Twisted Boundary Conditions and Effective Mass in Heisenberg-Ising and Hubbard Rings

B. Sriram Shastry
AT&T Bell Laboratories, Murray Hill, New Jersey 07974

Bill Sutherland
Department of Physics, University of Utah, Salt Lake City, Utah 84112
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We identify the boundary energy of a many-body system of fermions on a lattice under twisted boundary conditions as the inverse of the effective charge-carrying mass, or the stiffness, renormalizing nontrivially under interactions due to the absence of Galilean invariance. We point out that this quantity is a sensitive and direct probe of the metal-insulator transitions possible in these systems, i.e., the Mott-Hubbard transition or density-wave formation. We calculate exactly the stiffness, or the effective mass, in the 1D Heisenberg-Ising ring and the 1D Hubbard model by using the ansatz of Bethe. For the Hubbard ring we also calculate a spin stiffness by extending the nested ansatz of Bethe-Yang to this case.

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It is intuitively clear that one can distinguish between a metal and an insulator by studying the variation of eigenvalues under changes in boundary conditions (BC's). This was proposed by Kohn[1,2] as a means of studying the Mott transition—a metal-insulator transition that requires the combination of strong correlations and a single-band model of fermions. We present here what we believe is the first application of this idea, in two nontrivial many-body problems in 1D exhibiting the metal-insulator transition. These are the Heisenberg-Ising model undergoing a CDW (charge-density-wave) transition, and the Hubbard model undergoing a Mott transition.

We first sharpen the arguments of Kohn, specializing to a one-band d-dimensional-lattice Fermi system, and deduce the main implications—some of which seem to be insufficiently appreciated in literature. Consider a d-dimensional hypercubic lattice of linear dimension L, with spinless fermions having a nearest-neighbor hopping matrix element t and arbitrary density-dependent interactions that are lattice-translation invariant, and assume periodic BC's. We now introduce a uniform vector potential $A_x\hat{\mathbf{x}}$, which modifies the hopping in $\hat{\mathbf{x}}$-directed bonds by the usual Peierls phase factor, $t \to t\exp(\pm i\Phi/L)$, where $\Phi = LA_x e/\hbar c$ and the lattice constant $a_0 = 1$. Expanding the exponential we find the perturbed Hamiltonian $H' = H - \Phi j_x/L - \frac{1}{2}\Phi^2 T_x/L^2 + O(\Phi^3)$, where $j_x = 2t\sum \sin k_x C_k^\dagger C_k$, $T_x = -2t\sum \cos k_x C_k^\dagger C_k$, and H is the Hamiltonian for the interacting Fermi system. The energy shift of the ground state (g.s.) in the presence of the field is $E_0(\Phi) - E_0(0) \equiv D\Phi^2/L^{2-d} + O(\Phi^4)$, with the stiffness constant D given by second-order perturbation theory as

$$D = \frac{1}{L^d}\left[\frac{1}{2d}\langle -T\rangle - \sum_{\nu\neq 0}\frac{|\langle 0|j_x|\nu\rangle|^2}{E_\nu - E_0}\right], \tag{1}$$

where $\langle T\rangle$ is the kinetic-energy expectation in the g.s. and $E_0(0) \equiv E_0$. We have assumed that $\langle j_x\rangle$ is zero. Higher-order (nonquadratic) terms in the energy-shift formula are important when the energy shift is comparable to the energy gaps in the spectrum of H. The latter are $O(1/L)$ in metals and so in this case corrections arise when Φ is $O(1/L^{(d-1)/2})$. Level crossings would occur and perturbation theory would break down for Φ of order π.

We next specialize to $A_x \to A_x^0 \exp(-i\omega t)$ leading to an electric field $\mathbf{E}_x = A_x(i\omega/c)\hat{\mathbf{x}}$, from which the usual linear-response formula[3] gives the imaginary part of the ac conductivity,

$$\mathcal{I}\sigma_{xx}(\omega) = \frac{2e^2}{L^d\hbar^2\omega}\left[\frac{1}{2d}\langle -T\rangle - \mathcal{P}\sum_{\nu\neq 0}\frac{|\langle 0|j_x|\nu\rangle|^2(E_\nu - E_0)}{(E_\nu - E_0)^2 - \hbar^2\omega^2}\right]. \tag{2}$$

From (1) and (2) we see that $\lim_{\omega\to 0}\omega\mathcal{I}\sigma_{xx}(\omega) = (2e^2/\hbar^2)D$ and $\lim_{\omega\to\infty}\omega\mathcal{I}\sigma_{xx}(\omega) = (e^2/d\hbar^2L^d)\langle -T\rangle$. The high-frequency behavior of the imaginary part of the conductivity implies for the real part, through the usual dispersion relations, the well-known[3] f-sum rule:

$$\int_{-\infty}^{\infty}\mathcal{R}\sigma_{xx}(\omega)d\omega = \frac{\pi e^2}{d\hbar^2 L^d}\langle -T\rangle.$$

More interesting is the small-ω behavior, implying that

$$\mathcal{R}\sigma_{xx}(\omega) = \frac{2\pi e^2}{\hbar}\left[D\delta(\hbar\omega) + \frac{1}{L^d}\sum_{\nu\neq 0}|\langle 0|j_x|\nu\rangle|^2\delta((E_\nu - E_0)^2 - \hbar^2\omega^2)\right]. \tag{3}$$

The coefficient of $\delta(\hbar\omega)$, if nonzero, implies free acceleration or infinite dc conductivity, which is reasonable here since there is no dissipative mechanism in the model at $T=0$. The coefficient is essentially the inverse of the effective current-carrying mass (for free electrons it is $\pi pe^2/m$). Therefore the f-sum rule is satisfied by the *sum of two terms of the same order*, the stiffness D and the "intraband dipole matrix elements." A method to calculate $E_0(\Phi)$ is to study different BC's—we can absorb the Peierls phases by a pseudo-gauge-transformation[4] and shift the effect of Φ into twisted BC's for the wave functions:

$$\Psi(\ldots,\mathbf{r}+L\mathbf{x},\ldots)=\exp\{i\Phi\}\Psi(\ldots,\mathbf{r},\ldots). \quad (4)$$

A crucial point (familiar from Landau's Fermi-liquid theory) is that for a Galilean-invariant interacting system, an analogous calculation would give the coefficient of $\delta(\hbar\omega)$ in (3) unrenormalized by interactions since $[j_x,H]=0$ [the first term in (1) becomes the particle density]. For lattice fermions the operator j_x commutes with the hopping part of H, but not with the interaction piece in general[5] and hence for *interacting lattice fermions* there is the possibility that the two terms in (1) cancel as some parameter is varied, signaling a metal-insulator transition. The absence of Galilean invariance thus allows the charge-carrying effective mass to vary with interactions, and in fact to diverge.[6]

We now consider the 1D Heisenberg-Ising (H-I) model of spinless fermions, with twisted BC's on a ring of length L described by

$$H=-\sum(C_n^\dagger C_{n+1}+\text{H.c.})-2\Delta\sum(\rho_n-\tfrac{1}{2})(\rho_{n+1}-\tfrac{1}{2}),$$

with $\rho_n=C_n^\dagger C_n$. Much is known about the model without the twist, and we merely note here that it has a gapless phase for $-1\le\Delta\le+1$ which is the conducting phase, and an ordered state with a gap for $-1>\Delta$, the insulating state. Bethe's ansatz is readily generalized to the case of twisted BC's (4) and the g.s. energy is known[7,8] for all Φ for the repulsive case ($0\ge\Delta\ge-1$). The angle Φ has the physical interpretation of a magnetic flux through the ring in units of $\hbar c/e$. In brief, the Bethe equations generalize to $Lk_n=2\pi I_n+\Phi-\sum_{m\neq n}\Theta(k_n,k_m)$ with the usual phase shift[9] Θ. In the sector with $M=L/2$ particles the g.s. quantum numbers are $I_n=-(L+1)/2+n$ for $1\le n\le L$; this is the half-filled band corresponding to $S^z_{\text{tot}}\equiv L/2-M=0$ in the spin representation. In general, a calculation of the stiffness D requires a precision in total energy of order $1/L$ in 1D. In this problem, however, it is possible to obtain D through a thermodynamic calculation[8] using a remarkable property of the generalized Bethe equations, and the result (with $\Delta=-\cos\mu$) is

$$D=\frac{\pi}{4}\frac{\sin\mu}{\mu(\pi-\mu)}.$$

As $\Delta\to-1$, $\mu\to0$ and D approaches a nonzero value $\frac{1}{4}$. For $\Delta<-1$ there is a gap in the spectrum and D is zero—thus the stiffness and the effective mass have a jump discontinuity.

This transition is tracked by the interesting variation of certain eigenvalues of the H-I model. The state of the H-I model obtained[8] from the g.s. by adiabatically increasing Φ from 0 to 2π is one with a total momentum π, and can be found from the set of generalized Bethe equations by shifting all g.s. integers by unity; the energy above the ground state is $\Delta E_1=4D\pi^2/L=\pi^3(\sin\mu)/\mu(\pi-\mu)L$. A third state of relevance is the g.s. in the sector $S^z=1$ (corresponding to removing a particle) with an energy (above the absolute g.s.) given by Yang and Yang[9] as $\Delta E_2=\pi(\pi-\mu)(\sin\mu)/\mu L$ in the entire gapless range, $-1\le\Delta\le+1$. These levels cross at the critical point where $\Delta\to-1$. This degeneracy is accounted for by the rotational invariance of the H-I model at $\Delta=-1$.

In the ordered state $\Delta<-1$, the second state above (with quantum numbers leading to ΔE_1) is asymptotically degenerate with the g.s. (the splitting vanishing more rapidly than $1/L^n$ for any n). Its energy splitting from the g.s. is fortunately available from the work of Baxter who calculated the interfacial tension of the six- and eight-vertex models.[10] Baxter's beautiful result translates into $D\sim\exp(-L/\xi)$, where the correlation length

$$\xi=1\Big/\ln\left[\frac{1}{2x^{1/2}}\left(\prod_{m=1}^{\infty}\frac{1+x^{4m-2}}{1+x^{4m}}\right)^2\right],$$

with $\Delta=-\cosh\lambda$, $x=\exp(-\lambda)$. This phase is therefore insulating in the thermodynamic limit. The third state above corresponds to removing a particle, and develops an energy gap in this region,[9] $\Delta<-1$, with

$$\Delta E_2=2(\sinh\lambda)\sum_{n=-\infty}^{\infty}\frac{(-1)^n}{\cosh(n\lambda)}.$$

The above behavior of D implies that although the system is insulating in the infinite-lattice limit, for a finite system, provided L/ξ is not too large, we should see a small "free acceleration" response arising from adiabatic sliding between the almost degenerate "ground" states.

We next consider the repulsive $U\ge0$ Hubbard model in 1D containing two species of particles, spin up and spin down. The boundary angles for the two are treated as independent parameters $\Phi_\uparrow$ and $\Phi_\downarrow$. There are two independent stiffnesses that we may calculate. Setting $\Phi_\uparrow=\Phi_\downarrow=\Phi$ the energy shift gives the "charge stiffness" D_c and setting $\Phi_\downarrow=-\Phi_\uparrow=\Phi$ gives the "spin stiffness" D_s. These have expressions identical to Eq. (1), with D_c involving the *sum* of the up and down currents and D_s the *difference* in the matrix element, and both containing the total kinetic-energy expectation. This general case requires a generalization of the Bethe-Yang ansatz that was employed by Lieb and Wu[11] for the solution of the model with periodic BC's. We present here, in brief, the analysis necessary to ensure that the model remains solvable with the twisted BC's.

The model is described by the usual Hamiltonian and we denote by L, N, and M the number of sites, particles, and down-spin particles. The Bethe wave function is written in the form

$$|\Psi\rangle=\sum_{\substack{1\le x_1\le\cdots\le x_N\le L\\ 1\le j_1\le\cdots\le j_M\le N}}\sum_{P}\left[\exp\left(i\sum_n k_{P_n}x_n\right)A(\{j_n\}\,|\,P)\right]$$

$$\times C^{\dagger}_{x_1\uparrow}\cdots C^{\dagger}_{x_{j_1}\downarrow}\cdots C^{\dagger}_{x_{j_M}\downarrow}\cdots C^{\dagger}_{x_N\uparrow}|0\rangle\,,$$

where P is a sum over the $N!$ permutations and $A(\{j_n\}\,|\,P)$ is the amplitude. The wave function satisfies the difference equations that follow from the Hubbard model in the interior of the chain as usual with energy $E=-2\sum\cos k_n$ (setting $t\to 1$), provided the amplitudes satisfy the usual consistency conditions.[11,12] We impose the boundary conditions Eq. (4) with different boundary angles for the two spin species by transporting the particle at x_1 to x_1+L, and this gives

$$\exp(ik_{P_1}L)A(\{j'_n\}\,|\,P')$$

$$=\{\exp(i\Phi_\uparrow\delta_{j_1,1})+\exp[i\Phi_\uparrow(1-\delta_{j_1,1})\}A(\{j_n\}\,|\,P)\,. \quad (5)$$

Here P' is obtained from P by a cyclic permutation and $j'_n=j_n-1\,(\mathrm{mod}N)$. It is convenient to write these in vector form by introducing $|A(P)\rangle=\sum|\{j_n\}\rangle A(\{j_n\}\,|\,P)$ with the vector $|\{j_n\}\rangle$ denoting the basis state with overturned "spins" located at the "sites" $j_1,\ldots,j_n$. The BC's Eq. (5) translate into the following N eigenvalue conditions that must be simultaneously satisfied: $\exp(ik_jL)\,|A_0\rangle=L_j\,|A_0\rangle$, where $|A_0\rangle$ is the vector for the identity permutation, the N-string operators are

$$L_j=X_{j+1,j}\cdots X_{N,j}D_jX_{1,j}\cdots X_{j-1,j}\,,$$

the operators $X_{i,j}=(y_{i,j}-P_{i,j})/(y_{i,j}-1)$, with $y_{i,j}=2i\times(\sin k_i-\sin k_j)/U$ and $P_{i,j}$ the usual permutation operator, and the new operator is

$$D_j=\exp(i\Phi_\uparrow)(1+\sigma^z_j)/2+\exp(i\Phi_\downarrow)(1-\sigma^z_j)/2\,.$$

We must now verify that the N operators L_j commute, and then diagonalize these. This task is neatly performed with a generating (monodromy) operator Υ_g acting on a $(N+1)$-site spin chain, $\Upsilon_g(\lambda)=D_g l_{N,g}(\lambda)\cdots l_{1,g}(\lambda)$, where g is the extra $(N+1)$th site and the scattering operator

$$l_{n,g}(\lambda)=[i(\sin k_n-\lambda)-U/2P_{n,g}]/[i(\sin k_n-\lambda)-U/2]\,.$$

The N-string operators L_j can be obtained from the generating operator by using that $\mathrm{Tr}_g\Upsilon_g(\lambda=\sin k_j)=L_j^{\dagger}(-[k_n])$. The commutation relations between L_j are guaranteed if $\mathrm{Tr}_g\Upsilon_g(\lambda)$ commutes with similar operators differing in the spectral parameter λ. This is in turn true[10] if an operator $R_{g,g'}$ exists such that $\Upsilon_g(\lambda)\Upsilon_{g'}(\mu)R_{g,g'}(\lambda,\mu)=R_{g,g'}(\lambda,\mu)\Upsilon_g(\mu)\Upsilon_{g'}(\lambda)$. In the present problem the Υ operator differs from the zero-flux case through the D_j operators with the property that $D_gD_{g'}=c\exp[d(\sigma^z_g+\sigma^z_{g'})]$. Noting that the $R_{g,g'}$ for the Heisenberg spin chain fulfills the commutation rules in the zero-flux case and further commutes with $\sigma^z_g+\sigma^z_{g'}$, we conclude that the twisted-BC case is also satisfied by the same R operator. The diagonalization of the L_j operators was done by a variant of the nested Bethe-Yang ansatz and the resulting transcendental equations are

$$Lk_n=2\pi I_n+\Phi_\uparrow+2\sum_{j=1}^{M}\arctan[4(\Lambda_j-\sin k_n)/U]\,, \quad (6)$$

$$2\sum_{n=1}^{N}\arctan[4(\Lambda_j-\sin k_n)/U]=2\pi J_j+\Phi_\downarrow-\Phi_\uparrow+2\sum_{i\neq j}^{M}\arctan[2(\Lambda_j-\Lambda_i)/U]\,, \quad (7)$$

with I_n,J_j as the usual quantum numbers (integer or half odd integer).

In order to study D_c, the charge stiffness, we set $\Phi_\uparrow=\Phi_\downarrow=2\pi$, and argue that the excitation energy is $(4\pi^2/L)D_c$. The underlying assumption here and in the next section (justified for the H-I model in Ref. 7) is that the energy $E_0(\Phi)$ remains quadratic in Φ out to this value, in spite of a level crossing that occurs prior to it. With this assumption, we can calculate D_c, in the general case, from the excitation energy of the state, obtained by adding unity to the g.s. quantum numbers I_n. An evaluation of D_c requires a detailed study of the finite-size effects. Here we are content to observe that the general structure of the equations forces D_c to vanish as $N\to L$, i.e., as we approach half filling for any nonzero value of U. This follows from the fact I_n+L and I_n lead to the same solution, and further, at half filling, the set of $N=L$ g.s. integers I_n exhaust all the allowed distinct values $-(L-1)/2,\ldots,(L-1)/2$, whereby $D_c=0$. To leading order in $1/U$ we can see this explicitly. Here Λ_j are of $O(U)$, and hence the two sets of equations decouple. It is readily seen that the charge stiffness is identical to that of spinless fermions with a density $\delta=(L-N)/L$, and hence $D_c\to 0$ linearly as $\delta\to 0$. It is also worth remarking that this vanishing stiffness can be equally well interpreted as a vanishing of the density of the effective carriers of charge, the "holons" of Anderson.[13]

The spin stiffness can, however, be related with the help of a remarkable identity to the bulk spin susceptibility, which in turn can be calculated readily by the method of integral equations for relevant densities. Consider the state for even N, with $M=N/2$ and $\Phi_\uparrow=\Phi_\downarrow$

$=0$; this is the g.s. for this filling and has the quantum numbers taking on values $I_n=-(N+1)/2+n$ for $1\le n\le N$ and $J_j=-(N/2+1)/2+j$ for $1\le j\le N/2$. Suppose that we have found the solutions for k_n and Λ_j. We now turn on Φ so that $\Phi_\uparrow=-\pi$ and $\Phi_\downarrow=\pi$, thereby "deforming" the previous solution. This case, however, can be solved by a neat observation (analogous to the H-I model in Ref. 8). The self-consistent solution is that $\Lambda_{\max}=+\infty$. Equation (7) for $j=j_{\max}$ is identically satisfied, and the remaining $N/2-1$ equations for $1\le j\le N/2-1$ can be written as

$$2\sum_{n=1}^{N}\arctan[4(\Lambda_j-\sin k_n)/U]=2\pi J_j'+2\sum_{i\neq j}^{N/2-1}\arctan[2(\Lambda_j-\Lambda_i)/U],$$

with $J_j'=J_j+\frac{1}{2}$; in Eq. (6) we drop the Φ and sum j over the $N/2-1$ finite Λ's. This set is recognizable as the g.s. equations in the sector $M=N/2-1$. Hence, the spin stiffness $D_s=(L/4\pi^2)[E_0(N,N/2)-E_0(N,N/2-1)]$. With the magnetization variable $y=1-2M/N$, the g.s. energy in a sector with fixed M is $E_0(N,M)=Ne_0(y)+\frac{1}{2}N\chi^{-1}y^2+O(y^4)$, defining the susceptibility. From the smallest allowed value of $y=2/N$ we conclude that $D_s=(1/2\pi^2)(L/N)\chi^{-1}$. This identity is true at all U and can be used to extract D_s from the calculation of the susceptibility. The latter has been calculated numerically[14] at several fillings and U. Qualitatively it is nonzero at all fillings, and resembles the Pauli susceptibility renormalized by U. Physically a nonvanishing D_s implies that the model has long-ranged (presumably power-law) spin correlations at all fillings.

The origin of the above relationship, between D_s and χ, is in the rotation invariance of the model for any U or filling. It follows from the degeneracy of the lowest excitations of $S_z=0$ with those of $S_z=1$ (with appropriate momenta). Apart from the normalization factor of L/N this is the same relation as in the Heisenberg-Ising model at $\Delta=-1$, i.e., the isotropic point. In general, the relation between the two for the H-I model is $D=[1/2(\pi-\mu)^2]\chi^{-1}$.

In conclusion, we have given two nontrivial examples where a metal-insulator transition occurs due to interactions and is reflected directly in the effective mass obtained by twisting the BC's. For the 1D Hubbard model the spin stiffness has been related to the bulk susceptibility through an interesting identity. It is clear that the ideas explored here have possible applications in higher-dimensional models, where numerical investigations with twisted BC's are possible for small systems.

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