

Spectral Functions of Strongly Interacting Isospin- $\frac{1}{2}$ Bosons in One Dimension

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We study a system of one-dimensional (iso)spin- $\frac{1}{2}$ bosons in the regime of strong repulsive interactions. We argue that the low-energy spectrum of the system consists of acoustic density waves and the spin excitations described by an effective ferromagnetic spin chain with a small exchange constant J . We use this description to compute the dynamic spin structure factor and the spectral functions of the system.

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Physics of one-dimensional Fermi systems has long attracted the interest of both theorists and experimentalists. Interactions between particles have a strong effect on the properties of these systems. Interacting fermions form the so-called Luttinger-liquid state [1], whose excitations are bosons with acoustic spectrum, $\varepsilon(q) \propto |q|$. Recently it has become possible to confine ultracold gases of bosons to elongated traps [2,3], effectively creating systems of one-dimensional bosons. The properties of interacting one-dimensional spinless bosons are in many respects similar to those of spinless fermions. In particular, they too form a Luttinger-liquid state at low energies.

In a recent experiment [4] bosons with two internal degrees of freedom, which can be viewed as components of (iso)spin- $\frac{1}{2}$, were confined to one dimension. For spin- $\frac{1}{2}$ particles the difference between the Bose and Fermi statistics is of fundamental importance. Indeed, spin-independent interactions between one-dimensional bosons favor ferromagnetic spin ordering [5], whereas for fermions the ground state spin is zero [6]. As a result, the low-energy spin excitations of the boson system are magnons with quadratic spectrum $\varepsilon(q) \propto q^2$, and the system is no longer a Luttinger liquid.

In the absence of the effective theory of interacting spin- $\frac{1}{2}$ bosons in one dimension, considerable progress has been made recently by focusing on the regime of very strong repulsive interactions [7,8]. In this Letter we show that this regime allows for a remarkably simple theoretical description, in which there are two types of low-energy excitations: acoustic density waves and the spin excitations described by a one-dimensional Heisenberg model with a very small ferromagnetic exchange constant J . The theory is applied to the calculation of the dynamic spin structure factor and the spectral functions of the system. Unlike Refs. [7,8], our conclusions are not limited to spin excitations of small momentum $q \rightarrow 0$. In addition, although the frequency ω is assumed to be small compared to the typical kinetic energy of the bosons $E_F \sim (\hbar n)^2/m$, it can be of order of the small exchange constant J . (Here n is the one-dimensional density of bosons and m is their mass.)

The model we consider is that of one-dimensional (iso)spin- $\frac{1}{2}$ bosons interacting with repulsive spin-independent potential $V(x-y)$. For simplicity, we concentrate on the most realistic regime of short-range interactions, $V(x-y) = g\delta(x-y)$; the generalization to the case of finite-range repulsion is relatively straightforward. The strong repulsion regime is achieved at $\gamma \gg 1$, where $\gamma = mg/\hbar^2 n$ is the dimensionless interaction strength.

As the first step, we show that at low energies the excitation spectrum of the system consists of independent phonon and magnon excitations. This effect is essentially equivalent to the well-known spin-charge separation in interacting one-dimensional electron systems [9]. Our arguments follow the discussion [10,11] of that phenomenon in the limit of strong repulsion.

In the Tonks-Girardeau limit $\gamma \rightarrow +\infty$ the repulsion effectively forbids any two particles to occupy the same point in space, regardless of their spin. Thus the density excitations of the system are those of a gas of spinless hard-core bosons, or, equivalently, those of noninteracting gas of spinless fermions [12], where the same constraint is enforced by the Pauli principle. It is convenient to treat the low-energy excitations of one-dimensional spinless Bose and Fermi systems in the framework of the hydrodynamic approach [1] and write the Hamiltonian in the form

$$H_{\text{ph}} = \frac{\hbar u_\rho}{2\pi} \int [K(\partial_x \theta)^2 + K^{-1}(\partial_x \phi)^2] dx. \quad (1)$$

Here ϕ and θ are bosonic fields satisfying the standard commutation relation $[\phi(x), \partial_y \theta(y)] = i\pi \delta(x-y)$. The Luttinger-liquid parameter K and the phonon velocity u_ρ are determined by the interactions. In the case of hard-core bosons $K = 1$, while the effective ‘‘Fermi velocity’’ $u_\rho = \pi \hbar n/m$.

In the limit $\gamma \rightarrow +\infty$ any collision of two bosons results in perfect backscattering. As a result the bosons become distinguishable particles. Indeed, if boson 1 is to the left of boson 2, i.e., $x_1 < x_2$ at some moment in time, then this property cannot be changed as a result of any collisions between particles. Thus one can number all particles by an integer l in accordance with their positions along the x axis.

In this limit the spins of the bosons do not interact, and each state of N bosons is 2^N -fold degenerate. A coupling of the spins appears only when γ is finite. At $\gamma \gg 1$ a collision of two bosons, l and $l+1$, may result in their forward scattering, in which case the particles exchange their spins. Since for spin- $\frac{1}{2}$ particles the spin permutation operator $P_{l,l+1}$ can be expressed as $P_{l,l+1} = 2\mathbf{S}_l \cdot \mathbf{S}_{l+1} + 1/2$, this gives rise to coupling of the spins of the nearest-neighbor particles:

$$H_\sigma = -\sum_l J S_l \cdot S_{l+1}. \quad (2)$$

Thus at $\gamma \gg 1$ the low-energy excitations of the system are given by the acoustic phonons, described by the Hamiltonian (1) and the spin excitations of the Heisenberg Hamiltonian (2).

A similar separation of the density and spin excitations is well known in the case of strongly interacting one-dimensional fermions, where it was first derived [13] from the exact solution of the infinite- U Hubbard model. The sign of the exchange constant J is determined by the requirement to either symmetrize or antisymmetrize the wave function with respect to the permutation $x_l \leftrightarrow x_{l+1}$; the coupling is antiferromagnetic for fermions, $J < 0$, and ferromagnetic for bosons, $J > 0$. On the other hand, the magnitude of the exchange constant J is determined by the amplitude of the forward scattering of two neighboring particles, regardless of their statistics. Thus we find the same value of J as in the case of fermions with strong short-range repulsion,

$$J = \frac{2\pi^2}{3} \frac{\hbar^2 n^2}{m\gamma}, \quad (3)$$

see Eq. (22) of Ref. [10]. The effective theory (2) and (3) of the spin subsystem is consistent with the recent thermodynamic Bethe ansatz results [14].

The Hamiltonian describing all the low-energy excitations of the system is the sum $H_{\text{ph}} + H_\sigma$. An important assumption in its derivation was that all the relevant energy scales in the problem, such as the temperature T , are small compared to the bandwidth (the ‘‘Debye frequency’’) of the phonons E_F . In the following we limit our discussion to the most interesting case of $T = 0$.

The ground state of the ferromagnetic spin chain (2) is fully spin polarized. The excitations near this state, the magnons, have the well-known spectrum

$$\varepsilon(Q) = J(1 - \cos Q), \quad (4)$$

where Q is the wave vector defined with respect to the lattice of the spin chain (2) and varying in the range $-\pi < Q < \pi$. Since the spins are attached to particles filling the real space with density n , the physical momentum of the magnon is $p = \hbar n Q$ [15,16]. In the limit of small p , the spectrum (4) is quadratic, $\varepsilon(p) = p^2/2m^*$. Using Eq. (3), one finds the effective mass $m^* = (3/2\pi^2)\gamma m$, in agreement with the result of Ref. [17].

Let us now illustrate our approach based on the separation of the density and spin excitations in the form (1) and (2) by calculating the dynamic spin structure factor

$$S_\perp(q, \omega) = \int \frac{dx dt}{2\pi} e^{-iqx + i\omega t} \langle S^+(x, t) S^-(0, 0) \rangle. \quad (5)$$

Here $S(x)$ is the spin density operator, $S^\pm = S^x \pm iS^y$, and the expectation value $\langle \dots \rangle$ is evaluated in the fully polarized ground state of the system, with the polarization assumed to be directed in the positive z direction.

We start by expressing the spin density operator $S(x)$ in terms of the particle density operator $n(x)$ and the spin operator S_l ,

$$S(x) = n(x) S_{l(x)}. \quad (6)$$

Here $l(x)$ is the operator of the number of particles to the left of point x , i.e., $\partial_x l(x) = n(x)$. Its presence in Eq. (6) accounts for the fact that the operator $S(x)$ acts on site l of the spin chain (2) attached to the boson at point x ; cf. [11].

The problem of zero-temperature properties of strongly interacting bosons is considerably simpler than that of fermions [11], because of the simplicity of the ground state of the ferromagnetic Heisenberg model (2) and its single-particle excitation spectrum (4). In particular, the correlator $\langle S_l^+ S_l^- \rangle_\sigma$ for the spin chain (2) is easily found as

$$\langle S_l^+(t) S_l^-(0) \rangle_\sigma = \int \frac{dQ}{2\pi} e^{iQ(l-l') - i\Omega(Q)t}, \quad (7)$$

where $\Omega(Q) = \varepsilon(Q)/\hbar$ is given by Eq. (4). Substituting Eq. (6) into (5) and using (7), we find

$$S_\perp(q, \omega) = \int \frac{dx dt dQ}{(2\pi)^2} e^{-iqx + i[\omega - \Omega(Q)]t} \times \langle e^{iQ[l(x,t) - l(0,0)]} n(x, t) n(0, 0) \rangle_{\text{ph}}. \quad (8)$$

The expectation value $\langle \dots \rangle_{\text{ph}}$ is performed in the ground state of the phonon Hamiltonian (1). To evaluate it, we use the standard hydrodynamic expression for particle density $n(x) = n + \frac{1}{\pi} \partial_x \phi(x)$, and the resulting expression for the particle number

$$l(x) = nx + \frac{1}{\pi} \phi(x). \quad (9)$$

In the low-energy limit one can neglect the $\partial_x \phi$ correction to $n(x)$, and replace it with the average value n . However, it is important to include the field ϕ in Eq. (9) when evaluating the exponential in the second line of Eq. (8). The latter calculation is performed using the standard techniques [1], resulting in

$$\langle e^{iQ[l(x,t) - l(0,0)]} \rangle_{\text{ph}} = \frac{e^{inQx}}{[(1 + iDt)^2 + (Dx/u_\rho)^2]^{(Q/2\pi)^2}}, \quad (10)$$

where $D \sim E_F/\hbar$ is the phonon bandwidth.

In the denominator of Eq. (10) one can neglect x compared to $u_\rho t$. Indeed, to this approximation one finds that

Eq. (10) falls off at $Q \sim 1/\sqrt{\ln(Dt)}$, resulting in the estimate $x \sim 1/nQ \sim \sqrt{\ln(Dt)}/n \ll u_\rho t$; cf. [8,18]. The remaining calculation is straightforward, and one finds

$$S_\perp(q, \omega) = \frac{\vartheta(\omega - \Omega(q/n))}{\Gamma(q^2/2\pi^2 n^2)} \frac{n}{D} \times \left[\frac{\omega - \Omega(q/n)}{D} \right]^{q^2/(2\pi^2 n^2) - 1}. \quad (11)$$

Here $\vartheta(\omega)$ is the unit step function. Its presence in Eq. (11) expresses the obvious fact that the minimum energy of a spin excitation with momentum q is $\varepsilon(q/n)$, Eq. (4).

The structure factor (5) is essentially a Fourier transform of the correlation function $G_\perp(x, t)$ discussed recently by Zvonarev, Cheianov, and Giamarchi [8]. Their treatment is limited to the regime $q \ll n$; in which case our results are consistent with Eqs. (13) and (14) of Ref. [8]. On the other hand, our calculations show interesting behavior at larger q , especially the additional features at $\omega \ll J/\hbar$ and $q \approx \pm 2\pi n, \pm 4\pi n, \dots$

We now apply our technique to the calculation of the single-particle spectral functions of the system

$$A_s^+(q, \omega) = \int \frac{dx dt}{2\pi} e^{-iqx + i\omega t} \langle \psi_s(x, t) \psi_s^\dagger(0, 0) \rangle, \quad (12)$$

$$A_s^-(q, \omega) = \int \frac{dx dt}{2\pi} e^{-iqx + i\omega t} \langle \psi_s^\dagger(0, 0) \psi_s(x, t) \rangle, \quad (13)$$

where $\psi_s(x)$ is the annihilation operator of bosons with spin $s = \uparrow, \downarrow$.

As discussed above, at strong repulsion ($\gamma \rightarrow +\infty$) the density excitations of the system are identical to those of a gas of spinless hard-core bosons, whose density $\Psi^\dagger(x)\Psi(x)$ equals the true particle density $n(x)$. (Here Ψ is the annihilation operator of the hard-core bosons.) Then, assuming that the ground state is polarized in the positive z direction, one concludes that operator ψ_\uparrow simply destroys a hard-core boson, i.e., $\psi_\uparrow(x) = \Psi(x)$. In the low-frequency regime $\omega \ll D$ the spectral functions $A_\uparrow^\pm(q, \omega)$ can then be obtained in the framework of the hydrodynamic approach based upon the Hamiltonian (1) with $K = 1$. In this method the annihilation operator Ψ is expressed in terms of the bosonic fields entering the Hamiltonian (1) as

$$\Psi(x) = \sqrt{n} e^{-i\theta(x)} + \sqrt{n} e^{-i\theta(x)} \sum_{j=1}^{\infty} [e^{i2\pi j l(x)} + e^{-i2\pi j l(x)}]. \quad (14)$$

Here one should use the hydrodynamic form (9) of the particle number operator $l(x)$.

Compared to the first term in the right-hand side of Eq. (14), the remaining ones are formally irrelevant; i.e., their contribution to the observable quantities is expected to show additional power-law suppression at low energies. The reason for writing the full expression (14) is that this form accounts for the discreteness of particles

by enforcing the condition of $l(x)$ being integer [1,19]. As a result, at $\omega \ll D \sim nu_\rho$ the spectral function $A_\uparrow(q, \omega) = A_\uparrow^+(q, \omega) + A_\uparrow^-(q, \omega)$ shows not only the expected feature near $q = 0$, but also weaker features at $q = \pm 2\pi n, \pm 4\pi n, \dots$,

$$A_\uparrow(q, \omega) = \sum_{j=-\infty}^{\infty} \frac{\rho_\infty A_{|j|}}{\pi n u} \frac{\vartheta(\omega^2 - u^2(q - 2\pi j n)^2)}{\Gamma((j - \frac{1}{2})^2) \Gamma((j + \frac{1}{2})^2)} \times \left(\frac{|\omega - u(q - 2\pi j n)|}{2\pi n u} \right)^{(j - 1/2)^2 - 1} \times \left(\frac{|\omega + u(q - 2\pi j n)|}{2\pi n u} \right)^{(j + 1/2)^2 - 1}. \quad (15)$$

The hydrodynamic approach does not enable one to obtain the numerical coefficients ρ_∞ and A_j . To find them, one can compare the equal-time Green's function computed within this approach with the exact results [20–22]. This results in $\rho_\infty = 0.92418$, $A_0 = 1$, $A_1 = 1/16$, $A_2 = 9/2^{16}, \dots$

In this Letter we are primarily interested in the spectral function A_\uparrow^+ , because unlike A_\uparrow^\pm , it is sensitive to the non-trivial spin properties of the system. (The other spin- \downarrow spectral function, A_\uparrow^- , obviously vanishes.) To evaluate $A_\uparrow^+(q, \omega)$, one needs to express the operator $\psi_\uparrow(x)$ in terms of the density and spin variables entering the Hamiltonians (1) and (2). Following the ideas of Refs. [11,16] we identify

$$\psi_\uparrow(x) = \Psi(x) Z_{l(x), \downarrow}. \quad (16)$$

The presence of the hard-core boson operator Ψ accounts for the change in the total number of particles in the system, when a particle with spin- \downarrow is destroyed. In addition, the number of sites in the spin chain (2) reduces by one. This effect is accounted for by the operator $Z_{l, \downarrow}$, which by definition removes a site at position l in the spin chain, provided that the spin at that site is \downarrow . (Otherwise, the result is zero.)

In the fully spin-polarized state of an infinite spin chain (2), the correlator $\langle Z_{l, \downarrow} Z_{l', \downarrow}^\dagger \rangle_\sigma$ coincides with the spin-spin correlator (7). Then the substitution of Eq. (16) into (12) gives

$$A_\uparrow^+(q, \omega) = \int \frac{dx dt dQ}{(2\pi)^2} e^{-iqx + i[\omega - \Omega(Q)]t} \times \langle \Psi(x, t) e^{iQ[l(x, t) - l(0, 0)]} \Psi^\dagger(0, 0) \rangle_{\text{ph}}. \quad (17)$$

To evaluate the expectation value in the ground state of the Hamiltonian (1), we use the hydrodynamic theory expression (14) for the hard-core boson operator. Upon substitution of Eq. (14) into (17), the effect of the $j \neq 0$ terms amounts to the extension of the range of Q -integration from $(-\pi, \pi)$ to $(-\infty, +\infty)$. Then the correlator in the second line of Eq. (17) is computed with the help of the relation

$$\begin{aligned} & \langle e^{-i\theta(x,t)+iQI(x,t)} e^{i\theta(0,0)-iQI(0,0)} \rangle_{\text{ph}} \\ &= \frac{e^{iQnx}}{[iD(t-x/u_\rho)+1]^{\lambda_Q^+} [iD(t+x/u_\rho)+1]^{\lambda_Q^-}} \end{aligned} \quad (18)$$

with $\lambda_Q^\pm = (Q/\pi \pm 1)^2/4$, obtained using the standard techniques [1].

Similarly to our derivation of the dynamic spin structure factor (11), at low frequencies one can neglect the x -dependence in the denominator of Eq. (18) and find

$$\begin{aligned} A_\downarrow^+(q, \omega) &= \frac{\vartheta(\omega - \Omega(q/n))}{\Gamma(q^2/2\pi^2n^2 + 1/2)} \frac{1}{D} \\ &\times \left[\frac{\omega - \Omega(q/n)}{D} \right]^{q^2/(2\pi^2n^2) - 1/2}. \end{aligned} \quad (19)$$

This expression is the main result of our Letter. It is worth noting, that similarly to the case of $A_\uparrow(q, \omega)$, Eq. (15), the hydrodynamic approach does not enable one to accurately determine the prefactor in Eq. (19), whose calculation at this time remains an open problem.

The spectral function $A_\uparrow^+(q, \omega)$ is defined as the Fourier transform (12) of the spin- \downarrow boson Green's function. The latter was discussed recently by Akhanjee and Tserkovnyak [7]. Their theory focused on the $Jt \rightarrow \infty$ limit, and accounted only for the long-wavelength magnons, $q \ll n$. Calculating the inverse Fourier transform of Eq. (19) under these assumptions, we get

$$\langle \psi_\downarrow(x, t) \psi_\downarrow^\dagger(0, 0) \rangle = \frac{n}{\sqrt{2\pi DJ/\hbar}} \frac{1}{it + 0} \exp\left(\frac{i\hbar n^2 x^2}{2Jt}\right). \quad (20)$$

Comparison with the considerably more complicated Green's function given by Eq. (7) of Ref. [7] shows the same oscillating exponential factor (up to a missing π^2 in their exponent). Further, assuming $|x| \ll u_\rho t$ in the result of Ref. [7], we find that their prefactor is consistent with our Eq. (20).

It is interesting to compare the spectral function (19) with that of strongly interacting fermions [11]. The latter calculation, performed in the limit $J \ll \hbar\omega$, shows the same Gaussian peak as a function of q at small ω as the expression (19) at $\Omega \propto J \rightarrow 0$. In both cases the peak gives the leading contribution to the density of states, obtained as q integral of $A_\uparrow^+(q, \omega)$, resulting in $\nu(\omega) \propto 1/\sqrt{\omega \ln(D/\omega)}$, cf. [18,23]. In addition to the peak at $q = 0$, the spectral function of the fermion system shows weaker features at the Fermi surface, $q = \pm k_F$, as well as the shadow-band features at $\pm 3k_F, \pm 5k_F$, etc., with the Fermi momentum $k_F = \pi n/2$. At $J/\omega \rightarrow 0$ the boson spectral function (19) does not show any additional features. However, at $\omega \lesssim J/\hbar$ we find a sequence of additional features at $q = \pm 2\pi n, \pm 4\pi n$, etc.

To summarize, we have developed a new approach to study the low-energy properties of a gas of one-dimensional (iso)spin- $\frac{1}{2}$ bosons with strong short-range

repulsion. Our method is based on the separation of density and spin variables in the form (1) and (2) and the expression (16) for the boson annihilation operator. We applied this technique to the calculation of the dynamic spin structure factor (11) and the spectral function (19). At small ω they both show Gaussian peaks as a function of q centered at $q = 0$, as well as sequences of additional features at $q = \pm 2\pi n, \pm 4\pi n, \dots$. Although the spectral functions (11) and (19) are obtained for the Tonks-Girardeau regime ($\gamma \gg 1$ and $K = 1$), we expect similar additional features away from this limit.

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