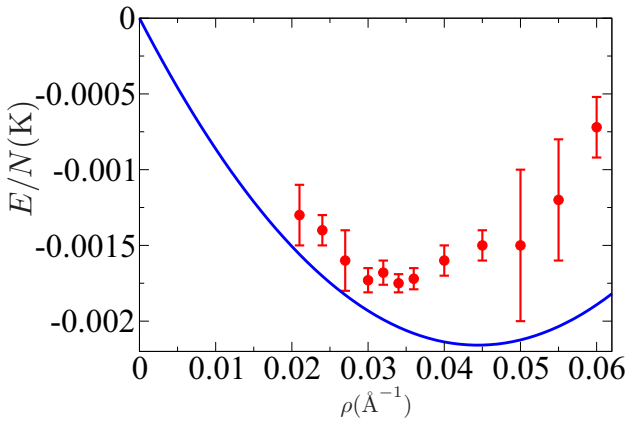

FIG. 4. Low-density equation of state from Eq. (8) (blue solid line). Red dots are the Monte Carlo data of Ref. [10].

by using $\partial_\rho \mu = 0$ at $\rho = \rho_*$, where $\mu = g\rho + \lambda_3 \rho^2$ is the chemical potential. This yields $\lambda_3 = (\hbar^2/m)/\rho_* a$ ($\propto \sqrt{r/a}$) and the equation of state (EOS) in this approximation is given by

$$\frac{E}{N} = \frac{\hbar^2 \rho}{ma}\left[-1 + \frac{1}{3}\frac{\rho}{\rho_*}\right]. \tag{8}$$

The EOS is shown in Fig. 4, where it is compared to the results of Ref. [10]. The EOS is in qualitative agreement with the Monte Carlo results at the densities where these are available, with the correct order of magnitude. The speed of sound v for $\rho > \rho_*$ can be calculated from the EOS in Eq. (8) as $mv^2 = \rho \partial_\rho \mu$. The Luttinger parameter then has the form

$$K_L = \pi \sqrt{\frac{\rho_* a}{2}} \left(\frac{\rho - \rho_*}{\rho}\right)^{-1/2}. \tag{9}$$

Even though the above result, in particular the factor $\pi/\sqrt{2}$, is not accurate quantitatively (see the inset of Fig. 3), because higher power terms of ρ, and possibly quantum fluctuations [39], contribute to the chemical potential at such densities, it does show that K_L diverges for $\rho \to \rho_*^+$ as $(\rho - \rho_*)^{-1/2}$, whose exponent agrees with Monte Carlo simulation results [10], and unveils the otherwise inaccessible factor of $\rho^{1/2}$ that renders the square root dependence dimensionless. If we assume the functional form of K_L given by Eq. (9), but leave the factor in front as a renormalizable parameter, i.e., $\pi/\sqrt{2} \leftrightarrow C$, then this can be extracted by fitting the Luttinger parameter for $\rho \in [0.035, 0.06]$ Å^{-1} to the values reported in [10]. For our calculated value of $\rho_* = 0.0296$ Å^{-1} we obtain $C = 1.388$, whereas for the Ref. [10] estimate $\rho_* = 0.026$ Å^{-1}, we obtain $C = 1.697$. In the inset of Fig. 3, we show the resulting renormalized K_L, which strongly suggests that the critical point of Ref. [10] is most accurate and that the functional dependence in Eq. (9) is indeed correct.

VII. CONCLUSION

In this Rapid Communication we have devised a remarkably simple method that uses only two-particle scattering data, that is, the phase shifts, to obtain nonperturbative approximations to the speed of sound and the Luttinger parameter of one-dimensional quantum many-body systems. The method reveals how strikingly large an amount of information the two-body problem in one dimension encodes about the low-energy physics of the many-body system near the Fermi points. We have given relevant examples, such as the Lieb-Liniger model, where third-order perturbation theory is recovered and the speed of sound interpolates deep into the regime where strong-coupling perturbation theory fails. For the simplest case of the hard-rod model our method is, moreover, exact. We have also applied the method to all isotopes of helium and hydrogen, finding excellent agreement with full-blown Monte Carlo simulations available in the literature. Our method, given its simplicity, can also be used as a valuable tool for efficiently recognizing possible interesting regions of parameter space that can then be explored via exact numerical calculations. We have also shown how well simple two-body theory can predict the critical or spinodal point in one-dimensional ^{4}He and extracted the effective three-body force that is largely responsible for the liquid-to-Luttinger liquid transition in this system. On the Bose gas side, we have also obtained the critical exponent with which the Luttinger parameter diverges at the spinodal point (1/2), in perfect agreement with Monte Carlo calculations. Our method is not restricted to continuous models, but works as well for lattice models and can be easily extended to systems with discrete translational invariance, i.e., many-body problems in one-dimensional periodic potentials, for which scattering is also characterized by phase shifts [40]. We expect variations of our method to also be able to describe electrons with spin or cold atoms with pseudospin. Of special interest are systems, such as electrons in a strong magnetic field [41,42], where spin-charge separation is destroyed and the microscopic calculation of the low-energy properties is quite challenging. An extension of our theory to higher-dimensional systems with restricted phase space around the Fermi energy, such as materials with Dirac cones, e.g., for the estimation of the renormalized Fermi velocity in graphene [43–45], would be highly desirable. More accurate approximations should also be feasible by extending our results to three- and four-particle problems, which may show the effects of nonintegrability, but would still be manageable from a theoretical and computational point of view by using recently developed methods such as the adiabatic projection method [46] that has been successfully applied to the nuclear few-body problem [47,48].

ACKNOWLEDGMENTS

We are indebted to G. E. Astrakharchik, A. J. Vidal, L. Vranjes Markic, and J. Boronat for sharing the Monte Carlo data of Refs. [11,12] and to G. Bertaina, M. Motta, M. Rossi, E. Vitali, and D. E. Galli for providing their Monte Carlo results of Ref. [10]. We thank L. Vranjes Markic for useful discussions about the JDW potential and for sharing her interpolated data. We thank B. Braunecker, J. Keeling, N. T. Zinner, and L. G. Phillips for their valuable feedback. We acknowledge support from EPSRC Grant No. EP/M024636/1.

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