Luttinger liquid behavior of one-dimensional $^3$He.

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The ground-state properties of one-dimensional $^3$He are studied using quantum Monte Carlo methods. The equation of state is calculated in a wide range of physically relevant densities and is well reproduced by a power-series fit. The Luttinger liquid theory is found to describe the long-range properties of the correlation function. The density dependence of the Luttinger parameter is explicitly found and interestingly it shows a non-monotonic behavior. Depending on the density, the static structure factor can be a smooth function of the momentum or might contain a peak of a finite or infinite height. Although no phase transitions are present in the system, we identify a number of physically different regimes, including an ideal Fermi gas, a “Bose-gas”, a “super-Tonks-Girardeau” regime, and a “quasi-crystal”.

The experimental realization and study of one-dimensional quantum fluids is nowadays an active research area. From conventional quantum liquids, $^4$He and $^3$He, to trapped ultracold Bose and Fermi gases there are a set of increasing data confirming the peculiarities of such a reduced geometry. Recently, Yager et al.\cite{1} have found clear evidence of the one-dimensional character of $^3$He when confined in the narrow nanapores of a MCM-41\cite{2} substrate. The Fermi statistics of $^3$He allowed for using nuclear magnetic resonance to study the dependence of spin relaxation time with the angular frequency, obtaining a dependence $\omega^{1/2}$ characteristic of one-dimensional diffusion. It was then claimed\cite{1} that NMR measures on $^3$He confined in these nanopores would provide access to the experimental determination of the Luttinger parameter. Nevertheless, the experiment was carried out at too high temperature (1.7 K) to achieve quantum degeneracy. There are additional evidences of the one-dimensional behavior of $^3$He by heat capacity measurements\cite{3,4}. These experimental achievements open the real possibility of obtaining a stable Fermi Luttinger liquid, with the relevant advantage of existing at any density since $^3$He does not sustain a many-body self-bound state. In addition, and from a theoretical point of view, the properties of $^3$He can be accurately determined because the helium interaction potential is known with high precision\cite{5}.

In this Letter, we present a quantum Monte Carlo study of one-dimensional $^3$He in the limit of zero temperature. From the obtained equation of state and static structure factors we determined the Luttinger parameter as a function of the density of the system. Contrarily to the monotonic behavior of the Luttinger parameter observed in purely repulsive systems, the Luttinger $^3$He fluid shows a novel feature: a reentrant behavior due to the attractive van der Waals tail of the helium interaction.

Helium atoms, confined to one-dimensional geometry, are described by the Hamiltonian

$$
\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_i + \sum_{i<j} V(|x_i - x_j|),
$$

where $m = 3.016u$ is the $^3$He mass and $x_i,i = 1, N$ are the positions of each one of the $N$ atoms. We take the two-body interaction potential $V(r)$ in Aziz II form\cite{5}. The system is simulated by imposing periodic boundary conditions (p.b.c.) on a box of size $L$. In the thermodynamic limit, the properties are governed by a single parameter, namely the linear density $\rho = N/L$.

We use the diffusion Monte Carlo (DMC) method to study the ground state properties at zero temperature\cite{6}. The DMC method is based on solving the Schrödinger equation in imaginary time so that the excited states are projected out when this time goes to $\infty$ (for more details on DMC technique see, for example, Ref.\cite{7}). The variance of the results is greatly reduced by introducing an importance sampling based on use of a guiding wave function. We choose the guiding wave function in a pair-product form

$$
\psi_T(x_1, \ldots, x_N) = \prod_{i<j} f_{2b}(x_i - x_j) \text{sign}(x_i - x_j),
$$

where $f_{2b}(x)$ is taken as the solution of the two-body scattering problem in a finite-size box with p.b.c., i.e., $f_{2b}(L/2) = 0$. The sign function in Eq. (2) ensures that the wave function changes its sign when any two fermionic atoms are exchanged. While the guiding wave function based on the two-body solution is known to produce poor results for the energy in three dimensions, we find that in one-dimensional geometry choice\cite{2} provides a remarkably precise description (the difference between variational and diffusion energy is smaller than 20%). A possible reason for that is that the three-body collisions are greatly suppressed in reduced geometry. Furthermore, wave function\cite{2} becomes exact in the limit of low density, $\rho \rightarrow 0$. Indeed, when the interparticle distance is
The ground-state energy, obtained in DMC calculations, is exact (apart from some controllable statistical error). In the low density limit, the interaction potential can be neglected and the system behaves as an ideal Fermi gas (IFG). In this limit, the energy per particle has a quadratic dependence with the density \( \rho \)

\[
E_{\text{IFG}} \approx \frac{\pi^2 \hbar^2 \rho^2}{6m}.
\]  

The dependence of the ground-state energy \( E \) on the linear density \( \rho \) is reported in Fig. 1 in units of \( E_{\text{IFG}} \). We find that the ideal Fermi gas limit realizes at densities \( \rho \lesssim 0.01\,\text{Å}^{-1} \). For larger densities, the interparticle distance becomes smaller and the attractive long-range part of the He-He interaction contributes significantly to the potential energy. This “softening” of the energy increases up to a density \( \rho \approx 0.1\,\text{Å}^{-1} \). For larger densities, the short-range repulsive part makes the system more rigid. At the density \( \rho \approx 0.2\,\text{Å}^{-1} \) the energy per particle becomes larger than that of an ideal Fermi gas and the energy diverges quickly as the density is further increased. The core size \( \sigma = 2.963\,\text{Å} \) of Aziz II potential imposes the maximal density \( \rho_{\text{max}} = 1/\sigma = 0.3375\,\text{Å}^{-1} \), up to which the system can be compressed. At this density, the excluded hard-core volume fills all available space, resulting in the formation of a true crystal with a diverging energy. It is important to note that the Aziz II model potential cannot be reliably used at such extreme densities. Nevertheless, we will show that at smaller densities, where the interaction potential is still valid, the system forms a quasi-crystal.

The DMC energy is well fitted in the range \( 0 < \rho < 0.2\,\text{Å}^{-1} \) with a polynomial series

\[
\frac{E}{N} = \frac{\pi^2 \hbar^2 \rho^2}{6m} \left(1 + \sum_{i=1}^{6} C_i \rho^i \right)
\]  

with coefficients \( C_1 = -15.076\,\text{Å}, \ C_2 = 230.78\,\text{Å}^2, \ C_3 = -2177\,\text{Å}^3, \ C_4 = 13266\,\text{Å}^4, \ C_5 = -44130\,\text{Å}^5, \) and \( C_6 = 64600\,\text{Å}^6 \). While compared to an ideal Fermi gas, \(^3\text{He}\) might be both softer or more rigid, the energy per particle always remains a monotonously increasing function of the density. This should be contrasted with \(^4\text{He}\), where its heavier mass leads to the existence of a minimum in the energy, physically reflecting the formation of a liquid (many-body self-bound) state. Contrarily, one-dimensional \(^3\text{He}\) always stays in a gas state.

In order to study the structural properties, we calculate the static structure factor \( S(k) \). We use the technique of pure estimators\(^{10}\) to ensure that the results are independent of a particular choice of the trial wave function. In the dilute the static structure factor approaches the one of an ideal Fermi gas. In this case, the low-momentum linear behavior

\[
S(k) = \frac{\hbar |k|}{2m c} \quad k \to 0
\]  

continues up to \( |k| = 2k_F \) with \( k_F = \pi \rho \) the Fermi momentum. The slope is fixed by the speed of sound which for the ideal Fermi gas coincides with the Fermi velocity \( c = v_F = \hbar k_F/m \). For any larger momenta, \( |k| > 2k_F \), the static structure factor is equal to the large-momentum asymptotic value \( S(k) = 1 \). The first derivative is discontinuous at \( |k| = 2k_F \) corresponding to a umklapp process in which an atom is flipped from one side of the Fermi surface to the other. The kink at \( |k| = 2k_F \) disappears as the density is increased and the attractive part of the interaction potential becomes relevant. In this regime, \( S(k) \) is a smooth monotonous function with the typical shape found in weakly interacting Bose gases. Indeed, in one dimension there are certain
analogies between an attractive Fermi gas and a repulsive Bose gas. According to the Girardeau mapping\cite{8}, an infinitely-repulsive Bose gas has the same \( S(k) \) as an ideal Fermi gas. Adding attraction to the Fermi gas results in a linear slope in \( S(k) \), similar to the one in a Bose gas with finite repulsion (for instance, in the bosonic Lieb-Liniger model\cite{11}). In the limit of weak interactions, the Bose gas is well described by the Gross-Pitaevskii equation, with the chemical potential linear with density \( \mu = g_{1D} \rho \), where \( g_{1D} \) is the coupling constant\cite{12}.

For weak interactions the speed of sound, \( c = \sqrt{\mu/m} \), is small and the linear slope in \( S(k) \) becomes larger than that of an ideal Fermi (or Tonks-Girardeau) gas. Although the Gross-Pitaevskii regime is never reached in helium system, still we see an increase in the slope of \( S(k) \) in the regime of equivalence to a Bose gas system (\( \rho \lesssim 0.05\) \( \AA^{-1} \)). On the contrary, at larger density the linear slope starts to decrease, reflecting the growth of the contribution coming from the hard-core part of the interaction potential. Eventually, a kink at \( k = 2k_F \) is formed which, as the density is increased further, gets transformed to a sharp peak. A diverging peak in \( S(k) \) manifests the formation of a quasi-crystal. In fact, in a crystal the wave number \( k = 2k_F \) corresponds to the width of the first Brillouin zone \( 2k_F = 2\pi/a \) with the crystal lattice spacing \( a = \rho^{-1} \).

In order to determine the boundaries between “Bose-gas”, “super-TG” and “quasi-crystal” regimes we make use of the Luttinger liquid theory\cite{12} \cite{15}. This effective theory relies on the presence of phonons in the gapless excitation spectrum \( E_k = \hbar |k|c \) and predicts the large-distance (or small-momenta) behavior of the correlation functions. The results are universally expressed in terms of the Luttinger parameter which, in a homogeneous system, is directly related to the Fermi velocity \( v_F \) and the speed of sound \( c \) as \( K = \frac{v_F}{c} \). The Fermi velocity \( v_F \) is completely fixed by the density while the speed of sound \( c \) takes into account the many-body interactions between particles. The description in terms of a Luttinger liquid is very broad and applies to a large number of one-dimensional systems, but a microscopic calculation is always necessary to relate the Luttinger parameter \( K \) to the linear density \( \rho \).

The dependence of \( K \) on \( \rho \) is reported in Fig. 8 and constitutes the main result of the Letter. We use two alternative approaches to find the speed of sound \( c \) and to establish the dependence of \( K \) on \( \rho \): (i) by differentiating the equation of state\cite{10} we obtain the chemical potential \( \mu = \partial E/\partial N \) and, from that, the speed of sound \( c, mc^2 = \rho \partial \mu/\partial \rho \) (ii) from the linear behavior of \( S(k) \) with \( k \) at low momentum\cite{5}. The fact that two different approaches are in agreement demonstrates the high precision of the calculations and the internal consistency of our approach.

In the low-density limit, the value of the Luttinger parameter, \( K = 1 \), corresponds to that of an ideal Fermi gas where \( c = v_F \). By increasing the density, the Luttinger parameter becomes larger, \( K > 1 \), corresponding to a Fermi system with dominant attraction and similarly to an interacting Bose gas (Lieb-Liniger model\cite{14} \cite{16}). The non-monotonous behavior with the density makes the Luttinger parameter to return at \( \rho = 0.123 \AA^{-1} \) to \( K = 1 \), which can be associated to the Tonks-Girardeau regime for bosons. For larger density, \( K \) becomes smaller than unity, \( K < 1 \). This regime corresponds to a Fermi system with a dominant repulsion and is similar in many aspects to the super-Tonks-Girardeau regime for bosons\cite{17}. The “quasi-crystal” regime is reached for \( K < 1/2 \), at \( \rho \geq 0.19 \AA^{-1} \), and is characterized by a diverging peak in the static structure factor at the momentum corresponding to the inverse lattice spacing. The reentrant behavior, when two different densities correspond to the same value of the Luttinger parameter, is a peculiar feature of the helium interaction and of the gas nature of \(^3\)He. This was not observed in purely repulsive systems, such as \( \delta \)-interacting bosons\cite{14}, hard rods\cite{18}, dipoles\cite{19} \cite{20} or Coulomb charges\cite{21}. This rich behavior in helium is a consequence of its interatomic potential: a hard core at short distance and an attractive van der Waals tail at long distance.

Within the Luttinger liquid theory, the pair distribution function \( g_2(x) \) can be expanded at large distances in a series of oscillating terms with a power-law envelope\cite{13}

\[
g_2(x) = 1 - \frac{K}{2(k_F)^2} + \sum_{l=1}^{\infty} A_l \frac{\cos(2l k_F x)}{|k_F x|^{2i l K}}.
\]

The terms on the r.h.s. in Eq. (6) describe (i) the long-distance asymptotic constant value of uncorrelated particles, (ii) \( 1/x^2 \) decay due to density fluctuations, with the amplitude fully fixed by \( K \), and (iii) oscillations with a power law envelope. The exponents in the power-law decay are fully fixed by \( K \), while the amplitudes \( A_l \) cannot be established within the Luttinger liquid approach. Such oscillations might cause divergencies at the multi-
The pair distribution function is shown in Fig. 4 for a
minimum and helium is superfluid according to Landau
argument, in one dimension the excitation spectrum al-
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tem always leads to dissipation of energy making the
gas being normal even at zero temperature. Moreover,
in one dimension quantum fluctuations destroy the di-
geonal long-range order and no phase transition is
possible at finite temperature. The system always
stays in the same phase which is not superfluid, is not
Bose-condensed and does not form a true crystal.

To summarize, we have studied the ground-state prop-
erties of one-dimensional $^3$He by means of the diffu-
sion Monte Carlo method. The helium-helium interac-
tion potential is known very precisely (Aziz et al., [5])
which permits us to make quantitative predictions for
the energy and the correlation functions, which can be
experimentally measured. The equation of state is ob-
tained for a wide range of physically relevant densities,
$0 < \rho < 0.2 \text{ Å}^{-3}$, and we provide a power-law series fit to it. The structural properties are addressed by studying the static structure factor $S(k)$ and the pair distribution function $g_2(r)$. We show that the long-range properties of the correlation functions are well reproduced by the Luttinger liquid theory. We extract the Luttinger parameter $K$ (i) from the compressibility by using the fit to the equation of state (ii) from the linear slope of $S(k)$ for small momenta. Both methods agree within the error bars which prove a high quality of the results and the internal consistency of the method. The obtained relation between the Luttinger parameter $K$ and the linear density $\rho$ can be used to predict the long-range asymptotics of stationary correlation functions (one-body density matrix, momentum distribution, etc.) as well as dynamic quantities (dynamic form factor $S(k, \omega)$ close to $k = 2k_F$, etc.). The non-monotonous dependence of $K$ and the den-
sity was not previously observed in fully repulsive sys-
tems and is a special feature of $^3$He. In particular, the
reentrant behavior if found, when two different densities

\[ S(k = 2l k_F) = A_l N^{1-2l^2 K} \]

diverges when $K < 1/(2l^2)$. In particular, the first
peak $l = 1$ diverges when $l > 1/2$, i.e., for densities
$\rho \geq 0.2 \text{ Å}^{-3}$. We call this regime a “quasi-crystal”. There
is a number of differences between “quasi” and “true”
crystals. A three-dimensional crystal possesses a dia-
gonal long-range order as the density oscillations remain
in phase for large distances. Instead, in one dimension
the order is lost in a power-law way. The height of the
peak is divergent in both cases, but in a true crystal
the Bragg peak grows linearly with the number of parti-
cles $S(k_{\text{peak}}) \propto N$, while in a quasi-crystal the exponent
is smaller than unity, as can be seen from Eq. (7). A
true crystal is characterised by a number of diverging
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pend on the value of $K$. There are no diverging peaks
for $K > 1/2$, one diverging peak for $1/2 > K > 1/8$, two
for $1/8 > K > 1/18$ and so on. Only when asymptoti-
cally $K \to 0$ (or $\rho \to \rho_{\text{max}}$) the true crystal is recovered.
The physics in 1D systems is unusual and easily might
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