

Quantum Phase Diagram of the t - J_z Chain Model

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We present the quantum phase diagram of the one-dimensional t - J_z model for arbitrary spin (integer or half-integer) and sign of the spin-spin interaction J_z , using an *exact* mapping to a spinless fermion model that can be solved *exactly* using the Bethe ansatz. We discuss its superconducting phase as a function of hole doping ν . Motivated by the new paradigm of high temperature superconductivity, the stripe phase, we also consider the effect the antiferromagnetic background has on the t - J_z chain intended to mimic the stripe segments.

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Introduction.—Phase diagrams of generic models of strongly interacting quantum particles are considered fundamental to understanding the complex physical behavior of cuprate superconductors, heavy fermion, and related compounds. It is rare to encounter situations where unambiguously these diagrams can be completely determined and only a few exceptional cases are exactly solvable. It is a purpose of this paper to show that the t - J_z chain belongs to this latter class of models.

A new paradigm in superconductivity springs up as a consequence of the growing body of experimental evidence suggesting that the quantum state of high temperature superconductors is a striped phase. Unlike conventional conductors where the charge carriers distribute in an spatially homogeneous way, the stripe paradigm assumes that carriers cluster into quasi-one-dimensional (1D) channels. These channels act as domain walls separating different antiferromagnetic (AF) domains. It is remarkable that experiments are consistent with a spin ordering that is π shifted across the wall [1], indicating the topological character of these extended defects [2].

Motivated by this new paradigm Ref. [3] argued that planar models, with appropriate inhomogeneous magnetic terms, breaking translational and local spin SU(2) symmetries are appropriate to understanding neutron scattering and angle-resolved photoemission experiments in cuprates [4]. It is interesting to understand why spin anisotropies are relevant to obtain substantial pair hole binding and whether the stripes themselves have important superconducting fluctuations. The simplest representation of a stripe segment is realized by a t - J_z chain model.

Model Hamiltonian.—The Hamiltonian representing the 1D t - J_z model with L sites (equal to the length of the chain, i.e., lattice constant $a = 1$) and M holes with open boundary conditions (BC) [5] [the thermodynamic limit (TL), $L, M \rightarrow \infty$ with $\nu = M/L$ finite, is performed at the end of the calculation], for arbitrary half-integer spin S , is $\hat{H} = \hat{T} + \hat{H}_{J_z}$ with

$$\hat{T} = -t \sum_{\substack{\alpha=1 \\ \sigma \in [-S, S]}}^{L-1} \hat{T}_{\alpha, \sigma}, \quad \hat{T}_{\alpha, \sigma} = c_{\alpha \sigma}^\dagger c_{\alpha+1 \sigma} + \text{H.c.},$$

$$\hat{H}_{J_z} = J_z \sum_{\alpha=1}^{L-1} S_\alpha^z S_{\alpha+1}^z, \quad S_\alpha^z = \sum_{\sigma \in [-S, S]} \sigma c_{\alpha \sigma}^\dagger c_{\alpha \sigma}.$$

Here, $c_{\alpha \sigma}^\dagger$ ($c_{\alpha \sigma}$) creates (annihilates) a fermion of z spin component σ in a Wannier orbital centered at α . The Hilbert space of states corresponds to a constrained space with no doubly occupied sites [6].

Consider the set of parent states, labeled by the string configuration $\vec{\sigma}$, with M holes and $L - M$ quantum particles, $|\Phi_0(\vec{\sigma})\rangle$, defined as

$$|\Phi_0(\vec{\sigma})\rangle = |\underbrace{\sigma_1 \sigma_2 \sigma_3 \cdots \sigma_{L-M}}_{L-M} \underbrace{\circ \circ \circ \circ \cdots \circ}_M \rangle, \quad (1)$$

where σ_α indicates the z component of the spin of the particle at site α . These states are eigenstates of \hat{H}_{J_z} with energy $E_M(\vec{\sigma}) = J_z \sum_{\alpha=1}^{L-M-1} \sigma_\alpha \sigma_{\alpha+1}$, and z component of the total spin $S_z = \sum_{\alpha=1}^{L-M} \sigma_\alpha$.

From a given parent state one can generate a subspace of the Hilbert space $\mathcal{M}(\vec{\sigma})$ by applying the hopping operators $\hat{T}_{\alpha, \sigma}$ to the parent state and its descendants $|\Phi_i(\vec{\sigma})\rangle$,

$$|\Phi_1(\vec{\sigma})\rangle = \hat{T}_{L-M, \sigma} |\Phi_0(\vec{\sigma})\rangle, \quad (2)$$

or, in general,

$$|\Phi_i(\vec{\sigma})\rangle = \hat{T}_{\alpha, \sigma} |\Phi_j(\vec{\sigma})\rangle. \quad (3)$$

The dimension \mathcal{D} of the subspace $\mathcal{M}(\vec{\sigma})$ is $\binom{L}{M}$. Moreover, these different subspaces are orthogonal and are not mixed by the Hamiltonian \hat{H} , although they can be degenerate. In the following we will consider only the AF case $J_z > 0$. At the end we will discuss two important generalizations: the ferromagnetic (FM) $J_z < 0$ and the arbitrary integer spin hard-core boson cases.

Among all possible initial configurations the one corresponding to the Néel string $\vec{\sigma}_0$ [i.e., $\sigma_\alpha = (-1)^\alpha S$], which is twofold degenerate, turns out to be special. We want to show now that for a given number of holes M the subspace generated by the Néel parent state, $\mathcal{M}(\vec{\sigma}_0) \equiv \mathcal{M}_0$, contains the ground state. To this end, one has to realize that the kinetic energy matrix elements $\langle \Phi_i(\vec{\sigma}) | \hat{T} | \Phi_j(\vec{\sigma}) \rangle$ are the same for the different subspaces \mathcal{M} . Nonetheless, the magnetic matrix elements $\langle \Phi_i(\vec{\sigma}) | \hat{H}_{J_z} | \Phi_j(\vec{\sigma}) \rangle = \delta_{ij} A_i(\vec{\sigma})$ are different for the different subspaces, with $A_i(\vec{\sigma}_0) \leq A_i(\vec{\sigma})$ [7]. Notice

that if one assigns $\sigma_\alpha = 0$ to the presence of a hole at site α , then $A_i(\vec{\sigma}) = J_z \sum_{\alpha=1}^{L-1} \sigma_\alpha \sigma_{\alpha+1}$. Therefore, the Hamiltonian matrices $H_{i,j}^{\mathcal{M}}$ (of dimension $\mathcal{D} \times \mathcal{D}$) in each subspace \mathcal{M} , consist of identical off-diagonal matrix elements ($H_{i,j}^{\mathcal{M}} = H_{i,j}^{\mathcal{M}'}$, $i \neq j$) and different diagonal ones. These Hermitian matrices can be ordered according to the increasing value of the energy E_M of their parent states (for fixed L and M). For any $E_M(\vec{\sigma}) < E_M(\vec{\sigma}')$, $H^{\mathcal{M}'} = H^{\mathcal{M}} + B$, where B is a positive semidefinite matrix. Then, the monotonicity theorem [8] tells us that

$$E_k(\vec{\sigma}) \leq E_k(\vec{\sigma}') \quad \forall k = 1, \dots, \mathcal{D}, \quad (4)$$

where $E_k(\vec{\sigma})$'s are the eigenvalues of $H^{\mathcal{M}}$ arranged in increasing order [$E_k(\vec{\sigma}) \leq E_{k+1}(\vec{\sigma})$]. Therefore, we conclude that the lowest eigenvalue of \hat{H} must be in \mathcal{M}_0 , is $E_1(\vec{\sigma}_0)$, and is twofold degenerate [9].

Spinless fermion mapping.—The next step consists in showing, within the ground state subspace \mathcal{M}_0 , that the Hamiltonian \hat{H} maps into an attractive spinless fermion model. If one makes the following identification

$$|\underbrace{\uparrow\downarrow\uparrow\downarrow \dots \circ \circ \circ \circ \dots}_{L-M} \rangle \rightarrow |\underbrace{\bullet \bullet \bullet \dots \circ \circ \circ \circ \dots}_{L-M} \rangle, \quad (5)$$

i.e., any spin ($c_{\alpha S}^\dagger$ or $c_{\alpha -S}^\dagger$) maps into a single spinless fermion (b_α^\dagger) in \mathcal{M}_0 , it is straightforward to show that all matrix elements of $H^{\mathcal{M}_0}$ are identical to the matrix elements of the interacting quantum lattice gas

$$H = -t \sum_{\alpha=1}^{L-1} (b_\alpha^\dagger b_{\alpha+1} + \text{H.c.}) - J_z S^2 \sum_{\alpha=1}^{L-1} n_\alpha n_{\alpha+1} \quad (6)$$

in the corresponding new basis. In Eq. (6), $n_\alpha = b_\alpha^\dagger b_\alpha$.

Quantum phase diagram.—The attractive spinless fermion model of Eq. (6) certainly has a superconducting phase (i.e., correlation exponent $K_\rho > 1$) [10]. For arbitrary values of $J_z S^2$, t , and hole density ν , the spinless model is equivalent (via a Jordan-Wigner transformation) to a Heisenberg-Ising spin- $\frac{1}{2}$ chain (also known as XXZ model) with Hamiltonian [11]

$$H_{\text{xxz}} = \sum_{\alpha=1}^L J_\perp (s_\alpha^x s_{\alpha+1}^x + s_\alpha^y s_{\alpha+1}^y) + J_\parallel (s_\alpha^z s_{\alpha+1}^z + s_\alpha^z) \quad (7)$$

and $J_\perp = 2t$, $J_\parallel = -J_z S^2$. In this new representation the spin up (down) density is ν ($1 - \nu$). $J_\perp = 0$ represents the classical Ising limit while $J_\parallel = 0$ is the extreme quantum limit (XY model). In general, the exchange anisotropy parameter $\Delta = J_\parallel/J_\perp < 0$ determines the physical nature of the correlations while J_\perp defines the energy scale.

There is a vast literature on this model that was exactly solved by the Bethe ansatz [12]. For $|\Delta| < 1$, solutions of this model belong to the universality class called ‘‘Luttinger liquids’’ [13], with correlation functions characterized by power laws with nonuniversal exponents continuously depending on Δ . The correlation exponent K_ρ is determined from

$$K_\rho = \frac{\pi}{2} \nu^2 \kappa v_\rho = \pi \sqrt{\frac{\nu^2 \kappa D_c}{2}}, \quad (8)$$

where the Drude weight (or charge stiffness) D_c is related to the velocity of charge excitations v_ρ by $D_c = v_\rho K_\rho / \pi$ with $D_c = \frac{1}{2} \partial^2 e(\Phi) / \partial (\Phi/L)^2$ as usual [10], and κ is the isothermal compressibility. On the other hand, κ can be calculated from the variation of the ground state energy per site $e(\nu)$ as $(\nu^2 \kappa)^{-1} = \partial^2 e / \partial \nu^2$.

At $\nu = 1/2$, several quantities and properties are known in closed analytic form. There is a Mott transition at $\Delta = 1$ (umklapp scattering becomes relevant at $\Delta = 1$, while it is irrelevant for $|\Delta| < 1$). Moreover, the exact expressions for K_ρ and v_ρ can be determined from the Bethe ansatz [14]

$$K_\rho = \frac{\pi}{4(\pi - \mu)}, \quad v_\rho = \frac{\pi t \sin \mu}{\mu}, \quad (9)$$

which implies $D_c = \pi t \sin \mu / [4\mu(\pi - \mu)]$ with $\cos \mu = \Delta$. The energy per site ($|\Delta| < 1$) is given by

$$e(1/2) = \frac{\Delta t}{2} - 2t \sin \mu \int_0^\infty dx \frac{\sinh(\pi - \mu)x}{\cosh \mu x \sinh \pi x}. \quad (10)$$

Thus, one obtains $\frac{1}{2} \leq K_\rho \leq 1$ in the region $0 \geq \Delta \geq -1/\sqrt{2}$, and $K_\rho > 1$ (superconducting correlations dominate at large distances) for $-1 < \Delta < -1/\sqrt{2}$. At $\Delta = -1$, there is a transition to a phase segregated state ($\kappa = 2\mu / [\pi t \sin \mu (\pi - \mu)]$ diverges).

For $\Delta = 0$, the system reduces to a free spinless fermion system with energy per site $e = -\frac{2t}{\pi} \sin(\pi \nu)$, stiffness $D_c = -e/2$, and $\kappa^{-1} = -\pi^2 \nu^2 e$. This trivially corresponds to $K_\rho = \frac{1}{2}$. Also the cases $\nu \rightarrow 0^+$ and $\nu \rightarrow 1^-$ map to free fermions independently of the value of Δ , therefore, $K_\rho \rightarrow \frac{1}{2}$. The value $\Delta = -1$ is also special: After the unitary transformation $s_\alpha^{x,y} \rightarrow (-1)^\alpha s_\alpha^{x,y}$, the Hamiltonian H_{xxz} maps into the FM Heisenberg model in a magnetic field J_\parallel [full SU(2) symmetry is recovered]. Here $e = -\frac{t}{2} + (\frac{1}{2} - \nu)$, implying the opening of a gap with a diverging κ , i.e., $\Delta = -1$ determines the line of phase segregation for all densities ν .

Away from $\nu = 1/2$ and the special limiting cases discussed above, the quantities K_ρ and v_ρ are obtained from the numerical solution of the Bethe ansatz integral equations [15,16]. To calculate v_ρ one needs to determine hole excitations with a well-defined momentum q and energy Δe with respect to the ground state e . We find the velocity of this elementary excitation from $v_\rho = \lim_{q \rightarrow 0} d\Delta e/dq$, and together with the numerical second order derivative of $e(\nu)$, we determine the correlation exponent K_ρ . For $|\Delta| < 1$ the excitations are gapless. The resulting quantum phase diagram is shown in Fig. 1(a). Notice that the largest superconducting region corresponds to $\nu = 1/2$.

It is interesting to determine the influence of the anti-phase domain wall (ADW), associated with each charge, on the spin-spin correlations of the metallic and the

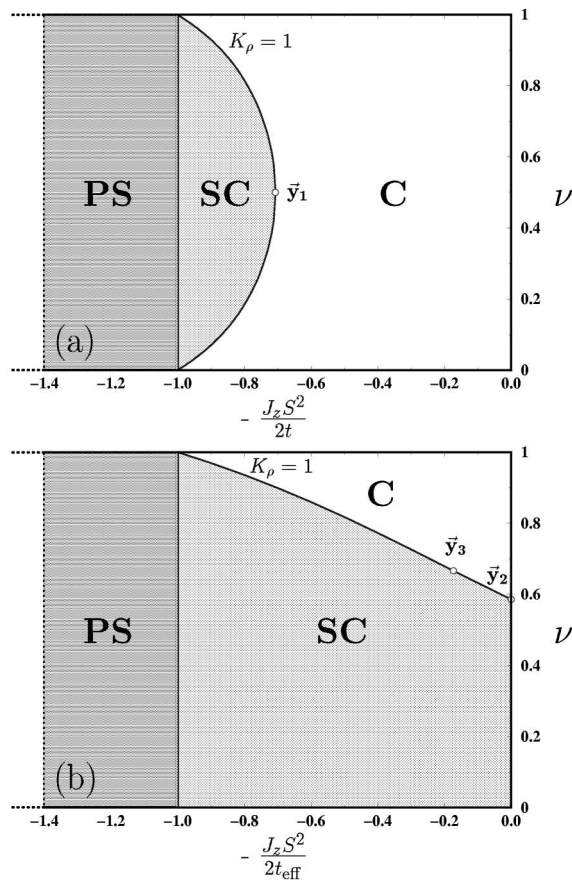


FIG. 1. Quantum phase diagrams of the (a) t - J_z chain, and (b) modified t - J_z model which includes the effects of the AF background where the chain is embedded [$\nu \in (0, 1)$]. There are three different quantum phases: phase segregated (PS), superconducting (SC), and metallic (C) phases. The last two belong to the “Luttinger liquid” universality class. Points with $K_\rho = 1$ known in closed analytic form are $\vec{y}_1 = (-\frac{1}{\sqrt{2}}, \frac{1}{2})$, $\vec{y}_2 = (0, 2 - \sqrt{2})$, and $\vec{y}_3 = (\cos\frac{5}{9}\pi, \frac{2}{3})$.

superconducting phases. It is well known [17] that the charge structure factor of the spinless model has a peak at $k = 2k_F = 2\pi\nu$. Since each charge of the effective model carries an ADW, the spin structure factor, $\mathbf{S}(k)$, will peak at $k = \pi \pm 2\pi\nu$ in the metallic phase. In the superconducting phase a broad peak at $k = \pi$ is obtained for $\mathbf{S}(k)$ since the pairs do not carry an ADW.

In the presence of a uniform magnetic field larger than the critical value leading to a saturated ferromagnetic state, the system maps onto a “repulsive” spinless model [Eq. (6) with the opposite sign for the interaction term]. In this way the magnetic field induces a transition from SC or PS phases to a metallic phase. For the special case $\nu = 1/2$ and $J_z S^2 / 2t > 1$ the transition is to an insulating charge density wave state.

Effect of AF boundaries on the chain.—We study now the effect of the AF background in which our stripe segments are embedded. This background provides a strong BC that results in an additional attractive (confining) poten-

tial for the holes on the stripe. In this way, an enhanced superconducting region is expected. In fact, the influence of the AF background on the stripe is equivalent to the effect a staggered magnetic field (STM) B_s (see Fig. 2). Since each hole carries an ADW, the staggered field gives rise to a confining linear potential between the α and the $\alpha + 1$ holes for even α . Therefore, the effect of a STM is to bind pairs of holes tightly by a string potential. These pairs interact as hard-core bosons. In the very dilute limit one expects these bosons to condense at $T = 0$ for any value of B_s/t and J_z/t lower than some critical value which gives rise to phase segregation.

In the limit $B_s/t \gg 1$ the model can be solved analytically for any concentration of hole pairs. In this limit the problem reduces to nearest-neighbors (NN) pairs of holes moving into an AF background (see Fig. 2). Each pair can hop to its NN with an effective hopping $t_{\text{eff}} = 2t^2/(B_s S + J_z S^2)$. In addition, there is an attractive $J_z S^2$ interaction between NN pairs which comes from the second term of Eq. (6). If we map each pair into a spinless particle and each spin into an empty site [18]

$$|\underbrace{\circ\circ\uparrow\downarrow\circ\circ\uparrow\downarrow\cdots}_{(L,M)}\rangle \rightarrow |\underbrace{\bullet\circ\circ\circ\bullet\circ\circ\cdots}_{(\tilde{L},\tilde{M})}\rangle, \quad (11)$$

the problem reduces to the spinless Hamiltonian Eq. (6). But as each pair is replaced by an effective particle, the number of particles and the length of the chain for the effective spinless problem are

$$\tilde{L} = L - \frac{M}{2}, \quad \tilde{M} = \frac{M}{2}, \quad (12)$$

where $\tilde{\nu} = \tilde{M}/\tilde{L} = \nu/(2 - \nu)$. Here, as in the FM case, we can use closed or open BC. The sign that arises after a cyclic permutation of fermions is absorbed in the BC. For an odd (even) number of fermions these BC are

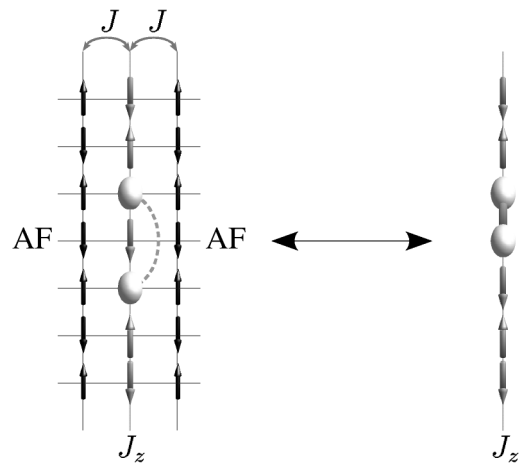


FIG. 2. Schematic representation of the effect of an AF background on a stripe segment. In this picture we assume that the concentration of holes in the stripe is such that there is no π shift between AF domains. If there were antiphase domains, then, there is no confining string potential even though two holes still like to be in adjacent sites.

periodic (antiperiodic). This corresponds to $M = 4n + 2$ ($M = 4n$) of the original problem. The relations between energies and charge velocities are [19]

$$e(\nu) = \tilde{e}(\tilde{\nu}) \left(1 - \frac{\nu}{2}\right), \quad v_\rho(\nu) = \tilde{v}_\rho(\tilde{\nu}) \frac{2}{2 - \nu}, \quad (13)$$

where $\tilde{e}(\tilde{\nu})$ and $\tilde{v}_\rho(\tilde{\nu})$ are the energy per site and charge velocity of the corresponding spinless model of concentration $\tilde{\nu}$. Therefore, simple algebraic manipulations lead to

$$K_\rho(\nu) = \tilde{K}_\rho(\tilde{\nu}) (2 - \nu)^2, \quad (14)$$

and the phase diagram is depicted in Fig. 1(b).

For completeness, we would like to mention that the mapping of the low energy spectra of the t - J_z model into the spinless Hamiltonian, Eq. (6), is also valid for the FM case, i.e., $J_z < 0$. In this case, the magnetic background, which is replaced by empty sites in the spinless model, is FM. Notice, however, that the effective spinless model is also attractive ($\Delta < 0$). This implies that the dynamics of the charge degrees of freedom in an AF background is the same as in the FM one. But in the latter case, the charges do not carry an ADW. Moreover, the mapping does not depend upon the statistics of the quantum particles. In other words, we could also apply these concepts to constrained quantum particles with integer spin S , i.e., hard-core bosons. In the large spin S limit, the quantum phase diagram of the t - J_z model approaches the one of the isotropic t - J Hamiltonian. Notice, however, the qualitative similarity between the phase diagram in Fig. 1(a) and the one for the isotropic spin- $\frac{1}{2}$ t - J model obtained numerically [20]. Finally, the solution can be trivially extended to the t - J_z - V model, where V represents a NN density-density interaction. The effect of V is simply to renormalize the spinless fermion interaction in Eq. (6). Furthermore, it is simple to prove that there is a family of bilinear-biquadratic spin-1 chain Hamiltonians that can be mapped onto a t - J_z - V model and, therefore, its low energy physics is exactly solvable [21].

In summary, we presented the exact quantum phase diagram of the t - J_z chain model for arbitrary spin S , particle statistics, and sign of the magnetic interaction J_z . We also exactly determined the phase diagram of a modified t - J_z chain that includes the effects of a strong antiferromagnetic background. While a superconducting phase exists in both cases, this phase is more prominent in the latter. Metallic, superconducting and segregated phases characterize these two phase diagrams.

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