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Adiabatic Transport Properties of an Exactly Soluble One-Dimensional Quantum Many-Body Problem

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We study an interacting one-dimensional quantum lattice gas, based on the Heisenberg-Ising ring. The particles are given a charge, and the ring is threaded by a magnetic flux. We then calculate exactly the energy of the state, which begins as the ground state with zero magnetic flux, when the magnetic flux is adiabatically increased. We find the result that the period of the ground state is two flux quanta, which can be interpreted as charge carriers with half-integer charge.

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In this Letter, we consider an interacting one-dimensional quantum many-body system on a ring of circumference L, with M particles—either one-component fermions or bosons—carrying a charge -q. The ring is threaded by a magnetic flux of strength $\hbar c\Phi/q$. Following Beyers and Yang, the sole effect of the magnetic flux is to impose twisted boundary conditions $\Psi(...,$ $x_1 + L, \ldots = e^{i\Phi} \Psi(\ldots, x_1, \ldots)$. If this system were a continuum system with Galilean invariance, the problem would be trivial, for then we could simply take an energy eigenstate for $\Phi = 0$ with total energy E and total momentum P, and multiply it by a phase factor $\exp(i\Phi\sum x_i/L)$. This new state will satisfy the correct twisted boundary conditions, and will also be an energy eigenstate with an energy $E(\Phi)$ equal to $E(\Phi) = E$ $+2\Phi P/L + M\Phi^2/L^2$. (We use units where $\hbar = 1$ and $2 \times \text{mass} = 1$.) On the other hand, if the particles move on a lattice, Galilean invariance is destroyed, and the problem is nontrivial.

Denoting by $E_0(\Phi)$ the ground-state energy for a given Φ , we can readily establish that $E_0(\Phi+2\pi)=E_0(-\Phi)=E_0(\Phi)$. On the other hand, if we begin with the ground state for $\Phi=0$, and then follow this state adiabatically for increasing Φ , we find the energy $E(\Phi)=E_0(0)+\Delta E(\Phi)$ to be a continuous function of Φ . It is this adiabatic variation that concerns us in this Letter. If the original spectrum has a gap above the ground state of order 1, then $E_0(\Phi)$ and $E(\Phi)$ will coin-

cide for all Φ , and in fact be independent of Φ . Otherwise they need not, and will only coincide up to the first level crossing of $E_0(\Phi)$. For the continuum case, $E_0(\Phi)$ and $E(\Phi)$ coincide only for $\pi \ge \Phi \ge -\pi$. At $|\Phi| = \pi$, there will be level crossings.

The model we study is the familiar Heisenberg-Ising spin chain governed by the Hamiltonian²

$$H = -\frac{1}{2} \sum_{j=1}^{N} \left\{ \sigma_{j}^{x} \sigma_{j+1}^{x} + \sigma_{j}^{y} \sigma_{j+1}^{y} + \Delta \sigma_{j}^{z} \sigma_{j+1}^{z} \right\}.$$

As is well known, ^{2,3} this has an interpretation as a lattice gas of either fermions or bosons, where spin up represents an empty lattice site and spin down represents a particle. The energy eigenfunctions are given by Bethe's ansatz in the form

$$\Psi(x_1,\ldots,x_M) = \sum_{P} A(P) \exp\left[i \sum_{j=1}^{M} p_{Pj} x_j\right].$$

In this expression, P is a permutation of the integers from 1 to M, A(P) are M! coefficients related by two-body scatterings, and the M variables p_j are given as solutions to a set of M coupled transcendental equations when we impose boundary conditions.

Much is known about this problem, especially in the thermodynamic limit. ^{2,4} For the considerations of this Letter, we quote a recent result of Hamer, Quispel, and Batchelor ⁵ who, using methods of Woynarovich and Eckle ⁶ which in turn were based on Wiener-Hopf techniques

of Yang and Yang,² find for the ground state with twisted boundary conditions, at $m = \frac{1}{2}$ and with $\Delta = -\cos(\mu)$,

$$E_{0,N}(\Phi) - E_{0,\infty}(0) \cong -\frac{\pi^2 \sin(\mu)}{6\mu N} + \frac{\pi \sin(\mu) \Phi^2}{4\mu (\pi - \mu) N},$$

$$E_0(\Phi) - E_0(0) = \pi \sin(\mu) \Phi^2 / 4\mu (\pi - \mu) N$$
.

We begin with the familiar coupled transcendental equations for the wave vectors of the Bethe-ansatz solution of the spin chain, modified only by the addition of the phase Φ of the twisted boundary conditions:

$$Np_j = 2\pi I_j + \Phi - \sum_{l=1(l\neq j)}^{M} \theta(p_j, p_l)$$
.

Since we wish to follow adiabatically the state which is the ground state at $\Phi = 0$, as we continuously vary Φ , we choose the quantum numbers I_j to be the ground-state quantum numbers: $I_1, \ldots, I_M = -(M-1)/2, \ldots, (M-1)/2$.

The phase shift $\theta(p,q) = -\theta(q,p)$ is the familiar function

$$\theta(p,q) = 2\arctan\left[\frac{\Delta\sin[(p-q)/2]}{\cos[(p+q)/2] - \Delta\cos[(p-q)/2]}\right].$$

In this Letter, we shall only treat the repulsive case $0 \ge \Delta \ge -1$, or $\pi/2 \ge \mu \ge 0$. This function θ , considered for now as a function of two real variables p and q, has branch points at $p = q = \pm (\pi - \mu)$, and periodic images of these. We choose the cuts so that as we vary Φ , the p's remain on the same sheet. (We find continuity in Φ to be extremely useful, as was continuity in Δ in previous investigations.) This criterion places branch cuts at $\pi - \mu \ge p = q \ge \pi + \mu$, and requires $\theta(p + 2\pi, q) = -2\pi + \theta(p,q)$.

There are three physical quantities of interest: (a) M, the number of particles, (b) the energy $E = -N\Delta/2 + 2\sum_{j=1}^{M} (\Delta - \cos p_j)$, and (c) the total momentum $P = M\Phi/N = \sum_{j=1}^{M} p_j/N$.

We want to start from the ground state and adiabatically vary the flux until we return to our initial state. The energy $E(\Phi)$ must then also return to its initial value, although it might return sooner (to order 1/N), so that the period of the wave function is an integer multiple of the period of the energy. Further, we see that the relation between the momentum and the flux, $P = M\Phi/N$, which can be proven generally, also places restrictions on the period of the wave function, since P must return to its initial value mod 2π . However, the energy may return to its initial value without P returning to its initial value (mod 2π), provided there is a degenerate state (to order 1/N) at the proper momentum. We will return to this point later.

Let us first review the case of free particles when $\Delta = 0$. Since this corresponds to free fermions, clearly the period of $E(\Phi)$ is $2\pi N$, and

$$E(\Phi) = -2 \frac{\cos(\Phi/N)\sin(\pi M/N)}{\sin(\pi/N)}.$$

For the interacting case with $0 > \Delta \ge -1$, or $\pi/2 > \mu \ge 0$, the situation is very different. We restrict ourselves in what follows to the most interesting case of a half-filled band or lattice when M = N/2. Following the p's, and thus the wave functions, as continuous functions as Φ , the behavior we find is the following. Starting from the ground-state p's characterized by the groundstate quantum numbers, we adiabatically turn up the flux Φ . As long as $|\Phi| \le 2(\pi - \mu)$, all p's stay within $|p| < \pi - \mu$. As Φ increases past $2(\pi - \mu)$, p_M —the maximum p—increases beyond $\pi - \mu$. It continues to increase, so that at $\Phi = 2\pi$, $p_M = \pi$, until finally at $\Phi = 2(\pi + \mu)$, p_M crosses $\pi + \mu$. During the time that $2(\pi-\mu) < \Phi < 2(\pi+\mu)$ and $\pi-\mu < p_M < \pi+\mu$, all the other M-1 p's stay within $|p| < \pi - \mu$. Finally, for $2(\pi + \mu) < \Phi < 2(3\pi - \mu)$ the p's are the same as for the original $|\Phi| \leq 2(\pi - \mu)$, mod (2π) , provided we relabel, so that $p_{M-1} > p_{M-2} > \cdots > p_1 > p_M - 2\pi$. The state is thus periodic in Φ with period 4π , which may be interpreted as implying charge carriers with charge -q/2. The remainder of this paper verifies this scenario and examines the consequences.

First let us consider some special points where the equations simplify.

(a) Let $p_M = \pi - \mu$, so $I_M = (M-1)/2$, and $\theta(p_j, p_M) = \pi - 2\mu$ for j < M. Remembering that a half-filled lattice implies N = 2M, the equation for p_M gives the flux to be $\Phi = 2(\pi - \mu)$. On the other hand, the remaining M-1 equations reduce to

$$Np = 2\pi I'(p) - \sum^{"} \theta(p, p') ,$$

where I'(p) are the ground-state quantum numbers for M-1 particles, and the double prime on the summation over p' indicates that both p and p_M are to be omitted. Thus neither p_M nor Φ appears in these equations, and the M-1 p's are just the ground-state distribution for M-1 particles and no flux. We find for the momentum and energy that

$$P = p_M = \pi - \mu = \Phi/2 ,$$

$$E = E_{0,M-1} + 2[\Delta - \cos(p_M)] = E_{0,M-1}$$
.

Yang and Yang² have calculated the susceptibility at zero magnetization, and thus give us the final result for $\Delta E(\Phi) = E(\Phi) - E(0) = E(\Phi) - E_{0,M}$,

$$\Delta E(\Phi) = E_{0,M-1} - E_{0,M} = \pi (\pi - \mu) \sin(\mu) / N\mu$$
$$= - \text{ (chemical potential)}.$$

This result agrees with Hamer, Quispel, and Batchelor, whose derivation is valid for $|\Phi| \le 2(\pi - \mu)$, or up to this point and not beyond.

(b) There is a similar point when $p_M = \pi + \mu$, $\Phi = 2(\pi + \mu) = 2P$, with the same energy as (a).

(c) If we let $p_M = \pi$, and assume that the remaining M-1 p's are symmetric about the origin so that $\sum \theta(p_j, p_M) = (M-1)\pi$, we then find the flux to be

 $\Phi = 2\pi$. Now, the remaining M-1 equations reduce to

$$Np = 2\pi I'(p) - \sum_{n=0}^{\infty} \theta(p, p') + [\pi - \theta(p, \pi)].$$

The last term is an odd function of p, justifying our original assumption. The total momentum is π ; however, the energy is not so easy to evaluate. It appears to give ΔE of order 1, when in fact, as we shall soon see, ΔE is really of order 1/N.

We now investigate the region when $|\Phi - 2\pi| < 2\mu$, $|p_M - \pi| < \mu$. We thus define new variables $\delta \Phi \equiv \Phi - 2\pi$, $\delta p \equiv p_M - \pi$, and find the equations become

$$Np = 2\pi I'(p) - \sum^{"} \theta(p, p') + \delta \Phi + [\pi - \theta(p, \pi + \delta p)],$$

$$N\delta p = \delta \Phi + \sum [\pi - \theta(p, \pi + \delta p)].$$

Thus the equations resemble a system of M-1 particles with flux, and some type of excitation.

The p variables are not the most useful for explicit calculations, since the two-body phase shift is so complicated. Therefore we now introduce a useful change of variables by first defining a function $f(\alpha|\mu)$ of a complex variable α and a real parameter μ :

$$f(\alpha|\mu) \equiv 2 \arctan[\cot(\mu/2)\tanh(\alpha/2)]$$
.

This function has branch points at $\alpha = \pm i\mu + 2\pi i$ (integer). We choose the branch so that

$$-\infty < \alpha < +\infty$$
 gives $-(\pi - \mu) < f < +(\pi - \mu)$,

and with $\alpha = i\pi + \beta$,

$$-\infty < \beta < +\infty$$
 gives $\pi - \mu < f < \pi + \mu$.

The derivative of f occurs so frequently that we give it a name,

$$\frac{df(\alpha|\mu)}{d\alpha} \equiv k(\alpha|\mu) = \frac{\sin(\mu)}{\cosh(\alpha) - \cos(\mu)},$$

and calculate the Fourier transform as

$$\tilde{k}(\gamma|\mu) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} d\alpha \, e^{-i\gamma\alpha} k(\alpha|\mu) = \frac{\sinh[(\pi-\mu)\gamma]}{\sinh(\pi\gamma)} \, .$$

An extremely important point is that this expression is only valid for $2\pi > \mu > 0$. For other values of the parameter we must use the symmetry relations

$$\tilde{k}(\gamma|\mu) = -\tilde{k}(\gamma|-\mu) = \tilde{k}(\gamma|\mu + 2\pi)$$

to extend the range of the parameter. We shall use the convention that when we write $\tilde{k}(\gamma|\mu)$, the argument μ will always be in the range $0-2\pi$. Note that $\tilde{k}(\gamma|\mu)$ is even in μ about π . The Fourier transform of f itself is given by $\tilde{f}(\gamma|\mu) = \tilde{k}(\gamma|\mu)/i\gamma$.

We now make a change of variables, so that

$$p_{j} = f(\alpha_{j} | \mu), \quad j = 1, \dots, M-1,$$

and

$$p_M = f(i\pi + \beta | \mu) = \pi - f(\beta | \pi - \mu),$$

so that

$$\delta p = -f(\beta | \pi - \mu) .$$

Also,

$$\theta(p,p') = \theta(f(\alpha|\mu), f(\alpha'|\mu)) = -f(\alpha - \alpha'|2\mu),$$

and

$$\pi - \theta(p, p_M) = \pi - \theta(f(\alpha|\mu), \pi - f(\beta|\pi - \mu))$$
$$= \pi - f(\alpha - \beta - i\pi|2\mu) = f(\beta - \alpha|\pi - 2\mu).$$

The basic equations thus now have the form

$$\begin{split} Nf(\alpha|\mu) = & 2\pi I'(\alpha) + \sum f(\alpha - \alpha'|2\mu) \\ & + f(\beta - \alpha|\pi - 2\mu) + \delta\Phi \;, \end{split}$$

$$Nf(\beta|\pi-\mu) = \sum f(\beta-\alpha|\pi-2\mu) - \delta\Phi$$
.

One further expression we need is the energy, given as

$$E = -N\Delta/2 - 2\sin(\mu) \left[\sum k(\alpha|\mu) - k(\beta|\pi - \mu) \right].$$

The coupled equations have terms of very different sizes, and consistency requires that they be satisfied to each order in 1/N. The lowest-order equations are

$$f(\alpha|\mu) = 2\pi I'(\alpha)/N + \sum f(\alpha - \alpha'|2\mu)/N,$$

$$f(\beta|\pi - \mu) = \sum f(\beta - \alpha|\pi - 2\mu)/N.$$

The first equation is familiar from Yang and Yang,² and requires that the α 's be distributed from $-\infty$ to $+\infty$ with a density $NR_0(\alpha)/2\pi$. Differentiating both equations and replacing sums by integrals, they become

$$k(\alpha|\mu) = R_0(\alpha) + \frac{1}{2\pi} \int_{-\infty}^{\infty} k(\alpha - \alpha'|2\mu) R_0(\alpha') d\alpha',$$

$$k(\beta|\pi - \mu) = \frac{1}{2\pi} \int_{-\infty}^{\infty} k(\beta - \alpha|\pi - 2\mu) R_0(\alpha) d\alpha.$$

Thus $R_0(\alpha)$ appears to be overconstrained. The integral equations can be easily solved by Fourier transforms, and we find that the first equation gives

$$R_0(\alpha) = \frac{\pi}{2\mu \cosh(\pi\alpha/2\mu)} .$$

The second equation is identically satisfied due to the remarkable identity between Fourier transforms,

$$\tilde{k}(\gamma|\pi-\mu)[1+\tilde{k}(\gamma|2\mu)] = \tilde{k}(\gamma|\mu)\tilde{k}(\gamma|\pi-2\mu).$$

This equation appears even more remarkable when rewritten as

$$k(i\pi+\beta|\mu) - \frac{1}{2\pi} \int_{-\infty}^{\infty} k(i\pi+\beta-\alpha|2\mu) R_0(\alpha) d\alpha = 0.$$

If we had taken the first equation and analytically continued α to $\beta + i\pi$, we would have had for the right-hand side of the second equation not zero, but instead $R_0(i\pi + \beta) \neq 0$. Analytically extending the equation is a trick that is often used, for instance, in the Wiener-Hopf techniques or the calculation of the excitations of the

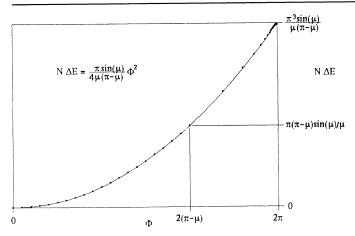


FIG. 1. The results for $\mu = \pi/3$. The curve is the exact theoretical result, while the small squares give numerical results for a ring of 64 sites.

Heisenberg-Ising ring. However, as we can easily see, it is not permissible to continue from the real axis to the line $i\pi$ because there is an essential singularity of the integral at $\pm i\pi/2$.

The corrections due to the extra terms in the equations are of order 1, and they add. There is a correction to $R_0(\alpha)$ from $\delta\Phi$, obtained by adjusting the finite limits, and very likely in fact of order 1/N, as was the case when $|\Phi| < 2(\pi - \mu)$. In addition, there is a shift of the α 's due to the β term, so that we write $R(\alpha) \cong R_0(\alpha) + R_1(\alpha - \beta)/N$. The first equation,

$$k(\alpha|\pi-2\mu) = R_1(\alpha) + \frac{1}{2\pi} \int_{-\infty}^{\infty} k(\alpha-\alpha'|2\mu) R_1(\alpha') d\alpha',$$

implies that $R_1(\alpha)$ is even, and so the second equation gives $\delta \Phi = 0$, since f is odd.

The energy to order 1 is given by $E = E_0 + E_1$, where E_0 is the ground-state energy of order N as found by Yang and Yang, ² while

$$E_{\perp} = 2 \sin \mu \left[k \left(\beta | \pi - \mu \right) - \frac{1}{2\pi} \int_{-\infty}^{\infty} k \left(\beta - \alpha | \pi - 2\mu \right) R_{\perp}(\alpha) d\alpha \right].$$

Again, we can solve for $R_1(\alpha)$ and evaluate E_1 by Fourier transforms. Remarkably, the same identity as before gives the surprising result that $E_1 = 0$.

To summarize, the whole region where β goes from $-\infty$ to $+\infty$ occurs with no change of energy to order 1, and with no variation of flux from $\Phi = 2\pi$.

Thus, the energy ΔE is order order 1/N, and all variation of both flux and energy occurs while $|p_M - \pi| \cong \mu$. An exact theoretical derivation using Wiener-Hopf techniques gives the final result for the energy as

$$\Delta E(\Phi) = [\pi \sin(\mu)/N4\mu(\pi - \mu)]\Phi^2, \quad |\Phi| \le 2\pi,$$

$$\Delta E(\Phi + 4\pi) = \Delta E(\Phi).$$

The derivation will be presented in a longer publication, but we have numerically iterated the equation, and the convergence is excellent. In Fig. 1, we show the results for $\mu = \pi/3$. The curve is the exact theoretical result, while the small squares give numerical results for a ring of 64 sites. The results are particularly impressive since different iteration schemes must be used on each side of the point $\Phi = 2(\pi - \mu)$. [The point at $\Phi = 2(\pi - \mu)$ is actually one point from each of the two schemes.] For any finite N, the curve is quadratic at $\Phi = 2\pi$, while in the limit $N \to \infty$, $N\Delta E$ has a cusp.

Since the spectrum is periodic in Φ with period 2π , $E(2\pi)$ must be a state in the spectrum with momentum $P = \Phi/2 = \pi$. This state has the energy of the first excited state in the M = N/2 sector with zero flux, it is the momentum π state at the bottom of the well-known des Cloizeaux and Gaudin⁴ dispersion curve, and it is degenerate with the ground state in the thermodynamic limit. If we had started from this state, we would have had an energy-flux relation $\Delta E(\Phi+2\pi)$, and these two curves intertwine as Φ is varied. In fact, our calculation gives an exact calculation of the energy gap above the ground state in the $S_z = 0$ sector,

$$\Delta E(2\pi) = \pi^3 \sin(\mu) / N\mu(\pi - \mu) ,$$

for the Heisenberg-Ising model with $0 \ge \Delta \ge -1$. This agrees with the numerical result π^2/N for $\Delta = -1$ of Bonner⁷ and the analytic result of Woynarovich.⁸

One can reverse the argument and give a partial explanation of the 4π periodicity for $\Delta E(\Phi)$ as follows: For finite N, we know the ground state to be nondegenerate. If we can sharpen this statement to show the ground state to be nondegenerate to order 1/N, then since P does not return to $0(\text{mod}2\pi)$ until Φ increases to 4π , the periodicity of $N\Delta E(\Phi)$ cannot be less than 4π . Of course for $\Delta=0$, we have a case where the period is much larger than 2π . And, on the other hand, we know that for $\Delta<-1$, the ground state is doubly degenerate to order 1/N, with a gap above of order 1, so $N\Delta E(\Phi)=0$ and the period is zero.

We define a topological winding number to be the number of times the flux Φ increases by 2π before the state returns to its initial value. Thus, the winding number of our state is 2, for $0 \le \mu < \pi/2$. However, we find for the free-particle case $\mu = \pi/2$ that the winding number is N. This result indicates that there are branch points in the μ - Φ plane at $\mu = \pi/2$ and $\Phi = 2(\pi \pm \mu)$, so that as we walk a closed curve in the μ - Φ plane, we do not necessarily return to our initial state. Or, in other words, zero interaction is fundamentally different from weak interaction.

To our knowledge, this is the first such calculation for an interacting many-body system. Results for the attractive case and for the Hubbard model will be presented in subsequent papers.

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