GAPS IN THE HEISENBERG-ISING MODEL

Rudolf A. Römer
Condensed Matter Theory Unit, Jawaharlal Nehru Centre for Advanced Scientific Research,
Indian Institute of Science Campus, Bangalore 560012, India

Hans-Peter Eckle
Department of Physics, Princeton University, Princeton, New Jersey 08544, U.S.A.

Bill Sutherland
Physics Department, University of Utah, Salt Lake City, Utah 84112, U.S.A.

(Version: March 2, 1995; printed March 23, 2022)

Abstract

We report on the closing of gaps in the ground state of the critical Heisenberg-Ising chain at momentum $\pi$. For half-filling, the gap closes at special values of the anisotropy $\Delta = \cos(\pi/Q)$, $Q$ integer. We explain this behavior with the help of the Bethe Ansatz and show that the gap scales as a power of the system size with variable exponent depending on $\Delta$. We use a finite-size analysis to calculate this exponent in the critical region, supplemented by perturbation theory at $\Delta \sim 0$. For rational $1/r$ fillings, the gap is shown to be closed for all values of $\Delta$ and the corresponding perturbation expansion in $\Delta$ shows a remarkable cancellation of various diagrams.

72.15Nj, 05.30.-d, 75.30Ds
I. INTRODUCTION

In recent years, there has been much interest in the finite-size spectra of one-dimensional (1D) quantum many-body Hamiltonians. This effort was largely motivated by the fascinating ideas of conformal invariance, which allow for a computation of scaling indices and classification of universality classes directly from the $1/L$ behavior of a given critical model [1].

For 1D systems, solvable by the Bethe-Ansatz (BA) method, the finite size spectra are accessible analytically by various methods and these models have thus been used as testing grounds for the general ideas of conformal invariance. In particular, the Heisenberg-Ising (H-I) model of an anisotropic spin-1/2 chain has been studied in great detail [2]. It has been shown that its low energy spectrum in the large $N$ limit can be classified as that of a $c = 1$ conformal field theory with marginally irrelevant operators giving rise to logarithmic corrections [3].

In the present work, we shall reexamine the behavior of the spectrum and the corresponding states of the H-I chain threaded by a magnetic flux $\Phi$. As shown in [4], the adiabatic ground state for half-filling is periodic in $\Phi$ with a period equal to $2 \cdot 2\pi - 2\pi$ is the flux quantum in appropriate units — for values of the interaction strength $\Delta = \cos(\pi/Q)$ with $Q$ not an integer. This is due to the presence of a finite gap at $\Phi = 2\pi$. We show that this gap scales as a power of the system size, with variable exponent depending on $\Delta$. For $\Delta \sim 0$, we calculate the exponent explicitly by perturbation theory. For $Q$ equal to an integer, however, the gap closes exactly and the periodicity of the ground state becomes macroscopic at half-filling, i. e. proportional to the system size. We show how this behavior can be understood in terms of the BA solution as a successive crossing of string solutions.

Furthermore, for $1/r$ filling with $r$ an integer, the periodicity is again not the expected $r$ flux quanta and we observe exact degeneracies between ground state and first excited state at various values of $\Phi$. This is true for all values of the interaction strength and not only at isolated points. We show that the numerical results are confirmed by second order
perturbation theory, due to a remarkable cancellation of various diagrams.

Lastly, we demonstrate that all degeneracies can be removed by simply adding a non integrable next-nearest neighbor term to the Hamiltonian.

II. CLOSING OF ENERGY GAPS AT HALF-FILLING

As is well known, the H-I model has an interpretation as a lattice gas of either fermions or bosons, where spin-down represents a particle and spin-up represents an empty site. The magnetic flux $\Phi$ modifies only the hopping term, s.t. the Hamiltonian is

$$H = -\frac{1}{2} \sum_{j=1}^{N} \{ e^{i\Phi/N} c_j \dagger c_{j+1} + \text{h.c.} \} + \cos \mu \sum_{j=1}^{N} n_j n_{j+1} + e_0,$$

where $e_0 = \Delta(2M - N/2)$, $N$ is the number of sites, $M$ the number of particles and we reparametrized the anisotropy as $\Delta = -\cos(\mu)$. We note that the total momentum induced into the system by the flux is given as $P = M\Phi/N$. We further remark, that the repulsive region $0 \leq \mu < \pi/2$ and the attractive region $\pi/2 < \mu \leq \pi$ of the H-I chain are related by an inversion of the spectrum: The behavior of the low-lying energy states in the attractive region will be mirrored to the behavior of the high energy states in the repulsive region and vice versa.

Let $E_0(\Phi)$ denote the ground state energy of the system with flux $\Phi$. As is easy to see, $E_0(\Phi)$ has a periodicity of $2\pi$ in $\Phi$, i.e. $E_0(\Phi + 2\pi) = E_0(-\Phi) = E_0(\Phi)$. However, the periodicity of a given state can be an integer multiple of the period of the energy. Following [4], we define a topological winding number $n$ to be the number of times the flux $\Phi$ increases by $2\pi$ before the state returns to its initial value.

We write the shift of the ground state energy as a function of flux as $\Delta E_0(\Phi) \equiv E_0(\Phi) - E_0(0) \equiv D\Phi^2/2N + O(\Phi^4)$, where $D$ has been called the stiffness constant [4]. For $0 \leq \mu \leq \pi/2$ and a half-filled band ($M = N/2$), the stiffness has been calculated exactly as $D = v_s/2(\pi - \mu)$ for flux values $|\Phi| \leq 2(\pi - \mu)$; the spin-wave velocity is given by $v_s = \pi \sin \mu/\mu$ [2].
At half-filling, we now adiabatically boost the zero momentum ground state until we have $\Phi = 2\pi$ and $P = \pi$. For $0 \leq \mu < \pi/2$, we then observe a finite gap $\Delta E$ between the boosted ground state and the first excited state in this momentum $\pi$ sector and so the winding number of the zero momentum ground state is $n = 2$. For the non-interacting case of $\mu = \pi/2$, the gap closes and $n = N$ which correctly implies free acceleration in the thermodynamic limit.

For $\mu > \pi/2$, the situation is more complicated: As has already been noted in [5], there are special values of the interaction strength $\mu_Q = (Q-1)\pi/Q$ at which the winding number becomes again macroscopic. In Fig. (1) we show as an example the spectrum at $\mu_3 = 2\pi/3$ and $N = 12, M = 6$. Note that not only the ground state gap closes at $\Phi = 2\pi$, but also various higher lying states become degenerate. Moreover, the closing of the gap at the special values $\mu_Q$ for $Q = 2, 3, \ldots, N$ occurs for all lattices sizes $N$.

In order to further understand this interesting behavior of the energy spectrum, we studied the Bethe Ansatz equations of the H-I chain with flux. The equations are given as

$$N\theta(\alpha, \mu) = 2\pi I + \Phi + \sum_{\alpha'} \theta(\alpha - \alpha', \mu),$$

(2)

where we have used Yang’s [3] change of variables for the pseudomomenta such that $p = \theta(\alpha, \mu) \equiv 2 \arctan[\cot(\mu/2) \tanh(\alpha/2)]$. The quantum numbers $\{I\}$ are integers or half-odd integers and specify the states. The ground state is given by $\{I\} = \{- (M-1)/2, \ldots, (M-1)/2\}$.

Let us briefly recall the behavior of the roots $\{\alpha\}$ for the ground state as we adiabatically turn on the flux: The largest root $\alpha_M$ goes to $\infty$ exactly at $\Phi = 2(\pi - \mu)$ and the remaining $M-1$ roots are distributed symmetrically around 0. The energy of the system is now equal to $M-1$ particles on a chain of length $N$ with $\Phi = 0$ — the ground state in the $S_z = 1$ sector. For $0 \leq \mu \leq \pi/2$, further increase of $\Phi$ renders $\alpha_M$ complex and it moves backwards along the line $i\pi$ with decreasing real part until at $\Phi = 2\pi$ it has the value $\alpha_M = i\pi \equiv \lambda_1$. Again, the remaining $M - 1$ real roots have been distributed symmetrically around 0. However,
the energy now is not related to the $S^z = 1$ ground state in a simple way.

For $\pi/2 \leq \mu \leq 2\pi/3$ and at $\Phi = 2\pi$, we have two complex roots with zero real part, i.e. $\lambda_{1,2} = i(\pi \pm (\pi - \mu))$, i.e. a two-string. And in general we find that at $\Phi = 2\pi$ in the interaction interval $(Q - 1)\pi/Q \leq \mu \leq (Q)\pi/(Q + 1)$, we have a $Q$-string sitting on the imaginary axis symmetrically around $i\pi$ with individual roots given by $\lambda_a = i\pi + i\beta_a \equiv i\pi + i(\pi - \mu)(Q + 1 - 2a) + i\delta_L$. $\delta_L$ represents an exponentially small finite-size correction, which is exactly zero for a 1-string, a 2-string and the two complex roots closest to $i\pi$ in a $Q$-string with $Q$ even. The remaining $M - Q$ real roots are distributed symmetrically around 0.

Note that at values of the interaction strength equal to $\mu_Q$, both a $(Q - 1)$-string and $Q$-string coexist in the degenerate ground state. The energies associated with these strings are $E_Q(\mu_Q) = 0$ and $E_{Q-1}(\mu_Q) = 2(\cos \mu_Q + 1)$ $[6]$. This suggests, that for $(Q - 1)\pi/Q \leq \mu \leq (Q)\pi/(Q + 1)$, when the $Q$-string corresponds to the ground state, the first exited state corresponds to the $(Q + 1)$-string.

We have therefore rewritten the BA equations (2) in order to incorporate the $Q$-strings sitting on the imaginary axis. The equations now are

$$\begin{align*}
N\theta_{00}(\alpha, \mu) &= 2\pi I + \sum_{\alpha'}^{M-Q} \theta_{00}(\alpha - \alpha', 2\mu) + \sum_{\beta'}^{Q} \theta_{01}(\alpha, \beta', \mu), \\
N\theta_{11}(\beta, \pi - \mu) &= 0 + \sum_{\alpha'}^{M-Q} \theta_{10}(\alpha', \beta, \mu) + \sum_{\beta'}^{Q} \theta_{11}(\beta - \beta', 2(\pi - \mu)),
\end{align*}$$

(3a)

(3b)

with

$$\begin{align*}
\theta_{00}(\alpha, \mu) &\equiv \theta(\alpha, \mu) \\
\theta_{10}(\alpha, \beta, \mu) &\equiv \operatorname{Re}\{2\arctanh[\tan(\beta/2)/\tan(\mu/2)]\}
\end{align*}$$

the phase shift of real roots $\alpha$, $\theta_{11}(\beta, \mu) \equiv \operatorname{Re}\{2\arctan[\coth((\alpha - i\beta)/2)/\tan(\mu)]\}$, $\theta_{01}(\alpha, \beta, \mu) \equiv -\frac{1}{2} \log[(\cos(\beta + 2\mu) + \cosh(\alpha))/(\cos(\beta - 2\mu) + \cosh(\alpha))]$ the mixed phase shifts of a real with a complex root. The quantum numbers for the $\{\beta\}$’s are zero and the flux $\Phi = 2\pi$ has been incorporated into the $\{I\}$ quantum numbers. We caution the reader that care has to be taken in regard to the branch cuts of these phase shifts. The existence of roots on different branches is equal to a net shift of the quantum numbers and thus a different state.
In Fig. (2), we show the results of iterating the BA equations (3) in the momentum \( \pi \) sector for the ground state and the first excited state on a chain with \( M = 4 \) particles on \( N = 8 \) sites. For \( 0 \leq \mu \leq \pi/2 \), the ground state corresponds to a 1-string state. As anticipated above, the first excited state is given by a 2-string state. At \( \mu_2 \), this 2-string state takes over as ground state and the 1-string state has vanished and in fact now corresponds to a higher lying state. An initially degenerate 3-string state appears and becomes the first excited state as \( \mu \) is further increased. At \( \mu_3 \), the 2-string now vanishes, the 3-string state takes over as ground state and a new 4-string state emerges. As there is no 5-string on a chain with \( M = 4 \) particles, this exchange of states ends here.

We have plotted the energy difference \( \Delta E \equiv E_1 - E_0 \) at \( \Phi = 2\pi \) as a function of \( \mu \) in Fig. (2). The closing of the gap at the special points \( \mu_Q \) can be clearly seen. Note that \( \Delta E/E_0 \) is already less than 2% at \( \mu = 7\pi/12 \) for this small system. For \( N = 12 \) and \( M = 6 \), \( \Delta E \sim 10^{-3} \) for the largest gap at \( \mu \sim 7\pi/12 \) and decreases approximately exponentially as \( \mu \to \pi \).

As \( N \to \infty \), the gaps for \( \mu \neq \mu_Q \) should close as \( \Delta E \sim N^{-\gamma} \). In Fig. (3), we have plotted \( \gamma \) versus \( \mu \) as extrapolated from calculations of up to \( N = 14 \) sites. Note that we can observe only \( Q \)-strings up to \( Q = 7 \) for these small sizes. Thus we can define \( \gamma \) only for \( \mu < \mu_7 = 6\pi/7 \). Moreover, for \( \mu \geq \mu_Q \), useful data can come only from systems with \( M = Q + 1 \) particles. The result shows that \( \gamma \) varies continuously for all \( 0 \leq \mu \leq \pi \).

Alcaraz et al. [3] have argued that both 1-string and 2-string for \( 0 \leq \mu \leq \pi/2 \) have the same scaling dimension. Therefore, the energy gap \( \Delta E \) measures finite size behavior beyond simple conformal \( 1/N \) formulas and we interpret the continuous variation of \( \gamma \) as indicating the presence of logarithmic corrections. A direct calculation of these corrections in the H-I chain has so far been done only at \( \mu = 0 \) and we are presently trying to extent these methods.

However, at \( \mu \sim \pi/2 \) (\( \Delta \sim 0 \)), we can calculate \( \gamma \) directly by perturbation theory in \( \Delta \). As a starting point, we choose the plane wave basis of free particles at \( \Phi = 0 \) and write

\[
c_j = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{i2\pi jm} d_m. \tag{4}
\]
We can then write the hopping term as
\[
T = -2 \sum_{m=1}^{N} \cos \left( \frac{2\pi}{N} m + \frac{\Phi}{N} \right) d_{m}^{\dagger} d_{m}.
\] (5)

Similarly, the interaction term is given as
\[
V = -\frac{2\Delta}{N} \sum_{m_{1},m_{2},m_{3},m_{4}} \cos \left( \frac{2\pi (m_{3} - m_{4})}{N} \right) \Delta_{m_{1}+m_{3},m_{2}+m_{4}} d_{m_{1}}^{\dagger} d_{m_{2}}^{\dagger} d_{m_{3}} d_{m_{4}},
\] (6)

where the periodic Kronecker symbol is defined as \(\Delta_{n,m} = 1\) if \(n = m \mod N\) and 0 otherwise.

We now wish to identify the ground state \(\Psi_{0}\) and the first excited state \(\Psi_{1}\) which are degenerate at \(\Phi = 2\pi\), i.e.,
\[
\Psi_{0}^{\dagger} T \Psi_{0} |_{\Phi=2\pi} = \Psi_{1}^{\dagger} T \Psi_{1} |_{\Phi=2\pi}.
\] (7)

Let \(M\) be odd and consider \(\Phi = 0\). We then construct the ground state simply by filling all available momenta symmetrically, i.e., \(\Psi_{0} = \prod_{m=-(M-1)/2}^{(M-1)/2} d_{m}^{\dagger} |0\). Turning on the flux, we find \(\Psi_{0}^{\dagger} T \Psi_{0} |_{\Phi=2\pi} = \Psi_{0}^{\dagger} T \Psi_{0} |_{\Phi=0} + 4 \sin(\pi/N)\). Keeping in mind Eqn. (7), we see that the first excited state is given by \(\Psi_{1} |_{\Phi=0} = d_{A}^{\dagger} d_{B}^{\dagger} d_{C} d_{D} \Psi_{0} |_{\Phi=0}\) with \(A = -(M+3)/2\), \(B = -(M+1)/2\), \(C = (M-1)/2\) and \(D = (M-3)/2\). A simple calculation shows that Eqn. (7) holds indeed.

For \(\Delta \neq 0\), \(\Psi_{0} |_{\Phi=2\pi}\) and \(\Psi_{1} |_{\Phi=2\pi}\) will not be degenerate anymore, and the interaction \(V\) gives rise to a mixing term \(\Psi_{0}^{\dagger} V \Psi_{1}\). An explicit calculation shows that \(\Psi_{0}^{\dagger} V \Psi_{1} = \frac{4\Delta}{N} [1 - \cos 2\pi/N] \sim 8\Delta \pi^{2}/N^{3}\). Therefore, we see that \(\gamma = 3\) at \(\Delta = 0\) and \(\Phi = 2\pi\). This agrees quite well with the numerical results of Fig. (3) which were obtained for small systems of up to \(N = 14\) sites and \(M = 7\) particles [7].

### III. CLOSING OF ENERGY GAPS AT 1/r-FILLING

Let us now study the behavior of the energy gap in the momentum \(\pi\) sector away from half-filling. As mentioned above, one generally expects the winding number of the ground state to be \(n = r\) for a 1/r filled band. As we have shown, this is true for the half-filled band except at isolated values of the interaction strength. For fillings equal to 1/3, 1/4, 1/5, 1/6, . . . , we have explicitly calculated the energy spectrum as a function of flux
and we find that the gap closes at $\Phi = \pi r$. In Fig. (4), we show a plot of the $1/3$ filled case with $\mu = 7\pi/12$ obtained by exact diagonalization of the H-I chain. This interaction strength corresponds to a large gap for the half-filled case. For $1/3$ filling, however, the gap at $\Phi = 3\pi$ is closed. Note that again various other degeneracies in the energy spectrum occur at this flux value. This behavior is unique to the $1/r$ filled chain — and by particle-hole symmetry to the $(r - 1)/r$ filled chain. It does not occur at all possible rational fillings such as, e.g., $2/5$.

The numerical results are again confirmed by perturbation theory. Let us, e.g., look at the $1/3$ filled case with $M$ odd and $N = 3M$. The ground state $\Psi_0$ is given as before and we need to identify the state $\Psi_1$ which is degenerate with $\Psi_0$ at $\Phi = 3\pi$. We find $\Psi_1|_{\Phi=0} = d_A^\dagger d_B^\dagger d_C^\dagger d_D d_E d_F \Psi_0|_{\Phi=0}$ with $A = -(M + 5)/2, B = -(M + 3)/2, C = -(M + 1)/2, D = (M - 1)/2, E = (M - 3)/2$ and $D = (M - 5)/2$.

For $\Delta \neq 0$, the exact diagonalization implies that $\Psi_0|_{\Phi=3\pi}$ and $\Psi_1|_{\Phi=3\pi}$ will remain degenerate. Due to the structure of $\Psi_1$, we see that the mixing term indeed vanishes in first order in $V$. The second order mixing term is given by

$$
\frac{1}{2} \Psi_0^\dagger V \cdot V \Psi_1 =
$$

$$
\frac{2\Delta^2}{N^2} \sum_{i_1,i_2,i_3,i_4,j_1,j_2,j_3,j_4} \cos 2\pi (i_3 - i_4)/N \Delta_{i_1+i_3,j_1+j_3} \cdot \cos 2\pi (j_3 - j_4)/N \Delta_{j_1+j_3,j_2+j_4} \times
$$

$$
\langle \Psi_0| d_{i_1}^\dagger d_{i_3}^\dagger d_{j_1}^\dagger d_{j_3}^\dagger d_{i_2} d_{j_2} d_{i_4} d_{j_4} d_A^\dagger d_B^\dagger d_C^\dagger d_D d_E d_F |\Psi_0\rangle. \quad (8)
$$

Explicitly performing the 576 possible contractions, we find that the diagrams arrange themselves into 36 groups corresponding to a given ordering of contractions over the indices $\{A, B, C, D, E, F\}$. Only one index is left to be summed over and it is exactly this sum that gives zero for all the 36 groups individually. Therefore, we have an exact cancellation of second order diagrams for all $\mu$ in the critical region $[8]$, too. A generalization of this calculation to other $1/r$ fillings is straightforward, but becomes increasingly tedious as the number of possible contractions increases as $(4 + r)!$. 

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IV. CONCLUSIONS

We have presented numerical and perturbative evidence for degeneracies in the momentum $\pi$ sector of the $1/r$ filled critical H-I model on a finite ring. Adding a non-integrable, say, next-nearest neighbor interaction $W = \omega \sum_{j=1}^{N} n_j n_{j+2}$ to the Hamiltonian (1), we find that all the degeneracies discussed above for $\mu \neq \pi/2$ are lifted and therefore all gap-closings disappear. The reader may now speculate that it is the integrability of the H-I chain which leads to the closed gaps. However, preliminary results from a related study of the repulsive Hubbard chain show that there the gap closes at $U = 0$ only. It is an interesting question, if our results can be found also in other one-dimensional quantum systems such as the long-ranged Haldane-Shastry chains.

Furthermore, we have shown by exact diagonalization and iteration of the BA equations that the gap at $\Phi = 2\pi$ ($P = \pi$) and half-filling scales as power of the system size with variable exponent $\gamma$. An analytical calculation of $\gamma$ is in preparation.

We close this paper by noting that as shown in [9], the here considered structure of low-lying states in the H-I chain is qualitatively the same in the SC model [10]. Therefore the results presented here will also hold in the SC model, up to the renormalization of quantities such as the spin wave velocity $v_s$.

ACKNOWLEDGMENTS

The authors would like to thank B. Sriram Shastry, Joel Campbell and Alexander Punnoose for many insights and fruitful discussions. R.A.R. and H.-P.E. acknowledge financial support from the Alexander von Humboldt foundation. H.-P.E. further acknowledges support at Tours through the European Union’s “Human Capital and Mobility” program. H.-P.E. and B.S. benefited from a stay at the Aspen Center for Physics.
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* Present address: LMPM, Département de Physique, Université François Rabelais, F–37200 Tours, France

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FIGURES

FIG. 1. The full spectrum of the H-I chain for \( N = 12 \) and \( M = 6 \) at \( \mu_3 = 2\pi/3 \). Note the level crossing for ground state and first excited state at \( \Phi = 2\pi \). Various other level crossings enhance the periodicity of the ground state such that its winding number is \( n = 6 \).

FIG. 2. Energy of the ground state and first excited state and their difference at \( \Phi = 2\pi \) (\( P = \pi \)) for \( N = 8 \) and \( M = 4 \). Note the closing of the gaps at \( \mu_2 = \pi/2 \), \( \mu_3 = 2\pi/3 \) and \( \mu_4 = 3\pi/4 \). The finite gaps in the regions \( \mu_2 \leq \mu \leq \mu_3 \) and \( \mu_3 \leq \mu \leq \mu_4 \) are just visible.

FIG. 3. Assuming \( \Delta E \sim N^{-\gamma} \), we extrapolate \( \gamma \) from finite size data of up to \( N = 14 \) sites and half-filling. The error bars get larger as \( \mu \to \mu_7 \) since we need \( M \geq Q \) for \( \mu \geq \mu_{Q-1} \). Data points for \( \mu > \mu_7 = 6\pi/7 \) are therefore not expected to obey the simple power-law behavior.

FIG. 4. The full spectrum for the H-I chain for \( N = 12 \) and \( M = 4 \) at \( \mu = 7\pi/12 \). Note the level crossing for ground state and first excited state at \( \Phi = 3\pi \) (\( P = \pi \)). Various other level crossings enhance the periodicity of the ground state such that its winding number is \( n = 6 \).