Integrable Impurity in the Supersymmetric *t-J* Model

Gerald Bedürftig,[1] Fabian H. L. Eßler,[2] and Holger Frahm[1]
[1]*Institut für Theoretische Physik, Universität Hannover, D-30167 Hannover, Germany*
[2]*Department of Physics, Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, Great Britain*
(Received 13 September 1996)

An impurity coupling to both spin and charge degrees of freedom is added to a periodic *t-J* chain such that its interaction with the bulk can be varied continuously without losing integrability. Ground state properties, impurity contributions to the susceptibilities and low temperature specific heat are studied as well as transport properties. The impurity phase shifts are calculated to establish the existence of an impurity bound state in the holon sector. [S0031-9007(96)01892-3]

PACS numbers: 71.27.+a, 05.70.Jk, 75.10.Lp

Quantum fluctuations are known to play an important role in the physics of low dimensional strongly correlated electron systems: the low temperature properties of such systems in one spatial dimension have to be described in terms of a Luttinger liquid rather than a Fermi liquid. From an experimental point of view the transport properties of these systems in the presence of boundaries and potential scatterers are of particular interest. Recently several attempts have been made to describe such a situation: Using renormalization group techniques the transport properties of a 1D interacting electron gas in the presence of a potential barrier have been studied by Kane and Fisher [1]. Their surprising findings triggered further work using different techniques like boundary conformal field theory [2] and an exact solution by means of a mapping to the boundary sine-Gordon model [3,4]. In particular, the low temperature properties of magnetic (Kondo) impurities in a Luttinger liquid [5,6] have been investigated in great detail. In the present work we will investigate the effects of a particular type of potential impurity in a Luttinger liquid (where both spin and charge degrees of freedom are gapless) by means of an exact solution through the quantum inverse scattering method (QISM) [7].

Attempts to study effects due to the presence of impurities in many-body quantum systems in the framework of integrable models have a long successful history [8–12]. As far as lattice models are concerned the underlying principle in these exact solutions is the fact that the QISM allows for the introduction of certain "inhomogeneities" into vertex models without spoiling integrability. The *local* vertices—so called $\mathcal{L}$ operators—are objects depending on a complex valued spectral parameter acting on an auxiliary matrix space in addition to the quantum space of the model. They are solutions of a Yang-Baxter equation with an $\mathcal{R}$ matrix which itself acts on two copies of the matrix space and depends on the difference of the corresponding spectral parameters only. This allows one to build families of vertex models with site-dependent shifts of the spectral parameters and even different quantum spaces on different sites. The first fact has been widely used in solving models for particles with an internal degree of freedom by means of the nested Bethe ansatz [13]. The second approach has been first applied by Andrei and Johannesson to study the properties of an $S = \frac{1}{2}$ Heisenberg chain with an additional site carrying spin S [8] (see also [9]).

In this Letter we study the properties of the supersymmetric *t-J* model with one vertex replaced by an $\mathcal{L}$ operator acting on a four-dimensional quantum space. This preserves the $gl(2|1)$ supersymmetry of the model but at the same time lifts the restriction of no double occupancy present in the *t-J* model at the impurity site. The existence of a free parameter in the four-dimensional representations of the superalgebra [14] allows one to tune the coupling of the impurity to the host chain. As will be shown below, the present model allows one to study some aspects of a more general situation than the ones mentioned above: the impurity introduced here couples to *both* spin and charge degrees of freedom of the bulk Luttinger liquid. The extension of our calculation to the case of many impurities is straightforward.

The solution of the model is completely analogous to that of the pure *t-J* model [15]: The transfer matrix generating the Hamiltonian and the other conserved quantities is the trace of a product of the local $\mathcal{L}$ operators chosen as $\mathcal{L}_{tJ} = (\lambda + i\Pi)/(\lambda + i)$ for the regular sites (Π is a graded permutation operator acting on the tensor product of the auxiliary and the quantum space) and $\mathcal{L}_{34} \propto \lambda - i(\frac{\alpha}{2} + 1) + i\tilde{\mathcal{L}}$ on the site associated with the impurity. Written as a matrix in the three-dimensional auxiliary space $\tilde{\mathcal{L}}$ reads

$$\tilde{\mathcal{L}} = \begin{pmatrix} X_2^{\downarrow\downarrow} + X_2^{00} & -X_2^{\downarrow\uparrow} & Q_\uparrow \\ -X_2^{\uparrow\downarrow} & X_2^{\uparrow\uparrow} + X_2^{00} & Q_\downarrow \\ Q_\uparrow^\dagger & Q_\downarrow^\dagger & \alpha + X_2^{\uparrow\uparrow} + X_2^{\downarrow\downarrow} + 2X_2^{00} \end{pmatrix}.$$

 0031-9007/96/77(25)/5098(4)$10.00

Here $Q_\sigma = \sqrt{\alpha + 1}\, X_2^{0\sigma} - \sigma\sqrt{\alpha}\, X_2^{-\sigma 2}$ with $\sigma = \pm$, where $+$ $(-)$ corresponds to $\uparrow$ $(\downarrow)$ and where the Hubbard projection operators are given by $X^{ab} = |a\rangle\langle b|$ with $a, b = \uparrow, \downarrow, 2, 0$. The Hamiltonian is then given by the logarithmic derivative of the transfer matrix at spectral parameter $\lambda = 0$. In general, the form of this Hamiltonian is rather complicated and will be given elsewhere [16]. In any case the precise form of the lattice (impurity) interactions is not essential as far as low-energy properties are concerned: in the continuum limit only a small number of terms with scaling dimensions smaller than two will survive (taking the continuum limit and identifying the scaling dimensions of the composite operators at the impurity site is rather nontrivial though). Physically the model describes an impurity with four allowed states (spin-up/down electrons, empty/doubly occupied site) that couples to two neighboring t-J sites and also modifies the interaction between the t-J sites (see Fig. 1). In the limiting cases $\alpha \to 0(\infty)$ the Hamiltonian simplifies essentially: In the first case the impurity acts as an ordinary t-J site in the ground state below half filling, for $\alpha \to \infty$ the impurity site is doubly occupied and induces a twist in the boundary conditions of the host chain.

The eigenstates of the Hamiltonian for $N_\uparrow$ $(N_\downarrow)$ electrons with spin $\uparrow$ $(\downarrow)$ are constructed by means of the nested algebraic Bethe ansatz (NABA) leading to a system of algebraic equations for the spectral parameters λ_j $(j = 1, \ldots, N_e = N_\uparrow + N_\downarrow)$ and $\lambda_\alpha^{(1)}$ $(\alpha = 1, \ldots, N_\downarrow)$

$$\left(\frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}}\right)^L \left(\frac{\lambda_j - \frac{\alpha+1}{2}i}{\lambda_j + \frac{\alpha+1}{2}i}\right) = \prod_{\alpha=1}^{N_\downarrow} \frac{\lambda_j - \lambda_\alpha^{(1)} - \frac{i}{2}}{\lambda_j - \lambda_\alpha^{(1)} + \frac{i}{2}},$$

$$\prod_{j=1}^{N_e} \frac{\lambda_\alpha^{(1)} - \lambda_j + \frac{i}{2}}{\lambda_\alpha^{(1)} - \lambda_j - \frac{i}{2}} = -\prod_{\beta=1}^{N_\downarrow} \frac{\lambda_\alpha^{(1)} - \lambda_\beta^{(1)} + i}{\lambda_\alpha^{(1)} - \lambda_\beta^{(1)} - i}.$$

The corresponding eigenvalues of the Hamiltonian in the grand canonical ensemble are $E = -\mu N_e - (H/2)(N_\uparrow - N_\downarrow) + \sum_{j=1}^{N_e} 1/(\lambda_j^2 + \frac{1}{4})$.

The configuration of spectral parameters leading to the lowest energy state for given chemical potential and magnetic field are found in complete analogy to the pure t-J chain: the ground state for finite H is described by two filled Fermi seas of λ-$\lambda^{(1)}$-"strings" $\lambda_\pm = \lambda^{(1)} \pm \frac{i}{2}$ with real $\lambda^{(1)}$ associated with the holon excitations and real solutions λ_j describing spin degrees of freedom. In the thermodynamic limit dressed energies ϵ_c and ϵ_s can be associated with the excitations of these objects. They are given in terms of coupled integral equations which are identical to those found for the chain without impurities [17]. In the resulting ground state energy the impurity contribution can be identified from its L dependence which allows one to compute the occupation, magnetization, and susceptibilities of the impurity site. Analytical results for these expectation values are available only in limiting cases close to half filling and for densities near or below the critical density n_c related to the magnetic field by $H = 4\sin^2(\pi n_c/2)$ where the ground state is ferromagnetic and only real λ_j are present [16]. For general values of band filling and magnetic field the magnetization and particle number on the impurity site can be determined by numerically solving a set of two coupled integral equations (see Fig. 2): For $\alpha \to 0$ the impurity mimics the bulk behavior as discussed above. For large α the impurity

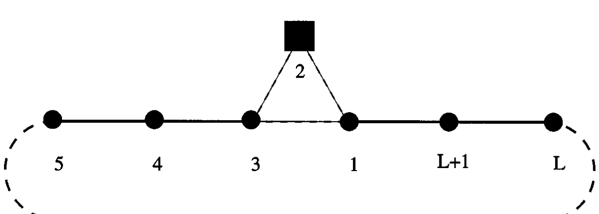

FIG. 1. Coupling of the impurity site (square) to the t-J bulk sites (circles).

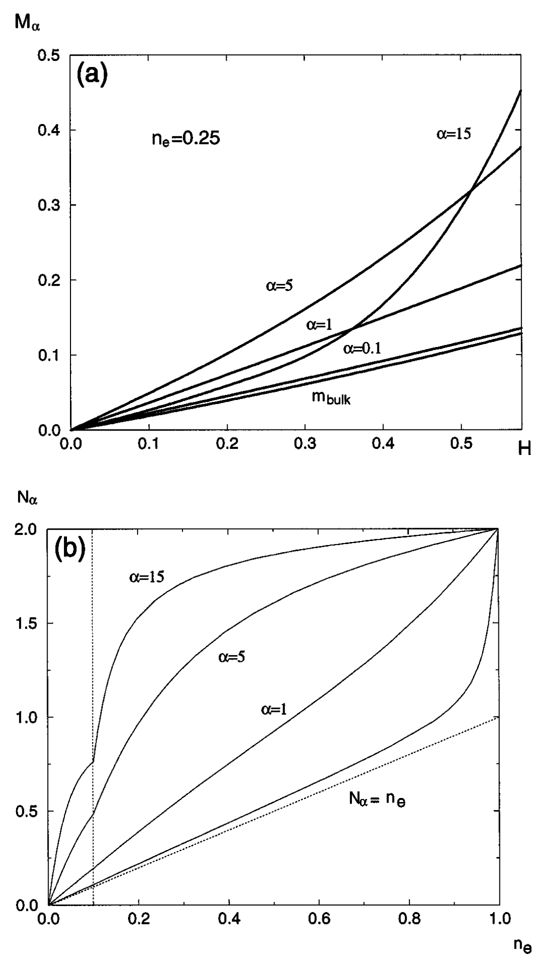

FIG. 2. (a) Impurity magnetization as a function of magnetic field for band filling $n_e = 0.25$ and several values of α. (b) Number of electrons located at the impurity as a function of the bulk electron density for fixed magnetic field $H = 0.1$ and several values of α. The dotted line denotes the critical electron density n_c below which the ground state is ferromagnetic.

occupation number is close to 1 (2) for $n_e < n_c$ ($> n_c$) leading to an enhanced (reduced) magnetization at small (large) electron densities. The magnetic susceptibility of the impurity near half filling is found to be $\sim\chi_{\rm bulk}/\alpha$. We note that the magnetization curves for sufficiently large α intersect the ones for small α.

In addition to the ground state properties the Bethe ansatz allows one to study the finite temperature behavior of the system. The thermodynamic Bethe ansatz equations for the system with impurity are the same as in the pure case [17]. Again the impurity contribution can be isolated in the free energy which can be evaluated explicitly in the limit $T \to \infty$ and for $H \gg T$ using Takahashi's method [18]. In the high temperature limit we find

$$\begin{aligned} F_{\rm bulk} &= -LT\ln\left(1 + e^{\mu/T}2\cosh\frac{H}{2T}\right), \\ F_{\rm imp} &= -\frac{2\alpha}{\alpha+2} \\ &\quad - T\ln\left(1 + e^{2\mu/T} + 2e^{\mu/T}\cosh\frac{H}{2T}\right), \end{aligned}$$

giving the correct entropy in this limit. Note that the parameter α enters the leading term in this expansion in a trivial way only.

For low temperatures $T \ll H$ we can determine the phase diagram of the system. Most interesting is the behavior at half filling where the impurity contribution to the specific heat is found to show a different temperature dependence than the one from the bulk: for $2\mu > H > 4$ the system is ferromagnetic and the low T free energy is given by (we suppress the contribution from the ground state energy)

$$\begin{aligned} F_{\rm bulk} &\approx -\frac{L}{2\sqrt{\pi}}T^{3/2}e^{(4-H)/T}, \\ F_{\rm imp} &\approx -Te^{(H/2-\mu)/T}. \end{aligned}$$

For smaller magnetic fields the thermodynamic equilibrium state is not ferromagnetically ordered, the bulk free energy is $F_{\rm bulk} \approx -\pi LT^2/(6v_s)$ with the spinon velocity v_s and the impurity contribution is $F_{\rm imp} \approx -\frac{2}{\alpha}T^{3/2}$ up to factors that cannot be calculated in closed form in general. Near $H = H_c$ this factor becomes

$$\sqrt{\frac{3}{8}}\,(4-H)^{-3/4}\exp\left[\frac{1}{T}\left(H/2 - \mu + \frac{2}{3\pi}(4-H)^{3/2}\right)\right].$$

The effect of the impurities on the transport properties of the system can be studied by calculating the spin and charge stiffnesses from the finite size corrections to the ground state energy of the model subject to twisted boundary conditions [19]. Following the analysis in [20] we introduce twist angles ϕ_c and ϕ_s affecting charge and spin degrees of freedom, respectively. The leading term in the resulting shift of the ground state energy can then be written as $\Delta E(\phi_c, \phi_s) = L^{-1}\phi_\alpha D_{\alpha\beta}(\alpha)\phi_\beta$ where charge (spin) stiffness are defined as $D^{(\rho)} = (L/2)\partial_\phi^2 \Delta E(\phi, 0) = D_{cc}$ $[D^{(\sigma)} = (L/2)\partial_\phi^2 \Delta E(\phi, -2\phi)]$. The analysis of the finite size corrections to the ground state energy yields the result that for the case of a single impurity the stiffnesses are not modified to leading order in L^{-1}. Hence, in spite of the presence of the impurity we find an infinite dc conductivity. This is completely different from the situation in the "weak-link"-type potential impurity discussed in [1,4]: such a weak link drives the Luttinger liquid to a strong coupling fixed point characterized by a vanishing conductivity. We believe that the behavior of the system considered here is related to its integrability and the absence of backscattering at the impurity.

The transport properties of the system do change if one considers a finite density n_i of impurity sites. In this situation the band filling can take values larger than 1 as the impurity sites allow for double occupancies. Comparing the charge stiffness to that of the pure t-J case one observes a reduction for densities just above the critical one. For larger band fillings the presence of the impurities leads to an enhancement of the stiffness (see Fig. 3). This is easily understood: $D^{(\rho)}$ vanishes at half filling in the t-J chain. The impurities do allow double occupancies thereby enlarging the phase space for the electrons which leads to an increase in the stiffness. At large fillings the stiffness increases as a function of α as the average occupation number of the impurity sites are close to doubly occupied which makes the movement of electrons between the t-J sites easier. In particular, the "absorption" of particles by the impurity sites for $\alpha = \infty$ leads to plateaus in the stiffness for $n_e < n_i$ (where it vanishes) and for $n_i + (1 - n_i)n_c < n_e < 2n_i + (1 -$

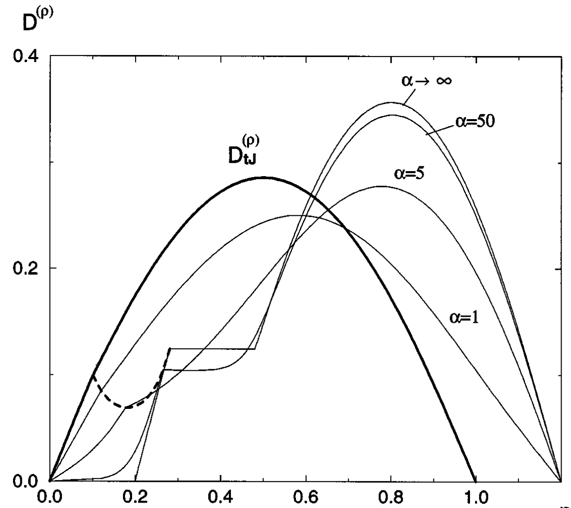

FIG. 3. Charge stiffness for a chain with 20% impurities as a function of the electron density at $H = 0.1$ for several values of α. The dashed line denotes the stiffness at the critical electron density $n_c(\alpha)$. (For comparison we have included the stiffness for the pure t-J chain $D_{tJ}^{(\rho)}$.)

$n_i)n_c$. For other fillings the stiffness is simply given by that of the t-J model (up to a rescaling). Similarly the reduction of the spin stiffness due to the addition of impurities can be understood.

Finally, to study the effects of the impurity on the excitations in the model we have computed the phase shifts acquired by holons and spinons due to scattering off the impurity in the case of a microscopic number of holes in the half filled ground state at vanishing magnetic field. The basic ingredient for this calculation is the quantization condition for factorized scattering of two particles with rapidities λ_1 and λ_2 on a ring of length N, namely, $\exp[iNk(\lambda_1)]S(\lambda_1 - \lambda_2)\exp[\psi(\lambda_1)] = 1$ where $k(\lambda)$ is the physical momentum in the infinite periodic system, $S(\lambda)$ is the bulk scattering matrix for scattering of particles 1 and 2, and $\psi(\lambda_1)$ is the phase shift acquired when scattering off the impurity (note that this incorporates the fact that there is no backscattering at the impurity). Using the known result for S [21] one extracts the impurity phase shifts using the method of [22,23]: both the spinon and holon impurity phase shifts are proportional to $\exp(-ik)$, where k denotes the physical momentum of spinons/holons in the t-J model *without impurity*. This reflects the fact that the impurity essentially decouples from the chain at half filling leading to a chain of $N - 1$ sites. In addition, the holons pick up a phase shift $(2i\lambda - \alpha)/(2i\lambda + i\alpha)$ due to the fact that the impurity site is charged. The pole at $\lambda = i\alpha/2$ corresponds to an impurity bound state for $\alpha < 2$.

To summarize, we have studied the effects of the addition of integrable impurities to the supersymmetric t-J model on certain zero and finite temperature properties of the system. The properties of the impurity, which couples to both spin and charge degrees of freedom, can be tuned by adjusting a continuous parameter α. Compared to the "weak-link" type impurities investigated by Kane and Fisher [1] it appears to be very special in that its dc conductivity is unchanged by the addition of a single impurity. We have argued that this is due to the absence of backscattering terms on the level of the dressed excitations (holons and spinons). Although the verification by explicit construction of the continuum limit for this system appears difficult, one may speculate that similar to the case of a Kondo impurity in a Luttinger liquid [6] a backscattering term would drive the system to a new fixed point. Hence the present model can be interpreted as an unstable fixed point from a renormalization group point of view (see also [24]).

F.H.L.E. is supported by the EU under Human Capital and Mobility fellowship Grant No. ERBCHBGCT940709. This work has been supported in parts by the Deutsche Forschungsgemeinschaft under Grant No. Fr 737/2-2.

[1] C. L. Kane and M. P. A. Fisher, Phys. Rev. B **46**, 15 233 (1992).
[2] J. L. Cardy, Nucl. Phys. **B324**, 581 (1989).
[3] P. Fendley and H. Saleur, Phys. Rev. Lett. **75**, 4492 (1995); P. Fendley, A. W. W. Ludwig, and H. Saleur, Phys. Rev. B **52**, 8934 (1995).
[4] A. M. Tsvelik, J. Phys. A **28**, L625 (1995).
[5] I. Affleck, Nucl. Phys. **B336**, 517 (1990); I. Affleck and A. W. W. Ludwig, Nucl. Phys. **B352**, 849 (1991).
[6] P. Fröjdh and H. Johannesson, Phys. Rev. Lett. **75**, 300 (1995); Phys. Rev. B **53**, 3211 (1996).
[7] V. E. Korepin, A. G. Izergin, and N. M. Bogoliubov, *Quantum Inverse Scattering Method, Correlation Functions and Algebraic Bethe Ansatz* (Cambridge University Press, Cambridge, 1993).
[8] N. Andrei and H. Johannesson, Phys. Lett. **100A**, 108 (1984).
[9] K. J. B. Lee and P. Schlottmann, Phys. Rev. B **37**, 379 (1988); P. Schlottmann, J. Phys. Condens. Matter **3**, 6617 (1991).
[10] H. J. de Vega and F. Woynarovich, J. Phys. A **25**, 4499 (1992); H. J. de Vega, L. Mezincescu, and R. I. Nepomechie, Phys. Rev. B **49**, 13 223 (1994); Int. J. Mod. Phys. B **8**, 3473 (1994).
[11] P.-A. Bares, Report No. cond-mat/9412011.
[12] N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983); A. M. Tsvelik and P. W. Wiegmann, Adv. Phys. **32**, 453 (1983).
[13] C. N. Yang, Phys. Rev. Lett. **19**, 1312 (1967).
[14] A. J. Bracken, M. D. Gould, Y.-Z. Zhang, and G. W. Delius, J. Phys. A **27**, 6551 (1994).
[15] F. H. L. Eßler and V. E. Korepin, Phys. Rev. B **46**, 9147 (1992); A. Foerster and M. Karowski, Nucl. Phys. **B396**, 611 (1993).
[16] G. Bedürftig, F. H. L. Eßler, and H. Frahm (to be published).
[17] P. Schlottmann, Phys. Rev. B **36**, 5177 (1987).
[18] M. Takahashi, Prog. Theor. Phys. **52**, 103 (1974).
[19] B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990); Sov. Phys. Solid State **32**, 905 (1990).
[20] P.-A. Bares, J. M. P. Carmelo, J. Ferrer, and P. Horsch, Phys. Rev. B **46**, 14 624 (1992).
[21] P. A. Bares, G. Blatter, and M. Ogata, Phys. Rev. B **44**, 130 (1991).
[22] V. E. Korepin, Theor. Math. Phys. **41**, 169 (1979).
[23] N. Andrei and J. H. Lowenstein, Phys. Lett. **80A**, 401 (1980).
[24] E. S. Sørensen, S. Eggert, and I. Affleck, J. Phys. A **26**, 6757 (1993).