Finite Drude weight for 1D low temperature conductors

Dariush Heidarian and Sandro Sorella

Istituto Nazionale di Fisica della Materia (INFM)-Democritos, National Simulation Centre, and Scuola Internazionale Superiore di Studi Avanzati (SISSA), I-34014 Trieste, Italy

We apply well established finite temperature Quantum Monte Carlo techniques to one dimensional Bose systems with soft and hardcore constraint, as well as to spinless fermion systems. We give clear and robust numerical evidence that, as expected, no superfluid density for Bosons or Meissner fraction for fermions, is possible at any non zero temperature in one dimensional interacting Bose or fermi lattice models, whereas a finite Drude weight is generally observed in gapless systems, in partial disagreement to previous expectations.

PACS numbers: 74.25.Fy, 71.27.+a, 71.10.Fd

I. INTRODUCTION

In the last decades there have been a lot of numerical and theoretical works to understand the role of strong correlation in lattice model Hamiltonians.1,2,3,4,5,6,7,8 Recently this issue has acquired an increasing attention and remarkable importance, due to the recent advances in the realization of optical lattices. In these experiments ultracold atoms behave as boson particles trapped on particular lattice sites, whereas the interaction and the hopping parameters can be tuned continuously. This important achievement has opened the possibility to verify directly the crucial role played by the electron correlation in very important model Hamiltonians defined on a lattice. An important example is the realization of a Mott insulating state in a system with strong on site repulsion.9,10 Moreover quite recently the possibility to include the Fermi statistics in optical lattices appears very promising and interesting.10

In 1D spinless fermion systems are equivalent to interacting Bose systems with hard-core constraint and are described by the same low energy theory -the Luttinger liquid theory-. Indeed this theory holds also for soft-core bosons, as shown in Ref.(7). Therefore, as far as the transport properties are concerned one should expect the same behavior both for fermions and bosons. On the other hand for lattice models, even in absence of disorder, the current does not commute with the Hamiltonian, implying its possible decay at finite temperature due to the backscattering processes.1,11 In this case the dynamical current-current correlation function also decays in time, leading to a current Fourier transform without \( \delta \) function at zero energy, namely without a finite Drude weight within the linear response theory.

Until few decades ago the absence of the Drude weight was the expected behavior of all interacting metals in lattice models or in real solids at finite temperature. However a quite clear numerical evidence has been reported in Ref(12) that current should not decay in integrable 1D models, namely for Hamiltonians that can be solved by Bethe ansatz techniques in 1D. These models essentially possess some hidden conservation law, that was conjectured to forbid the current decay process.12,13 Later several groups have reproduced this surprising effect14,15, with a noticeable exception that a finite Drude weight at finite temperature was found also for non-integrable models.12 On the other hand, from purely theoretical grounds this issue is not settled yet: in Ref(11) it was argued that backscattering processes can be effective also at finite temperature and in 1D non integrable models, whereas in Ref(10) it was proposed that also some particular non integrable model could provide a conserved current.

In this work we propose that the general behavior of 1D gapless systems is eventually characterized by a finite Drude weight at finite temperature, and we have found no exception in the models that we have studied. This conclusion is based on a careful and systematic numerical work on fairly generic one dimensional Bose and Fermi systems, that all show the same behavior, even though strong finite size effects are observed in the non integrable cases.

In the following we investigate the behavior of the Drude weight in 1D systems in the thermodynamic limit and finite temperature.

Model and Method : We have studied hardcore and softcore bosons in a 1D lattice with periodic boundary conditions. The Hamiltonian studied reads,

\[
H = \sum_i \left( -t(a_i^\dagger a_{i+1} + h.c.) + \frac{U}{2} n_i(n_i - 1) + V n_i n_{i+1} + W n_i n_{i+2} - \mu n_i \right)
\]

(1)

The sum is over all lattice sites \( i \), \( a_i^\dagger/a_i \) is the boson creation/annihilation operator at site \( i \), henceforth \( n_i \) is the particle number at site \( i \) and \( \mu \) is the chemical potential. \( t \) is the hopping amplitude which is set to one, \( U \) is the on-site repulsion, whereas \( V \) and \( W \) are the nearest and the next-nearest neighbor interactions, respectively. For hardcore bosons in the \( U \rightarrow \infty \) limit the Hamiltonian can be mapped onto an \( S = 1/2 \) spin system with \( S_i^z = n_i - 1/2 \) and \( S_i^+ = a_i^\dagger \). In this work we present our results for the half filled case of hardcore and softcore models. Most of our results have been obtained by Quantum Monte Carlo (QMC), using the stochastic series expansion (SSE) with the directed loop update.
Superfluid density $\rho_s$ (or spin stiffness in the equivalent spin model), is defined as the second derivative of the free energy with respect to a twist in the boundary conditions. In order to compute this quantity by QMC, it is convenient to apply linear response theory, relating this quantity to the current current response function $\Lambda(q, \omega_n) = \int_0^\beta d\tau \exp(i\omega_n \tau) \langle J(q, \tau)J(-q,0)\rangle/N$, where $J$ is the current operator and $\omega_n$ is Matsubara frequency. Then the following expression for the superfluid density is obtained:

$$\rho_s = \langle -K \rangle - \Lambda(q = 0; i\omega_n = 0) = \frac{(W^2)}{\beta}$$

(2)

where $\langle -K \rangle$ is the average kinetic energy per site, $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies and $W$ is the winding number. Similarly the Drude weight is obtained with the same expression but with a different order in the limit $\omega \rightarrow 0$ and $q \rightarrow 0$, namely $^{15, 19, 20}$

$$D = \langle -K \rangle - \text{Re} \Lambda(q = 0, \omega \rightarrow 0).$$

(3)

In SSE one can obtain $\Lambda$ very accurately in terms of Matsubara frequencies. Therefore analytic continuation of the data is required. In order to avoid difficulties of extrapolation to $i\omega_n \rightarrow 0$ at large temperatures, we have worked at relatively low temperatures ($\beta \geq 10$).

In principle, due to the different order of limits, the Drude weight and the superfluid density may be different when the following quantity remains finite in the thermodynamic limit $^{11, 15}$:

$$D - \rho_s = \sum_{E_n = E_m} \beta \exp(-\beta E_n) \langle \psi_n | J | \psi_m \rangle^2 / L,$$

where, $J$ is the current operator, while $E_n$ and $\psi_n$ are the $n$th eigenvalue and eigenstate of the many body system, respectively.

The current operator can be written as $J(q = 0) = \sum_b (H^b_0 - H^-_b)$ where $H^b_0 = t a^\dagger a_{i+1} + b$ is the bond index, corresponding to the site index $l$. The ensemble average of product of two local operators $H^b_{0l1}$ and $H^{b_2}_1(\tau)$ is:

$$\langle H^{b_2}_{0l1}(\tau) H^{b_1}_{1l1}(0) \rangle = \frac{1}{Z} \sum_{k,n,m=0} \sum_{\infty} \frac{(\tau - \beta)^n}{n!m!} \langle \psi_k | H^n H^{b_2}_1 H^m H^{b_1}_1 | \psi_k \rangle$$

(4)

where $\tau$ is the imaginary time, $Z$ is partition function and the summation over $n$ and $m$ comes from Taylor expansion of $e^{(-\beta + \tau)H}$ and $e^{-\tau H}$. Following Ref $^{14}$ the relation $^{14}$ can be simplified to

$$\langle \sum_{m=0}^{n-2} \frac{(\beta - \tau)^{n_s - m - 2} \tau^m}{\beta^{n_s}} \frac{(n_s - 1)!}{(n_s - m - 2)!m!} N_{m,b_1,b_2,\sigma_1,\sigma_2}^{b_1,b_2,\sigma_1,\sigma_2} \rangle_W$$

(5)

where $n_s$ is the length of sequence of the local operators and it changes in each QMC sampling. $N_{m,b_1,b_2,\sigma_1,\sigma_2}^{b_1,b_2,\sigma_1,\sigma_2}$ is the number of times that two operators $H^{b_1}_1$ and $H^{b_2}_1$ appear in this sequence with distance of $m$ local operators, and $\langle \cdots \rangle_W$ indicates an arithmetic average using configurations with relative weight $W$. In this work we introduce an efficient way to sample by SSE the current-current response function. To this end, we multiply expression (5) by $e^{i\omega_n \tau}$ and integrate over the imaginary time $\tau$, we obtain:

$$\frac{1}{\beta} \sum_{m=0}^{n-2} F_1(m + 1, n_s; 2i\pi n) N_{m,b_1,b_2,\sigma_1,\sigma_2}^{b_1,b_2,\sigma_1,\sigma_2} \rangle_W$$

(6)

where

$$F_1(m + 1, n_s; z) = \frac{(n - 1)!}{(n - m - 2)!m!} \int_0^1 dx \exp(2\pi n x) (1 - x)^{n - m - 2}$$

(7)

is the confluent hypergeometric function.

Therefore, the current-current correlation acquires contributions determined by length of operator string $n_s$. All these contributions are stochastically sampled in an efficient way, and in each statistical measurement the correlation function $\Lambda(q = 0, i\omega_n)$ has the following estimator:

$$\frac{1}{\beta} \sum_{\sigma_1,\sigma_2 = \pm} \left\langle \sum_{m=0}^{n-2} F_1(m + 1, n_s; 2i\pi n) N_{m,b_1,b_2,\sigma_1,\sigma_2}^{b_1,b_2,\sigma_1,\sigma_2} \right\rangle_W$$

(8)

where $N_{m,b_1,b_2,\sigma_1,\sigma_2}^{b_1,b_2,\sigma_1,\sigma_2}$ is the partition function.$^{15}$

**Discussion:** At zero temperature, for non degenerate ground state, the Drude weight and the superfluidity are the same. In a 1D system at any finite temperature $\rho_s$ is expected to be zero in the thermodynamic limit, whereas the Drude weight can be non-zero. For hardcore and soft-core bosons in a 1D lattice, a systematic size scaling of the superfluid density $\rho_s$ clearly shows that this quantity vanishes in the thermodynamic limit and for any finite temperature (see figures $^{1}$ and $^{2}$). Further, we find that, for a fixed set of parameters and at half filling, all superfluidity data versus $1/L$ collapse to one curve whenever the $x$-axis is appropriately scaled with the temperature $T$ (see figures $^{1}$ and $^{2}$). This analysis suggests the scaling $\rho_s(L) \sim \rho_s(L/L_c)$. If one takes the order of limit $T \to 0$ after $L \to \infty$, superfluidity remains zero even at zero temperature. Notice that by taking first the limit $T \to 0$ and then $L \to \infty$ superfluidity has a finite value for the gapless phase, but this is not a signature of superfluidity, rather the occurrence of a finite zero temperature Drude weight. Though in 1D is not possible to have a finite superfluid density at any non zero temperature, several authors have identified the finite zero temperature Drude weight with the superfluid density for a superfluid with vanishing critical temperature. We believe that this identification is a bit confusing and therefore we prefer to think about absence of superfluidity and superconductivity in 1D systems, as commonly reported in the textbooks.

Fig $3$ shows the current-current correlation versus $\omega_n$ in the metallic and insulating phases of an integrable...
FIG. 1: (color online) Superfluid stiffness for an integrable (a) and a non-integrable (b) model versus $\beta/L$. The system size $L$ is ranging from 50 to 1200.

FIG. 2: (color online) Superfluidity of the soft-core bosons versus scaled system size at half filling, the on-site interaction is $U = 4$

model ($W = 0, U = \infty$). The zero-frequency value is the superfluid density $\rho_s$ and the limit $\omega_n \to 0$ gives the Drude weight $D$. For $W = 0$ at zero temperature, there exists a critical value $V_c/t = 2$ below which the Drude weight is finite. In the first case (a) shown in Fig. 3 with $V/t = 2$ the Drude weight has a finite value at any finite temperature, which is consistent with the previous work. In the insulating phase (case b) with $V/t = 3$, the superfluid density coincides with the Drude weight and they both tend to zero as the system size increases.

In a non-integrable model such as hard-core bosons with nearest and next nearest neighbor interactions earlier works have suggested zero Drude weight as system size increases. With SSE we can go to very large system sizes and low temperatures and check the scaling dependence of the Drude weight. In Fig. 4 we have plotted current-current correlation versus Matsubara frequency for different $L$, and a fixed temperature $T = 1/100$. As shown in the same Figure 4 we have also found a finite Drude weight at finite $T$ in the celebrated Bose-Hubbard model with softcore constraint and in several other models (not shown). Although some evidence that few particular non integrable models could have a finite Drude weight at finite temperature have been reported before, here we have found a very convincing evidence that this behavior should be generic for 1D gapless system regardless from their integrability. We have supported this statement by state of the art numerical calculations obtained for very large system sizes and low temperature so that all possible extrapolations are perfectly under con-
In conclusion it turns out that, at low energy, all gapless lattice models studied scale to the Luttinger liquid fixed point where the backscattering is a marginally irrelevant coupling and the current is therefore conserved at the fixed point. This is therefore a peculiar and generic feature of 1D. Indeed in 2D systems, such as hardcore bosons with n.n. repulsion in a square and triangular lattice, we found no difference between $\rho_s$ and $D$.

Acknowledgments

We thank M. Troyer for useful discussions. This work is partially supported by COFIN-2005 and CNR.