Quantum Coherence in an Exactly Solvable One-Dimensional Model with Defects.

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Abstract. – Using the Quantum Inverse Scattering Method we construct an integrable Heisenberg-XXZ model, or equivalently a model for spinless fermions with nearest-neighbour interaction, with defects. Each defect involves three sites with a fine tuning between nearest-neighbour and next-nearest-neighbour terms. We investigate the finite-size corrections to the ground-state energy and its dependence on an external flux as a function of a parameter v, characterizing the strength of the defects. For intermediate values of v, both quantities become very small, although the ground-state wave function remains extended.

Introduction. – Three recent experiments have demonstrated that persistent currents, periodic in the magnetic flux, exist in mesoscopic metal [1] and semiconductor [2] rings at very low temperatures. Surprisingly, though the current is found to be small, of the order of $\sim ev_F/L$ for single rings (v_F is the Fermi velocity, and L the circumference), it is still two orders of magnitude larger than expected theoretically, at least for the metal rings studied in [1]. In the latter, the electron motion is diffusive, *i.e.* the elastic mean free path is much smaller than the circumference. While it is well established that the Coulomb interaction gives an important contribution to the current for a measurement on an ensemble of rings [3], the interaction effect in single rings is far from being understood theoretically.

In this article, we consider a one-dimensional, interacting model in the presence of a magnetic flux, or, equivalently, with twisted boundary conditions. We introduce very special «defects» into the model describing spinless fermions with nearest-neighbour interaction. Despite this inhomogeneity, the model remains integrable and we present exact results for the finite-size corrections to the ground-state energy, and its dependence on the magnetic flux, as a function of a parameter v characterizing the strength of the defects. Clearly, our investigation does not provide an answer to the questions raised by the experiments (there, the number of transverse channels is much larger than one). Instead, our work is closely related to, and an extension of, various recent theoretical studies [4-9] of quantum coherence in strongly interacting electron systems.

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Construction of the model. – Using the Quantum Inverse Scattering Method (QISM), we construct our model from the $\mathscr{R}$ and $\mathscr{L}$ matrices of the Heisenberg-XXZ model on an inhomogeneous lattice as, for example, described in [10]. The central equation of the QISM is the Yang-Baxter equation, which guarantees that a scattering process factorizes in two-particle scattering processes and does not depend on the order of these. In order to construct a model with defects, we allow that the local $\mathscr{L}_n$ matrix depends, in addition to the spectral parameter λ, on a parameter v_n, $\mathscr{L}_n(\lambda) = \mathscr{L}(\lambda + v_n)$. The transfer matrix is given by $T(\lambda) = \mathrm{Tr} \prod_{n=1}^{M} \mathscr{L}(\lambda + v_n)$, where M denotes the number of lattice sites. To include twisted boundary conditions, we multiply the $\mathscr{L}_M$ matrix of the Heisenberg-XXZ ring by $\exp[i\phi\hat{\sigma}^z/2]$.

The Hamiltonian is then given as the logarithmic derivative of the transfer matrix with respect to λ, at a specific value [10]. In particular, in the special case in which all $v_n = 0$, we obtain the usual XXZ model, which can be transformed to a spinless fermion model by a Jordan-Wigner transformation. For a general set of parameters, $\{v_n\}$, it is difficult to determine the Hamiltonian explicitly, with one exception, namely where there are no defects on neighbouring sites, *i.e.* $v_n v_{n+1} = 0$ for all n. This is the situation we study in the following. As an illustration, consider a vanishing nearest-neighbour interaction, and a single defect at the site n_1 characterized by the parameter v. The resulting Hamiltonian is given by

$$\mathscr{H} = \mathscr{H}^0 + \mathscr{H}_{n_1}^{\mathrm{I}}(v) = - \sum_{n=1}^{M} (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \mathscr{H}_{n_1}^{\mathrm{I}}(v), \tag{1}$$

$$\mathscr{H}_{n_1}^{\mathrm{I}}(v) = \left(1 - \frac{1}{\cosh v}\right)(c_{n_1-1}^\dagger c_{n_1} + c_{n_1}^\dagger c_{n_1+1}) - \exp[i\pi/2]\,\mathrm{tgh}(v)\,c_{n_1-1}^\dagger c_{n_1+1} + \mathrm{h.c.}, \tag{2}$$

where the $\{c_n^\dagger\}$ and $\{c_n\}$ are the standard fermion creation and annihilation operators. The generalization to r defects is straightforward (assuming $v_n v_{n+1} = 0$),

$$\mathscr{H} = \mathscr{H}^0 + \sum_{l=1}^{r} \mathscr{H}_{n_l}^{\mathrm{I}}(v_{n_l}), \tag{3}$$

where n_l denotes the location of a defect with strength v_{n_l}. An illustration is given in fig. 1. The expression for the Hamiltonian in the presence of a finite nearest-neighbour interaction is more lengthy but similar in structure, *i.e.* a defect located at n_l affects the lattice sites $n_l - 1$, n_l, and $n_l + 1$ only [11].

Single defect, no interaction. – As is apparent from eq. (2), for $v = 0$, the Hamiltonian reduces to $\mathscr{H}^0$, *i.e.* the standard single-band tight-binding model (the hopping matrix element is chosen to be unity). In the opposite limit, $v = \infty$, the lattice site n_1 is cut out of the ring. As a result, the model represents free fermions on a ring of $M - 1$ sites, however, with an additional phase factor $\exp[i\delta_1]$, $\delta_1 = \pi/2$, for the hopping between $n_1 - 1$ and $n_1 + 1$, plus one uncoupled site. We emphasize that the parameters, $\cosh^{-1}(v)$ and $\mathrm{tgh}(v)$, as well as the
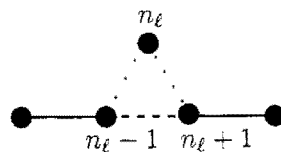

Fig. 1. – Graphical representation of a defect at the site n_l, compare eq. (2). Note that for $v \to 0$ ($v \to \infty$) the dashed (dotted) lines representing the corresponding hopping contributions are effectively cut.
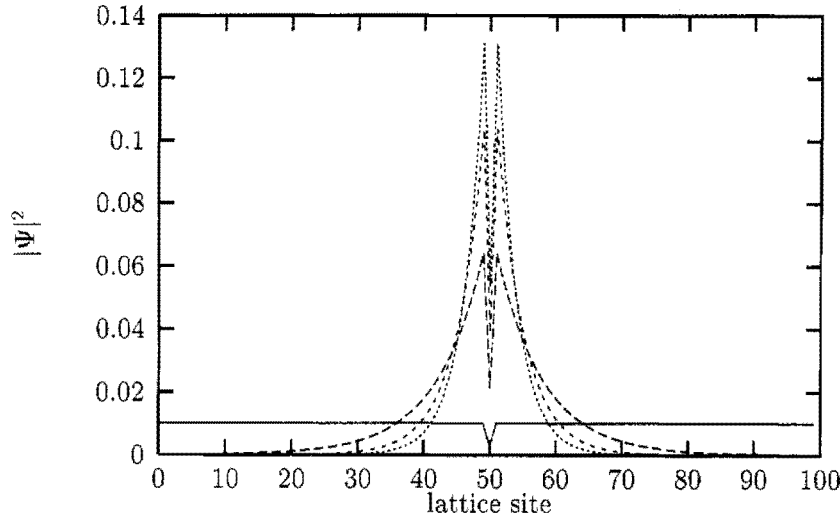
Fig. 2. – Squared modulus of the wave function of the lowest-energy eigenstate for the non-interacting limit in the presence of a single defect ($v = 1$) at the site $n_1 = 50$ ($M = 100$). For the integrable case ($\delta_1 = \pi/2$), the eigenstate is extended, though reduced at the defect, while a detuning of the defect phase ($\delta_1 \neq \pi/2$) leads to a localization of the wave function. —— $\delta_1 = \pi/2$, – – – $\delta_1 = 3\pi/8$, – – – – $\delta_1 = \pi/4$, ····· $\delta_1 = 0$.

phase factor $\delta_1 = \pi/2$, are fine-tuned in the following sense: a generic impurity breaks translational invariance and lifts the degeneracies of the single-particle spectrum, which are found at $\phi = 0$, $\pm\pi$. While our defects also break translational invariance, this symmetry is replaced by another, of not as clear physical origin. As a result we find that even when changing v, no degeneracies are lifted—they only occur at different, v-dependent values of ϕ. The corresponding v-dependent symmetry operators can be constructed[10].

The localization of electronic states is another, well-established phenomenon, in one-dimensional disordered systems. In fig. 2, we plot the squared modulus of the wave function for the single-particle level lowest in energy. Clearly, for the integrable case, the wave function is extended though reduced at the defect. Allowing, however, the phase δ_1 to be different from $\pi/2$, which corresponds to the non-integrable case, we find a drastically different behaviour with a clear localization of the wave function near the defect.

Several defects, finite interaction. – The results for a finite nearest-neighbour interaction, and in the presence of several defects, are obtained from the Bethe equations, which we derive from the algebraic Bethe ansatz, with the result

$$\left[\frac{\cosh(\lambda_j - i\eta)}{\cosh(\lambda_j + i\eta)}\right]^{M-r} \prod_{l=1}^{r} \frac{\cosh(\lambda_j + v_{n_l} - i\eta)}{\cosh(\lambda_j + v_{n_l} + i\eta)} = \exp[i\phi] \prod_{\substack{k=1 \\ k \neq j}}^{N} \frac{\sinh(\lambda_j - \lambda_k - 2i\eta)}{\sinh(\lambda_j - \lambda_k + 2i\eta)}. \quad (4)$$

Here, N is the number of fermions and M and r denote the number of lattice sites and defects, respectively. The nearest-neighbour interaction, in units of the hopping matrix element, is parametrized as $\Delta = \cos(2\eta)$ (we consider $-1 < \Delta < 1$ only, $\Delta > 0$ corresponds to an attractive interaction). For the spin model and for the fermion model with an odd number of fermions, $\phi = 0$ (π) represents periodic (antiperiodic) boundary conditions, and *vice versa* for an even number of fermions. The phase ϕ is directly related to the magnetic flux Φ, for odd N according to the relation $\phi = 2\pi\Phi/\Phi_0$, $\Phi_0 = h/e$. (For even N, $\phi = 2\pi\Phi/\Phi_0 - \pi$.)

Equations (4) have a remarkable consequence: given a set of defect parameters $\{v_n\}$ the roots $\{\lambda_j\}$ of the Bethe equations do not depend on the distribution of the defects over the

sites. This implies that the defects can be moved or permutated without any change in the energy spectrum, which is quite different from the observation that in mesoscopic physics, thermodynamic and transport properties can vary considerably by moving only one impurity by a few lattice constants.

In the following, we simplify our defect model further, by assuming that $|v_{n_i}| = v$, and choosing an equal number of defects of strength $+v$ and $-v$. With this choice, the ground-state energy is an even function of the phase ϕ. We define $x = \lim_{r, M \to \infty} (r/M)$ to be the density of defects. Assuming in addition $N = M/2$, i.e. a half-filled band, we calculate in a first step the ground-state energy per lattice site in the thermodynamic limit, $e_\infty = \lim_{M \to \infty} e_M$, $e_M \equiv E_M/M$. Using the standard method [10,12], we find

$$e_\infty = -\sin^2(2\eta) \int_{-\infty}^{\infty} \frac{\rho_\infty(\lambda)}{\cosh(\lambda + i\eta)\cosh(\lambda - i\eta)} d\lambda - \frac{\cos(2\eta)}{2}, \qquad (5)$$

$$\rho_\infty^0(\lambda) = \left\{ 2(\pi - 2\eta)\cosh[\pi\lambda/(\pi - 2\eta)] \right\}^{-1}, \qquad (6)$$

$$\rho_\infty(\lambda) = (1 - x)\rho_\infty^0(\lambda) + x[\rho_\infty^0(\lambda + v) + \rho_\infty^0(\lambda - v)]/2. \qquad (7)$$

The last equation relates the density of roots for the infinite system, ρ_∞, to the corresponding density of roots of the homogeneous system, ρ_∞^0. For $v = 0$, clearly, $\rho_\infty = \rho_\infty^0$, and we recover the results of [12]. On the other hand, for $v \to \infty$, it follows from (7) that $\rho_\infty = (1 - x)\rho_\infty^0$; as a direct consequence, the integral in eq. (5) is simply multiplied by the factor $(1 - x)$ compared to the homogeneous case, and e_∞ is easily calculated. Apparently, for all values of v, the ground-state energy e_∞ is a linear function of the defect concentration (and it is independent of ϕ, i.e. the boundary conditions).

The leading-order finite-size corrections can be determined with the help of the Wiener-Hopf technique, as described in [4], with the result

$$e_M(\phi) - e_\infty = -\frac{(\pi^2/6)\sin(2\eta)/(\pi - 2\eta)}{1 - x + x\cosh[\pi v/(\pi - 2\eta)]}\left(1 - \frac{3\phi^3}{4\pi\eta}\right)\frac{1}{M^2}, \qquad (8)$$

which for $x = 0$ is in agreement with [4]. In contrast to e_∞, the finite-size corrections depend in a non-linear way on the defect density, and they are exponentially suppressed, $\sim \exp[-\pi v/(\pi - 2\eta)]$, in the limit of large v. The finite-size corrections, $(e_M - e_\infty)M^2$, obtained by solving numerically the Bethe equations (4), are plotted in fig. 3 as a function of the defect parameter v, for half-filling ($N = M/2$), and $\Delta = 0.5$, $x = 0.2$. The system size is varied from 10^2 to 10^4. The numerical result is in perfect agreement with the analytical expression (8), but we also observe that the limits $M \to \infty$ and $v \to \infty$ do not commute. Taking $v \to \infty$ first, we obtain a system with r sites cut out; however, the occupancy of these sites still appears in the Hamiltonian, but as a good quantum number. The finite-size corrections thus correspond to a system of $M - r$ sites, i.e. they are enhanced in magnitude by the factor $(1 - x)^{-1} = 5/4$ as compared to a system with $x = 0$. For large values of v, the asymptotic result (8) (applicable for v finite, $M \to \infty$) is only reached for extremely large systems.

Finally, we consider the phase sensitivity of the ground-state energy, similar to ref. [4-6], where the homogeneous system was studied. Here we choose $M = 10^3$ and $x = 0.2$, and we plot $[e_M(\pi) - e_M(0)]M^2$ as a function of v in fig. 4 for different fillings N/M. Close to half-filling ($N = 440, 490$), the dependence on v is very similar to the result described above for the finite-size corrections, i.e. the phase sensitivity is very small between $v \approx 4$ and $v \approx 8$.
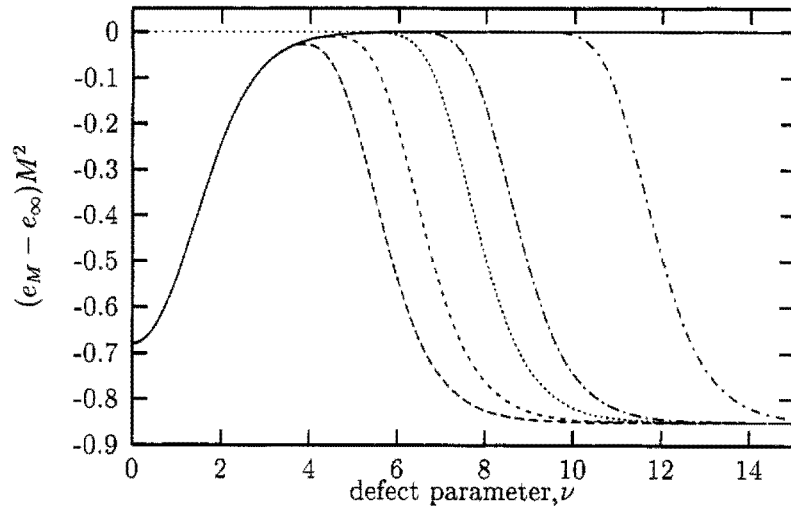
Fig. 3. – Finite-size corrections to the ground-state energy, $(e_M - e_\infty)M^2$, as a function of the defect parameter, ν, for half-filling, $N = M/2$. The system size is varied from $M = 10^2$ to $M = 10^4$ (respectively, — — —, - - - -, · · · · ·, — · —, — · · — · ·); the results for large systems fit perfectly with the analytical expression (———), eq. (8) for $\phi = 0$. The nearest-neighbour interaction is chosen to be $\Delta = 0.5$, and the defect density is $x = 0.2$.

In this context, note that eq. (8) implies that $[e_M(\pi) - e_M(0)]/[e_M(0) - e_\infty] = -3\pi/(4\eta)$; but note also that different Δ's have been chosen in fig. 3 and 4.

The asymptotic (large ν) results shown in fig. 4 can be explained as follows: in this limit (and for the given parameters), 200 sites are cut out from the system of 1000 sites. But, as discussed above, the occupancy of these sites still enters into the Hamiltonian. The defect phases, δ_l, are found to be $\pm 2\eta$, and, as a result, we find additional cusps in the energy-phase relation, for example, for η slightly less than $\pi/4$, at $\phi = \pm 4\eta$. Consequently, the number of discontinuities in the persistent current, $I = -\partial E_M/\partial\Phi$, increases, implying a reduction of the phase average of the current over half a period, i.e. $e_M(\pi) - e_M(0)$, compared to its $\nu = 0$ value.

For low filling, $N \ll M$, on the other hand, the interaction is unimportant and we may apply the free-electron result, $I = -(e v_F/L)\phi/\pi$, which implies that $E_M(\pi) - E_M(0) \approx \pi^2 N/M^2$
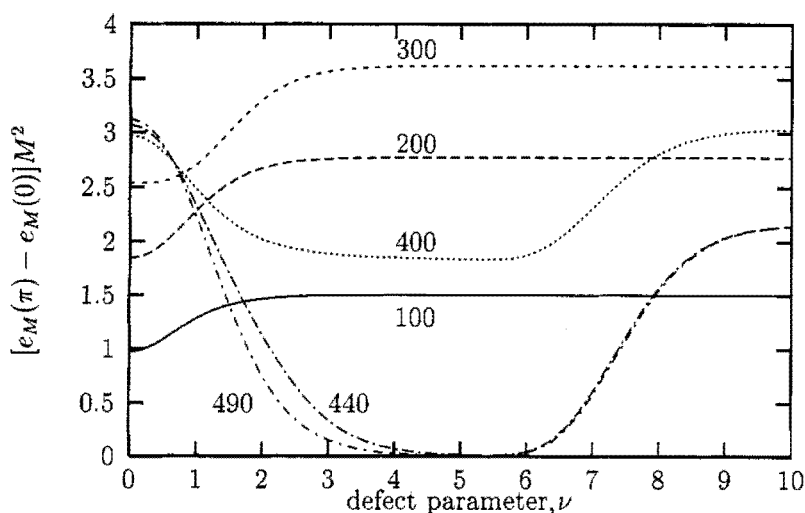

fig. 4. – Phase sensitivity of the ground-state energy, $[e_M(\phi = \pi) - e_M(0)]M^2$, as a function of ν for different fillings, i.e. numbers of fermions, N ($M = 10^3$, $\Delta = 0.2$).

for small N. (In our units, $L = M$ and $\hbar v_F = 2 \sin(\pi N/M)$.) Comparing the limits $\nu = 0$ and $\nu \to \infty$, the phase sensitivity is thus approximately enhanced in the latter case by the factor $(1 - x)^{-2}$, which is apparent in fig. 4.

Conclusions. – We have presented exact results for the finite-size corrections to the ground-state energy and its flux sensitivity for a one-dimensional, interacting model in the presence of defects. Through its construction, the model remains integrable. The defects are «magnetic» in the sense that a defect triangle, compare fig. 1, encloses a finite magnetic flux. This means that time-reversal symmetry is broken and, for general $\{\nu_n\}$, the energy is not an even function of ϕ. Surprisingly, the energy spectrum is independent of the spatial distribution of defects, and we find neither level repulsion nor localized states, which are considered to be generic properties of a «real» impurity. We believe that the absence of these effects is strongly related to the integrability of the model. Nevertheless, the finite-size corrections and the phase sensitivity, *i.e.* the persistent current, can become very small.

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