The Effective Charge Velocity of Spin-$\frac{1}{2}$ Superlattices

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We calculate the spin gap of homogeneous and inhomogeneous spin chains, using the White's density matrix renormalization group technique. We found that the spin gap is related to the ration between the spin velocity and the correlation exponent. We consider a spin superlattice, which is composed of a repeated pattern of two spin-$\frac{1}{2}$ XXZ chains with different anisotropy parameters. The behavior of the charge velocity as a function of the anisotropy parameter and the relative size of sub-chains was investigated. We found reasonable agreement between the bosonization results and the numerical ones.

Keywords: Heinsenberg; DMRG; Plateaus; Luttinger liquid

I. INTRODUCTION

The study of one dimensional spin systems has increased in the last decade, impelled by theoretical results such as the Haldane conjecture[1, 2], which affirms that the ground state of isotropic Heisenberg chains with integer spin are gapful, whereas half-integer spin ones are gapless. Also, the synthesis of new materials has been crucial, because interesting phenomena such as the magnetization plateaus were observed[3]. Oshikawa, Yamanaka and Affleck[4] derived the condition $p(S-m^z) =$ integer, necessary for the appearance of the magnetization plateaus in 1D systems. Here, p is the number of sites in the unit cell of the magnetic ground state, S is the magnitude of the spin and m^z is the magnetization per site (taken to be in the z-direction).

The low-energy properties of spin chains with spin S in partially magnetized phases are described by the one-component Luttinger liquid theory. The first parameter of this theory is the location of the Fermi points $\pm k_F$, given by $2k_F = 2\pi(S-m)$, where m is the magnetization. The second parameter, the spin velocity is just an energy scale, whereas the third parameter determines the universality class and the critical exponents. Spin chains with $S = 1/2$ can be solved exactly using the Bethe Ansantz, particularly for the anisotropic model Yang and Yang[5] found a Luttinger liquid (gapless) phase for $-1 < \Delta < 1$, where Δ is the anisotropy parameter. The validity of the Luttinger liquid theory has also been checked numerically for $S = 1$[6], and in fact, it is conjectured in general for higher S[7].

Different Inhomogeneous spin chains has been studied in the last years[8–10]. These systems are obtained when we consider the spatial variation of the coupling constants or an inhomogeneous magnetic field. The special case of spin superlattice (SS) composed of a repeated pattern of two long and different spin-$\frac{1}{2}$ XXZ chains, was considered by one of us in a previous work[10]. We found that the magnetization curve presents a nontrivial plateaus whose magnetization value depends on the relative size of sub-chains $\ell = L_2/L_1$ and is given by $M_s = 1/(1+\ell)$. For away from the plateaus gapless phases appears, which were described in terms of Luttinger liquid superlattice model parameterized by an effective velocity and an effective correlation exponent[11]. Here we extent the previous study of the gapless region using the White's density matrix renormalization group technique[12, 13]. We considered lattice sizes up to 100 sites with up to $m = 600$ states per block. The truncation errors were below 10^{-9}.

II. MODEL AND RESULTS

Consider a SS whose unit cell consists of two $S = 1/2$ XXZ chains with different anisotropy parameters Δ_λ and sizes L_λ ($\lambda = 1,2$) (but the same planar coupling) in the presence of a magnetic field h applied along the anisotropy (z-)axis. Its Hamiltonian is

$$H = J\sum_{n=1}^{L}\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta_\lambda S_n^z S_{n+1}^z\right) - h\sum_{n=1}^{L} S_n^z, \quad (1)$$

where S^x, S^y and S^z denote the spin-$\frac{1}{2}$ operators and $L = N_c(L_1+L_2)$ is the superlattice size. Here, N_c is the number of unit cells, each of which has a basis with L_1+L_2 sites. We assume the chain is subjected to periodic boundary conditions. The homogeneous situation is recovered when $\Delta_\lambda = \Delta$, independent of the position.

We then take advantage of the fact that *each sub-chain is a LL connected at its ends to reservoirs* (the rest of the lattice) to describe the low-energy properties of the SS in terms of a LL superlattice (LLSL)[11] with Hamiltonian

$$H = \frac{1}{2\pi}\int dx \left\{u(x)K(x)\left(\partial_x\Theta\right)^2 + \frac{u(x)}{K(x)}\left(\partial_x\Phi\right)^2\right\}. \quad (2)$$

Here, we have introduced the sub-chain-dependent parameters $u(x)$ and $K(x)$. For x on the sublattice λ, one has $K(x) = K(J,\Delta_\lambda,h)$ and $u(x) = u(J,\Delta_\lambda,h)$, *i.e.,* the usual uniform LL parameters for each sub-chain, which can be obtained directly from the Bethe Ansatz solution[14].

In the Hamiltonian (2), $\partial_x\Theta$ is the momentum field conjugate to Φ: $[\Phi(x), \partial_y\Theta(y)] = i\delta(x-y)$. Φ and Θ are dual fields,

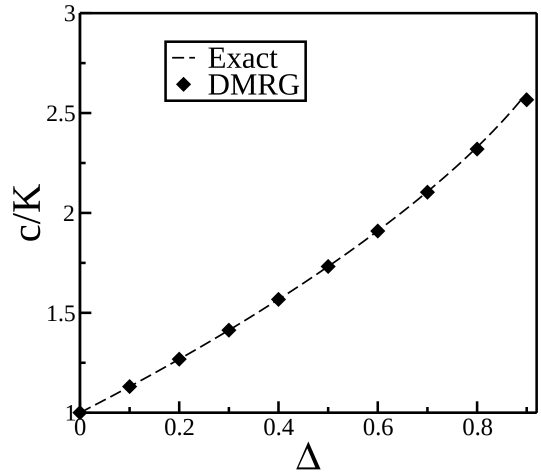

FIG. 1: The charge velocity for a homogeneous spin chain as a function of the anisotropy parameter. The dashed line was obtained from the exact solution using the Bethe Ansantz.

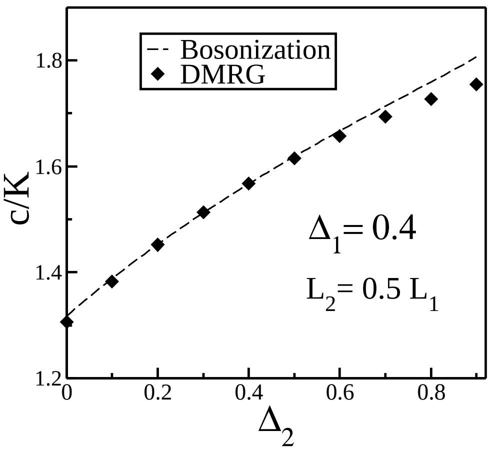

FIG. 2: c/K^* as a function Δ_2 for a SS with $\Delta_1 = 0.4$, $\ell = 1/2$ and $L = 100$. The continuous line was obtained using bosonization.

since they satisfy both

$$\partial_t \Phi = u(x) K(x) \partial_x \Theta \qquad (3)$$

and the equation obtained through the replacements $\Phi \to \Theta$, $\Theta \to \Phi$, and $K \to 1/K$. These equations can be uncoupled to yield

$$\partial_{tt}\Phi - u(x)K(x)\partial_x\left(\frac{u(x)}{K(x)}\partial_x\Phi\right) = 0, \qquad (4)$$

and a dual equation for Θ. The equations of motion are subject to the continuity of Φ and Θ[15]. This guarantees the continuity of the spin field. Since the time derivatives of these functions are continuous, the right hand side of Eq. (3) and its dual yield, as additional conditions, the continuity of $(u/K)\,\partial_x\Phi$ and $uK\partial_x\Theta$ at the contacts. Physically, this reflects the conservation of the z-axis magnetization current density $j = \sqrt{2}\partial_t\Phi/\pi$ at the interfaces between the sub-chains, see Eq. (3).

We diagonalize the Hamiltonian (2) through a normal mode expansion of the phase fields

$$\Phi(x,t) = -i\sum_{p\neq 0} \mathrm{sgn}(p)\frac{\phi_p(x)}{2\sqrt{\omega_p}}[b_{-p}e^{i\omega_p t} + b_p^{\dagger}e^{-i\omega_p t}] \qquad (5)$$

$$\Theta(x,t) = i\sum_{p\neq 0} \frac{\theta_p(x)}{2\sqrt{\omega_p}}[b_{-p}e^{i\omega_p t} - b_p^{\dagger}e^{-i\omega_p t}] \qquad (6)$$

where $b_p^{\dagger}$ are boson creation operators ($p > 0$). Plugging (5) into (4) we see that the normal mode eigenfunctions $\phi_p(x)$ and eigenvalues ω_p satisfy

$$\omega_p^2\phi_p(x) + uK\partial_x\left(\frac{u}{K}\partial_x\phi_p\right) = 0, \qquad (7)$$

subject to the same boundary conditions at the contacts as before, with $\phi_p(x)$ replacing $\Phi(x)$. The eigenvalues are given by

$$\begin{aligned}\cos p(L_1+L_2) &= \cos(\frac{\omega_p L_2}{u_2})\cos(\frac{\omega_p L_1}{u_1}) \\ &\quad -\frac{\eta}{2}\sin(\frac{\omega_p L_2}{u_2})\sin(\frac{\omega_p L_1}{u_1}), \qquad (8)\end{aligned}$$

where $\eta = K_1/K_2 + K_2/K_1$.

For $p \ll \pi/(L_2+L_1)$, $\omega_p \cong c\,|p|$, and the effective velocity for the SS is

$$c = \frac{u_1(1+\ell)}{\sqrt{1+\eta\ell u_1/u_2 + (\ell u_1/u_2)^2}}, \qquad (9)$$

where $\ell = L_2/L_1$. Clearly, $c \to u_2$ as $\ell \to \infty$, and $c \to u_1$ as $\ell \to 0$. In terms of the bosonic fields, the spin operators read

$$\begin{aligned} S_x^z &= \frac{M}{2} - \frac{1}{\sqrt{2\pi}}\partial_x\Phi + \frac{1}{\pi\alpha}\cos\left[2\Phi(x) - 2\overline{\phi}(x)\right], \\ S_x^+ &= \frac{1}{\sqrt{2\pi\alpha}}e^{-i\Theta(x)}\left\{1 + e^{2i\overline{\phi}(x)}\cos\left[2\Phi(x)\right]\right\}, \end{aligned}$$

where $\overline{\phi}(x) = k_F x - \phi_0(x)$, the Fermi momentum k_F is related to the magnetization by $k_F = (1+M)\pi/2$ and α is a cutoff parameter[16]. Thus, the correlation functions of the SS (for well separated x and y) are given by

$$\langle S^z(y)S^z(x)\rangle \sim \frac{C}{2\pi^2|x-y|^2} + A\frac{e^{2i\left(\overline{\phi}(y)-\overline{\phi}(x)\right)}}{m\,|x-y|^{2K^*}}, \qquad (10)$$

$$\left\langle S^+(y)S^-(x)\right\rangle \sim \frac{B_1}{|x-y|^{\overline{K}/2}} + B_2\frac{e^{2i\left(\overline{\phi}(y)-\overline{\phi}(x)\right)}}{|x-y|^{\overline{K}/2+2K^*}}, \qquad (11)$$

where the LLSL effective exponent is

$$K^* = \frac{\sqrt{1+\eta\ell u_1/u_2 + (\ell u_1/u_2)^2}}{\frac{1}{K_1} + \ell\frac{1}{K_2}\frac{u_1}{u_2}} \equiv f(K_1,K_2), \qquad (12)$$

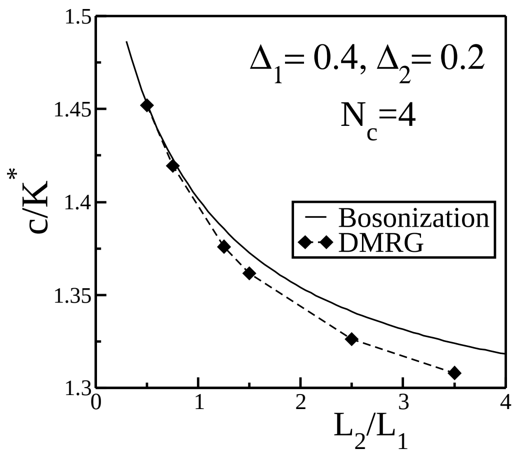

FIG. 3: c/K^* as a function ℓ for a SS with $\Delta_1 = 0.4$ and $\Delta_2 = 0.2$.

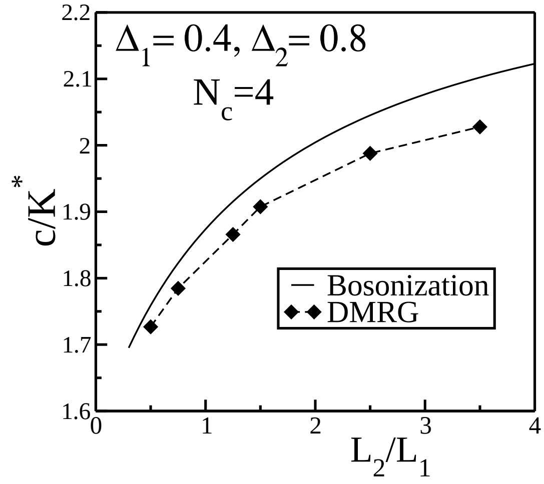

FIG. 4: c/K^* as a function ℓ for a SS with $\Delta_1 = 0.4$ and $\Delta_2 = 0.8$.

$\overline{K} = f(1/K_1, 1/K_2)$ and C is a function of system parameters and the sub-chain[11]. From Eqs. (10,11), we see how the correlation functions of the homogeneous system are recovered when $K_1 = K_2$ and $u_1 = u_2$. The important feature to notice in Eqs. (9) and (12) is the fact that the effective SS parameters represent a certain weighted average of the individual sub-chain velocities and correlation exponents. This weighted average is induced by the superlattice structure and it is a feature ubiquitous in TLLS's.[10, 11] It is straightforward to extract from the Hamiltonian (2) the finite-size spin gap of the system. It is given by

$$E\,(S^z_{tot} = 1, h = 0) - E\,(S^z_{tot} = 0, h = 0) = \frac{\pi c}{2K^* L}. \qquad (13)$$

From this relation we can estimate the charge velocity, which is given by the ration between the spin velocity and the correlation exponent.

First, we will calculate the charge velocity for a homogeneous spin chain as a function of the anisotropy parameter. In Fig.1 we observe that the charge velocity increases with the anisotropy parameter and an excellent agreement between the exact results and DMRG ones. But near the critical value we can see a slight discrepancy.

Now we can calculate the charge velocity from the scaling of the spin gap with the system size and to verify the predictions of Eqs. (9) and (12) for the effective Tomonaga-Luttinger parameters.

For a SS with $\Delta_1 = 0.4$, $N_c = 4$, $L = 100$ and $\ell = 1/2$ the numerically determined ratio c/K^* as a function of the anisotropy parameter Δ_2 is shown in Fig.2. For comparison, we also show the TLLS prediction obtained from the ratio of Eqs. (9) and (12) and from the known values of u_λ and K_λ for homogeneous chains. We can see that the ratio c/K^* increases gradually with the anisotropy parameter. When $\Delta_2 = 0.4$ the SS becomes a homogeneous chain and the exact value, obtained by Bethe Ansantz $u_1/K_1 = 1.57$ is recovered. Also we observed a good agrement between the bosonization results and the numerical ones for $\Delta_2 < 0.7$, but the scenario changes for bigger values, because the parameter Δ_2 is near the critical value, and we know that the results are poor in this case (see Fig. 1). The ration c/K^* as a function of ℓ for a SS with $\Delta_2/\Delta_1 < 1$ and $\Delta_2/\Delta_1 > 1$ is shown in Fig.3 and Fig.4 respectively. We used $N_c = 4$, $\Delta_1 = 0.4$, $\Delta_2 = 0.2$ and 0.8. The considered SS sizes were $L = 100, 76, 100, 52, 76, 100$, for $\ell = 1/2, 3/4, 5/4, 3/2, 5/2, 7/2$, respectively. The TLLS predictions are shown again for comparison. Note that c/K^* decreases (increases) with ℓ if $\Delta_2/\Delta_1 < 1$ ($\Delta_2/\Delta_1 > 1$). We can see that there is reasonable agreement, with slightly larger discrepancies at larger ℓ for both $\Delta_2/\Delta_1 < 1$ and $\Delta_2/\Delta_1 > 1$. The ratio u/K for homogeneous chains with anisotropy parameters $\Delta = 0.2$, $\Delta = 0.4$ and $\Delta = 0.8$ are equal to $u/K = 1.28$, $u/K = 1.57$ and $u/K = 2.33$, respectively (see Fig.1). c/K^* interpolates smoothly between u_1/K_1 and u_2/K_2 as ℓ increases, a manifestation of the spatial averaging due to the superlattice structure. We believe that the small discrepancies between the curves in Fig.3 and Fig.4 are due to the finite sizes of the sub-chains. We recall that the TLLS predictions are expected to hold asymptotically for very long sub-chains. For a gapless phase, the inhomogeneities created by the boundaries between sub-chains will give rise to Friedel oscillations which die out only as power laws.[17] These disturbances are expected to give rise to finite-size corrections to the TLLS predictions. We stress, however, that although the TLLS analysis predicts a sort of weighted average for the dependence of c/K^* on ℓ, the detailed form of this average is highly nontrivial. Yet, precisely this non-linear dependence is strikingly confirmed by the numerical data. We consider this as a stringent test of the predictions of the theory.

III. CONCLUSIONS

We found that using the scaling of the spin gap with the system size, the Tomonaga-Luttinger parameters for homogeneous and inhomogeneous spin chains can be estimated. For a spin chain with a superlattice structure the previous bosonization results for the effective spin velocity and effective correlation exponent were recovered numerically using density matrix renormalization group for finite systems. The ration c/K^* decreases (increases) with ℓ if $\Delta_2/\Delta_1 < 1$ ($\Delta_2/\Delta_1 > 1$). Thus, the low energy properties of spin superlattices are well described in terms of Luttinger liquid superlattice theory.

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