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ADIABATIC TRANSPORT PROPERTIES AND BERRY'S PHASE IN HEISENBERG-ISING RING

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In a recent paper, B. Sutherland and B. S. Shastry have constructed an adiabatic process for the Heisenberg spin chain (spin $\frac{1}{2}$) with respect to a change of boundary conditions. In this paper we calculate Berry's phase for this process. We also evaluate the dependence of energy levels on boundary conditions which permits us to calculate the effective charge-carrying mass.

1. Introduction

Consider the Heisenberg spin $\frac{1}{2}$ antiferromagnet on a lattice with L sites, described by the Hamiltonian

$$H = -\sum_{n=1}^{L} \{\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta(\sigma_n^z \sigma_{n+1}^z - 1)\} . \tag{1.1}$$

Here $\sigma^{x,y,z}$ are the three Pauli matrices (describing spin $\frac{1}{2}$), Δ is the anisotropy parameter, which we shall denote as

$$\Delta = \cos 2\eta . \tag{1.2}$$

We shall consider the region $\pi/2 < 2\eta \leq \pi$. It is also possible to make a Jordan-Wigner transformation ($c = \frac{1}{2}(\sigma^x + i\sigma^y)$) and rewrite the Hamiltonian (1.1) in terms of spinless lattice fermions: (their anticommutation relations are $\{c_j, c_k^\dagger\} = \delta_{jk}$)

$$H = -2\sum_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - 4\Delta \sum_n \left[\left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right) - \frac{1}{4}\right] . \tag{1.3}$$

The complete set of eigenfunctions $\Psi_N(x_1 \ldots x_N)$ of the Hamiltonian (1.1) is known,[1] we shall write them down below.

Recently, B. Sutherland and B. S. Shastry[2] have constructed an adiabatic process for this Heisenberg chain with respect to a change of boundary conditions. Consider N fermions (described by (1.3)), each carrying a charge $(-q)$ on a ring of length L. A magnetic flux $\hbar c\Phi/q$ threads the ring. Each particle, in going around the ring (while not seeing the magnetic field), picks up a phase Φ. Sutherland-Shastry pointed out that this Aharonov-Bohm effect is accounted for by replacing the usual periodic boundary condition by the twisted boundary condition:

$$\Psi_N(x_1, \ldots, x_j + L, \ldots, x_N) = e^{i\Phi}\Psi_N(x_1, \ldots, x_j, \ldots, x_N) . \tag{1.4}$$

The Aharonov-Bohm effect on a quantum many-body system was first discussed qualitatively by Beyers and Yang.[3] Now it plays an extremely important role.[4] (Below we shall fix our units to be equal to $\hbar = 1$, mass $= \frac{1}{2}$.) Following Ref. 2, we shall consider half-filled lattice $2N = L$.

The partition function, $Q = \mathrm{tr}(\exp[-H/T])$ as well as the whole spectrum of the Hamiltonian (1.1) is periodic with respect to Φ with the period 2π. (Consequences were discussed in Ref. 1.) But if we adiabatically follow an individual energy level this is not necessarily true. B. Sutherland and S. Shastry noticed that (under the described conditions) the adiabatic period of the ground state is 4π.

During this process some level crossings occur. Nevertheless during each of these level crossings two different wave functions have the same energy but different quantum numbers. These quantum numbers are eigenvalues of conservation laws: momentum, number of particles and so on. Actually the Hamiltonian (1.1) has infinitely many conservation laws. This shows that during energy-level crossing we can follow an individual wave function looking at other quantum numbers. Roughly speaking, if we keep in mind all the conservation laws, there is no level crossing during this adiabatic process.

In view of the fact that a Berry phase[5–8] usually exists for a general adiabatic process, it is of interest to evaluate the Berry phase related to this adiabatic process. Here we show that it is equal to π. We found Ref. 7 to be very useful, because the process considered there is similar to the case we consider.

Another interesting question is the dependence of ground state energy on Φ. In the gapless case (in the thermodynamic limit $L \to \infty$) the leading term in the variation of energy is

$$\delta E(\Phi) = (D/L)\Phi^2 + o(1/L) . \tag{1.5}$$

In Ref. 9, it is explained that the coefficient D is essentially the inverse of the effective current carrying mass. This coefficient D is also called stiffness. The value of D was evaluated only for a half-filled lattice ($L = 2N$).[9] Here we present formula for D at arbitrary filled lattice. Coefficient D is especially important because it defines the long distance asymptotics of the correlation functions.

The spin-stiffness was evaluated for the Hubbard model.[9] Finite size corrections (formulas similar to (1.5)) were obtained for a general Bethe-Ansatz solvable model.[10]

Long distance asymptotics of correlation functions in the 1-D Hubbard model were evaluated by means of finite size corrections.[11]

Our paper is organized as follows. In Sec. 2 we remind the reader of the exact solution of the model (1.1). In Sec. 3 we evaluate the Berry phase. In Sec. 4 we discuss the dependence of energy levels on the magnetic flux Φ. We also evaluate the effective charge carrying mass for arbitrary filling and relate it to the correlation functions.

2. Exact Solution of Heisenberg Antiferromagnet

We shall discuss the Heisenberg antiferromagnet:

$$H = -\sum_{n=1}^{L} \{\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta(\sigma_n^z \sigma_{n+1}^z - 1)\} . \tag{2.1}$$

Eigenfunctions of the model

$$H|\Psi\rangle = E|\Psi\rangle \tag{2.2}$$

can be represented in the form:

$$|\Psi\rangle = \sum_{x_1=1}^{L} \cdots \sum_{x_N=1}^{L} \chi_N(x_1, \dots, x_N) \prod_{j=1}^{N} \sigma_{x_j}^- |\uparrow\rangle . \tag{2.3}$$

Here $|\uparrow\rangle$ is a ferromagnetic state, σ_x^- is lowering spin operator at the point x. χ_N is N-body wave function, it should be symmetric with respect to all x and should vanish if two x's coincide. It depends on coordinates and momenta and is equal to:

$$\begin{aligned}\chi_N(x_1, \dots, x_N | p_1, \dots, p_N) = &\left\{\prod_{N \geq b > a \geq 1} \varepsilon(x_b - x_a)\right\} \\ &\times \sum_Q (-1)^{[Q]} \exp\left[i \sum_{a=1}^{N} x_a p_{Q_a}\right] \\ &\times \exp\left[i/2 \sum_{N \geq b > a \geq 1} \theta(p_{Q_b}, p_{Q_a}) \varepsilon(x_b - x_a)\right] .\end{aligned} \tag{2.4}$$

Here $\varepsilon(x)$ is the sign function, the summation is with respect to permutation Q of the momenta p and θ is the two-particle scattering phase. Dependence of θ on momenta can be simplified by introducing the spectral parameter λ:

$$p(\lambda) = i \ln \frac{\sinh(\lambda - i\eta)}{\sinh(\lambda + i\eta)} . \tag{2.5}$$

In terms of the spectral parameter, the scattering phase can be represented as:

$$\theta(p_1, p_2) = \theta(\lambda_1 - \lambda_2) = i \ln \frac{\sinh(2i\eta + \lambda_1 - \lambda_2)}{\sinh(2i\eta - \lambda_1 + \lambda_2)} . \tag{2.6}$$

Energy of this state is equal to:

$$E = \sum_{j=1}^{N} \frac{2\sin^2 2\eta}{\sinh(\lambda_j + i\eta)\sinh(\lambda_j - i\eta)} . \tag{2.7}$$

The energy is real for $\mathrm{Im}\,\lambda = 0$ and $\mathrm{Im}\,\lambda = \pi/2$. The last case is more important because at $\mathrm{Im}\,\lambda = \pi/2$ the energy is negative, so the ground state corresponds to $\mathrm{Im}\,\lambda = \pi/2$. This is the reason why it is convenient to introduce a new variable

$$s = \lambda - i\frac{\pi}{2} . \tag{2.8}$$

The momentum p and the scattering phase θ now look like:

$$p(s) = i \ln \frac{\cosh(s - i\eta)}{\cosh(s + i\eta)} , \tag{2.9}$$

$$\theta(p_1, p_2) = \theta(s_1 - s_2) = i \ln \frac{\sinh(2i\eta + s_1 - s_2)}{\sinh(2i\eta - s_1 + s_2)} . \tag{2.10}$$

We define the branch of the logarithm in the following way

$$\begin{aligned} p(0) &= 0 , \quad p(s) = -p(-s) , \\ \theta(0) &= 0 , \quad \theta(s) = -\theta(-s) . \end{aligned} \tag{2.11}$$

Derivatives of these functions are also important in order to follow the adiabatic process:

$$p'(s) = \frac{\sin 2\eta}{\cosh(s + i\eta)\cosh(s - i\eta)} \geq 0 \quad \text{for} \quad \mathrm{Im}\, s = 0 , \tag{2.12}$$

$$\theta'(s) = \frac{\sin 4\eta}{\sinh(s + 2i\eta)\sinh(s - 2i\eta)} \leq 0 \quad \text{for} \quad \mathrm{Im}\, s = 0 . \tag{2.13}$$

Let us now impose twisted boundary conditions $\chi(x_1 + L, \ldots) = \chi(x_1, \ldots) \exp i\Phi$. This leads to the system of transcendental equations for the set of $\{s\}$:

$$Lp(s_k) + \sum_{j=1, j\neq k}^{N} \theta(s_k - s_j) = 2\pi I_k + \Phi . \tag{2.14}$$

Here the set of N integers (or half integers, depending on the parity of N) are

$$\begin{aligned} I_{k+1} - I_k &= 1 , \\ I_k &= -(N-1)/2, \ldots, (N-1)/2 . \end{aligned} \tag{2.15}$$

This is the ground state for the half-filled lattice $L = 2N$. The wave function χ_N is antisymmetric with respect to the permutation of any two momenta and symmetric with respect to the permutation of x's.

Later we shall need to apply the space parity reflection $\{x\} \to \{-x\}$, $\{p\} \to \{-p\}$ to the wave function (2.4). First of all, it is convenient to change the enumeration of the sites of the lattice in such a way that the set of x_j coincide with the set of $(-x_j)$. As we have a lattice of even length $L = 2N$ this can be achieved in the following way:

$$x_j = -(L-1)/2, -(L-1)/2 + 1, \ldots, (L-1)/2 . \tag{2.16}$$

All coordinates here are half-integers. Now the behavior of the wave function under reflection is the following:

$$\chi_N(-x_1, \ldots, -x_N \mid -p_1, \ldots, -p_N) = (-1)^{N(N-1)/2} \chi_N(x_1, \ldots, x_N \mid p_1, \ldots, p_N) . \tag{2.17}$$

Here we used the symmetry of χ_N with respect to x_j.

3. Berry Phase

Consider the twisted boundary conditions

$$Lp(s_k) + \sum_{j=1, j\neq k}^{N} \theta(s_k - s_j) = 2\pi I_k + \Phi . \tag{3.1}$$

Let us describe the adiabatic process. For the ground state where $\Phi = 0$, all s_k are real and symmetric with respect to $s = 0$: $\{s_k\} = \{-s_k\}$, let us denote them by s_k^0. For small Φ, all Im s_k are still equal to zero. For $\Phi = 4\eta$ $(\pi < 4\eta \leq 2\pi)$, the biggest s_k (it is s_N) will reach infinity and all other s_k will form the ground state of the $(N-1)$ particle sector. When $4\eta < \Phi \leq 2\pi$, the value of S_N will be on the Im $\lambda = 0$ axis ($\lambda = s + i\pi/2$) and all other s_k's will stay on the Im $s = 0$ axis (they will move non-monotonically). At $\Phi = 2\pi$, the configuration will be $s_N = -i\pi/2$ $(\lambda_N = 0)$, all other s_k will be real and symmetric with respect to the $s = 0$.

This is the eigenstate (excited) for periodic boundary conditions. Let us denote this set of s_k by s_k^e. For $\Phi = 4\pi$, we shall denote the configuration of s_k by $\{s_k^a\}$. It is related to the original ground state configuration in the following way:

$$s_N^a = s_1^g, \quad s_k^a = s_{k+1}^g, \quad k = 1, \ldots, N-1\ , \tag{3.2}$$

$$p_N^a = p_1^g + 2\pi\ , \quad p_k^a = p_{k+1}^g\ , \quad k = 1, \ldots, N-1\ , \tag{3.3}$$

$$\theta(p_N^a, p_k^a) = \theta(p_1^g, p_{k+1}^g) - 2\pi\ , \tag{3.4}$$

$$\theta(p_l^a, p_k^a) = \theta(p_{l+1}^g, p_{k+1}^g)\ , \quad N-1 \geq l > k \geq 1\ .$$

So the set of s^a coincides with the set of s^g. This is the adiabatic process of Sutherland and Shastry.[2]

If we adiabatically follow the excited state (which is mentioned above), we shall discover that its period is also $\Delta\Phi = 4\pi$. In this case it is more convenient to change Φ in the interval $-2\pi \leq \Phi \leq 2\pi$. The value $\Phi = 0$ correspond to the ground state, the values $\Phi = \pm 2\pi$ correspond to the excited state. At an arbitrary value of in this region, we have:

$$\{-\mathrm{Re}\, s_1(\Phi), \ldots, -\mathrm{Re}\, s_N(\Phi)\} = \{\mathrm{Re}\, s_N(-\Phi), \ldots, \mathrm{Re}\, s_1(-\Phi)\}\ . \tag{3.5}$$

Imaginary parts are the same.

We shall use this for the evaluation of the Berry phase. To do this, we must consider the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\phi(t)\rangle = H|\phi(t)\rangle\ . \tag{3.6}$$

Solution of this equation is related to the eigenfunction of the time independent Schrödinger equation (2.2) in the following way:

$$|\phi(t)\rangle = \exp\left[\frac{-i}{\hbar}\int_0^t dt'\, E(\phi(t'))\right] \exp(i\gamma(t))\, |\psi(t)\rangle \tag{3.7}$$

Since this process is adiabatic, we have:

$$\dot{\gamma} = i\,\frac{\left\langle \psi(t) \left| \frac{\partial}{\partial t} \right| \psi(t) \right\rangle}{\langle \psi(t) | \psi(t) \rangle}\ . \tag{3.8}$$

When the system goes around the circle with $\Delta\Phi = 4\pi$, the wave function $|\phi(t)\rangle$ will get an additional phase factor

$$\exp\left[\frac{-i}{\hbar}\int_0^T dt'\, E(\phi(t'))\right]\exp(i\gamma) \tag{3.9}$$

where T is period of adiabatic change of Φ from 0 to 4π and γ is the Berry phase

$$\gamma = \mathrm{Re}\left[i\int_0^T dt\,\frac{\left\langle \psi(t)\left|\frac{\partial}{\partial t}\right|\psi(t)\right\rangle}{\langle\psi(t)\,|\,\psi(t)\rangle}\right]. \tag{3.10}$$

After a change of variables, we get

$$\gamma = \mathrm{Re}\left[i\int_{-2\pi}^{2\pi} d\Phi\,\frac{\left\langle \psi(\Phi)\left|\frac{\partial}{\partial \Phi}\right|\psi(\Phi)\right\rangle}{\langle\psi(\Phi)\,|\,\psi(\Phi)\rangle}\right]. \tag{3.11}$$

The time independent wave function should satisfy the following condition

$$\psi(\Phi + 4\pi) = \psi(\Phi)\ . \tag{3.12}$$

Let us check our wave function (2.4) with reference to (2.16). In (2.4), all p and θ are functions of $\{s_j\}$ (see (2.9) and (2.10)) which depend on Φ by means of system (3.1). Formulas (3.2)–(3.4) and (2.4), (2.16) show that

$$\chi_N(\Phi + 4\pi) = -\chi_N(\Phi)\ . \tag{3.13}$$

Thus we can substitute in (3.11) the following wave function:

$$|\psi(\Phi)\rangle = \exp(i\Phi/4)\,\chi_N(\Phi) \tag{3.14}$$

which satisfies (3.12). Putting this in Eq. (3.11), we get

$$\gamma = -\pi$$
$$-\,\mathrm{Im}\left[\int_{-2\pi}^{2\pi} d\Phi \sum_{\{x_i\}} \frac{\overline{\chi}_N(x_1,\ldots,x_N\,|\,p_1(\Phi),\ldots,p_N(\Phi))\,\frac{\partial}{\partial\Phi}\,\chi_N(x_1,\ldots,x_N\,|\,p_1(\Phi),\ldots,p_N(\Phi))}{\|\chi_N(\Phi)\|^2}\right] \tag{3.15}$$

where summation is with respect to each x_j through the region of (2.16) which is invariant under the reflection. Now let us use (3.5), (2.4) and (2.17) to show that:

$$\chi_N(x_1,\ldots,x_N)\,|_{\Phi} = \chi_N(-x_1,\ldots,-x_N)\,|_{-\Phi} \tag{3.16}$$

$$\|\chi(\Phi)\|^2 = \|\chi(-\Phi)\|^2 \tag{3.17}$$

and the following expression is an odd function of Φ

$$\sum_{\{x_j\}} \frac{\bar{\chi}_N(x_1, \ldots, x_N | p_1(\Phi), \ldots, p_N(\Phi)) \frac{\partial}{\partial \Phi} \chi_N(x_1, \ldots, x_N | p_1(\Phi), \ldots, p_N(\Phi))}{\|\chi_N(\Phi)\|^2} . \tag{3.18}$$

Thus the integral in (3.15) vanishes and the Berry phase is equal to:

$$\gamma = -\pi . \tag{3.19}$$

The answer $\gamma = \pi$ is also correct because γ is a phase.

The interesting question is the following: Is it possible to define the Berry phase for the smaller change of twisted boundary conditions $\Delta\Phi = 2\pi$? In this case, the ground state and excited state exchange their positions. At $\Phi = \pi$, the levels cross, but they have different momenta. This permits us to follow the levels individually. We can introduce a matrix which relates the adiabatically continued wave functions ψ_e^a, ψ_g^a to the original ones ψ_e, ψ_g

$$\begin{pmatrix} \psi_e^a \\ \psi_g^a \end{pmatrix} = M \begin{pmatrix} \psi_e \\ \psi_g \end{pmatrix} , \tag{3.20}$$

$$M = \begin{pmatrix} 0 & m_{21} \\ m_{12} & 0 \end{pmatrix} . \tag{3.21}$$

The square of matrix M describes the original adiabatic process $\Delta\Phi = 4\pi$. Comparing with formulas (3.9) and (3.19), we get

$$m_{12} m_{21} = -\exp\left[\frac{-i}{\hbar} \int_0^T dt'\, E(\phi(t'))\right] . \tag{3.22}$$

This shows that the matrix M has two eigenvalues $\pm m$

$$m = i \exp\left[\frac{-i}{2\hbar} \int_0^T dt'\, E(\phi(t'))\right] \tag{3.23}$$

where T is the period corresponding to $\Delta\Phi = 4\pi$. This means that there exist two different linear combinations of the ground state and the excited state which get factors $\pm m$ after adiabatic continuation for $\Delta\Phi = 2\pi$.

4. Effective Charge-Carrying Mass

Under the twisted boundary conditions (1.4), the ground state energy changes by

$$\delta E(\Phi) = \frac{D}{L} \Phi^2 + o(1/L) . \tag{4.1}$$

In Ref. 9, it is explained that D is essentially the inverse of effective current carrying mass, and was evaluated for a half-filled lattice only. Here we shall evaluate it for arbitrary filling. To do this, let us generalize the Hamiltonian (1.1) by introducing a one-dimensional magnetic field h:

$$H = -\sum_{n=1}^{L} \{\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta(\sigma_n^z \sigma_{n+1}^z - 1) + h(\sigma_n^z - 1)\} . \tag{4.2}$$

In the fermionic language of (1.3) this means the introduction of a chemical potential (one should add term $2h \, \Sigma_n \, c_n^\dagger \, c_n$ to (1.3)). (A one-dimensional magnetic field should not be confused with two-dimensional which produced twisted boundary conditions.) The one-dimensional magnetic field changes the ground state, since now the magnetization

$$\langle \sigma^z \rangle = \sigma \tag{4.3}$$

is non-zero. One can introduce the magnetic susceptibility

$$\chi = \frac{\partial \sigma}{\partial h} . \tag{4.4}$$

From Ref. 12 and Ref. 13, it is clear that

$$D = \frac{1}{8} v^2 \chi . \tag{4.5}$$

Here v is Fermi velocity

$$v = \frac{\partial \varepsilon}{\partial p}\Big|_{\text{Fermi level}} . \tag{4.6}$$

Here ε and p are energy and momentum of the excitation. It is explained in more detail in Ref. 12. For a half-filled lattice both the Fermi velocity and the susceptibility were calculated in Ref. 1:

$$v = \frac{2\pi \sin 2\eta}{\pi - 2\eta} , \quad \chi = \frac{(\pi - 2\eta)}{2\pi\eta \sin 2\eta} . \tag{4.7}$$

This permits us to reproduce the result of Ref. 2 for D,

$$D = \frac{\pi \sin 2\eta}{4\eta(\pi - 2\eta)} \tag{4.8}$$

and the energy gap in the $S^z = 0$ sector:

$$\delta E(2\pi) = \frac{\pi^3 \sin 2\eta}{L\eta(\pi - 2\eta)} + o(1/L) . \tag{4.9}$$

Results of Refs. 12 and 13 also permit the evaluation of the energy which is necessary to remove d particles from the ground state at arbitrary filling:

$$\delta E_d = \frac{(vd)^2}{4LD} + o(1/L) . \tag{4.10}$$

At half-filling for one particle we reproduce:[1]

$$\delta E_1 = \frac{4\pi\eta \sin 2\eta}{L(\pi - 2\eta)} + o(1/L) . \tag{4.11}$$

Considering once again arbitrary filling, let us remove d particles and impose twisted boundary conditions. The energy change is additive:

$$\delta E = \frac{2\pi v}{L}\left(\frac{D}{2\pi v}\Phi^2 + \frac{vd^2}{8\pi D}\right) + o(1/L) . \tag{4.12}$$

It is also important to note that the ideas of conformal field theory[14] permit us to relate finite size corrections[15,16] (see (4.12)) and long distance asymptotics of correlation functions. For example from Ref. 12, one can get:

$$\langle \sigma^+(x,t)\sigma^-(0,0)\rangle \to \frac{c}{|x^2-(vt)^2|^{\beta/2}}, \quad \beta = \frac{v}{4\pi D}, \tag{4.13}$$

$$\langle \sigma^z(x,t)\sigma^z(0,0)\rangle - \sigma^2 \to \frac{a}{(x-vt)^2} + \frac{a}{(x+vt)^2} + b(-1)^x \frac{\cos \pi\sigma x}{|x^2-(vt)^2|^{(1/2\beta)}} . \tag{4.14}$$

This illustrates the relation of coefficient D with transport properties. It is also interesting to mention that the calculation of this section was done for the Hubbard model in Ref. 11.

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