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MOTT TRANSITION IN THE HUBBARD MODEL*

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In this article, I discuss W. Kohn's criterion for a metal insulator transition, within the framework of a one-band Hubbard model. This and related ideas are applied to 1-dimensional Hubbard systems, and some interesting miscellaneous results discussed. The Jordan–Wigner transformation converting the two species of fermions to two species of hardcore bosons is performed in detail, and the "extra phases" arising from odd-even effects are explicitly derived. Bosons are shown to prefer zero flux (i.e., diamagnetism), and the corresponding "happy fluxes" for the fermions identified. A curious result following from the interplay between orbital diamagnetism and spin polarization is highlighted. A "spin-statistics" like theorem, showing that the anticommutation relations between fermions of opposite spin are crucial to obtain the SU(2) invariance is pointed out.

1. Introduction

In this article, I will give a brief introduction to the Mott Transition in the Hubbard model. This subject is in a state of considerable flux, since it is believed by a large number of theorists, to be at the heart of the High-T_c phenomenon. This point of view was suggested by Anderson[1] as early as in 1986, at the Bangalore ICVF conference. It is less clear as the years go by, that the problem has an easy solution. However the validity of the Mott–Hubbard point of view as a starting point, in the spirit of providing at least the analog of H_0 seems very probable to me, of course it may well be that there is a mystery H_1 remaining to be discovered! The scope of this article is much more limited. I would like to describe the transition, and discuss some powerful techniques that have been recently brought to bear on this problem, within a well defined problem, the 1-d Hubbard model. These ideas have also been applied with considerable success in higher dimensions, by clever numerical work, and I will direct attention to these articles at the end.

In Sec. 2 we survey the problem of the Mott transition in various Hubbard like models. In Sec. 3, I discuss the criterion of Kohn for the Mott transition, and define the charge stiffness from the Kubo formula point of view as well as the energy point of view. In Sec. 4, I carry out the Jordan–Wigner transformation and identify extra phases arising from it. The diamagnetic inequality for bosons

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is stated, and an amusing spin statistics like theorem for two-component hard core boson/fermion system remarked on. Amusing odd-even effects in diamagnetism and weak spontaneous magnetism in the Hubbard model are pointed out. In Sec. 5, I discuss the Bethe Ansatz equations for the 1-d Hubbard model, which turn out to be very useful in extracting the charge stiffness.

2. The Mott Transition

We will first of all dispose of the long ranged Coulomb interaction by confining ourselves to the single-band Hubbard model: there is no good reason to do this beyond achieving simplicity. The conducting state, by definition, has metallic screening, making the neglect of the long ranged Coulomb interaction a reasonable approximation. The nature of the insulating state obtained within a purely short ranged Hubbard model is surely incorrect with regard to the excitations involving promotion to the upper Hubbard band, i.e., optical excitations.

The situation in say the 2-dimensional square lattice is complicated by magnetic LRO. At half-filling, i.e., one electron per site, the ground state is presumably magnetically ordered and insulating. The usual statement of a Mott–Hubbard gap is in terms of an energy gap towards adding an extra particle to a half-filled band: the existence of a gap of $O(1)$ distinguishes the insulator from a metal. This formulation, applied to the magnetically ordered Antiferromagnet, is confused by the existence of a Spin Density Wave gap, and the subtlety of the Mott–Hubbard gap is swamped by the essentially trivial SDW gap. We need to consider situations where the band structure inhibits the formation of an SDW state: many possibilities arise (a) The triangular lattice: here the band structure does not have a strong maximum at any Q at half-filling[2] although a three-sublattice ordered AFM state is the ultimate large U fate of the model; (b) Random hoppings: this is a doubly hard problem with disorder and interactions and no really convincing studies exist so far; (c) The Hubbard model on a special lattice in 2 dimensions constructed by Shastry and Sutherland[3]: (see Fig. 1). This is an interesting two-dimensional lattice with a unit cell consisting of four squares of the square lattice with diagonal bonds (existing in only two of these squares) running NE–SW in one square and NW–SE in the square which shares no bonds with the first. We consider a Hubbard model on this lattice with hoppings t and $t\sqrt{2\alpha}$. The band structure gives a semi-metal at half-filling, with a quadratic touching of the filled valence band, and an empty conduction band, for generic α. At large U, the model reduces to a Heisenberg Antiferromagnetic model with $S = 1/2$ on this lattice, with bond strengths say $J = 4t^2/U$ and $J' = 2J\alpha$; the really interesting fact is that the Heisenberg model can be solved exactly, and has frozen dimer order for the region $\alpha \geq 1$. For $\alpha < 1$, the model has not been solved, and approaches the usual nearest neighbour model as $\alpha \to 0$. This is the only case of an exactly solvable Heisenberg model with $S = 1/2$ in 2 dimensions that I am aware of, and is of interest from a Mott–

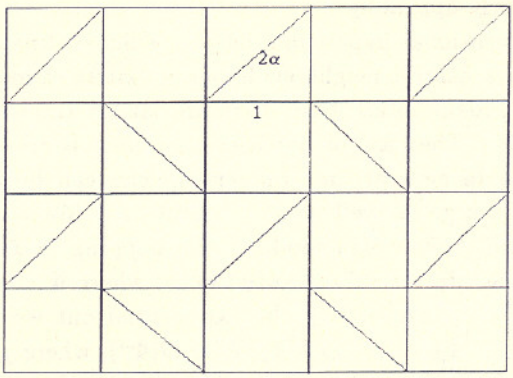

Fig. 1. The special lattice in two dimensions for which the Heisenberg $s = 1/2$ antiferromagnet is exactly solvable.

Hubbard point of view, since one expects the semi-metal to insulator transition, to be quite representative of the phenomenon, uncomplicated by magnetic LRO.

We confine ourselves in this article to the 1-d Hubbard model, which has the great virtue of being solvable exactly by the Bethe Ansatz,[4] and also of exhibiting a Mott Transition, uncomplicated by magnetic LRO. The model turns out to possess algebraically decaying spin correlations, which are by uncertainty principle arguments, the maximal remnants of magnetic LRO in 1-dimension. The tool that we bring to bear on this problem, is a powerful and beautiful argument due to W. Kohn.[5] This argument of Kohn, recently sharpened and revived by us[6] after many decades of neglect, turns out to be quantitatively implementable in the 1-d Hubbard model. In essence, Kohn's argument is that we can distinguish between a metal and an insulator, and hence track the Mott transition, by studying the ground state energy as a function of the boundary angle. This involves studying the solution of the many-body problem with twisted boundary conditions, and happily, the Bethe Ansatz method admits this complications and remains tractable.[6]

3. Kohn's Criterion for the Mott Transition

We first review the arguments of Kohn, specializing to a 1-band d-dimensional lattice fermi system, and deduce the implications, which concern the utility of studying the effect of twisting the boundary conditions in a many-body system. The second derivative of the ground state energy under variation of the flux is related to the zero frequency physics of the electrical conductivity. The economy of the Kohn argument is noteworthy: we talk of the properties of the conductivity directly, and do not worry about one electron gaps. It should be mentioned that several works have appeared in literature, trying to use various indirect probes of the Mott transition, including the double occupation, binding between holes and doubles,

and various fictitious fermi-bose fields. The directness of the Kohn argument, in contrast, is particularly appealing.

Consider a d-dimensional hypercubic lattice of linear dimension L, with spinless fermions having a nearest neighbour hopping matrix element 't', and with arbitrary density dependent interactions that are lattice translation invariant and assume periodic bc's. The case of particles with spin is trivially obtained from these considerations, in general, the different species can be twisted in differing degrees, leading to charge as well as a spin stiffness. We now introduce a uniform vector potential $A_x\hat{x}$, which modifies the hopping in $\hat{x}$ directed bonds by the usual Peierls phase factor $t \to t\exp(\pm i\Phi/L)$, where $\Phi = L(A_x e/\hbar c)$ and the lattice constant $a_0 = 1$. Expanding the exponential out we find the perturbed Hamiltonian $H' = H - \Phi j_x/L - 1/2\Phi^2 T_x/L^2 + O(\Phi^3)$, where $j_x = 2t\Sigma \sin k_x C_x^\dagger C_k$ and $T_x = -2t\Sigma \cos k_x C_k^\dagger C_k$, 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 $E_0(\Phi) - E_0(0) \equiv D\Phi^2/L^{2-d} + O(\Phi^4)$, or equivalently, we define the charge stiffness D:

$$D = \left(\frac{L^{2-d}}{2}\right) \frac{d^2 E_0(\Phi)}{d\Phi^2} \Bigg/_{\Phi=0}. \tag{1}$$

The stiffness constant D is given by second order perturbation theory as

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

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, this is not always true, and some examples are given in Sec. 4. Higher order (non-quadratic) 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 of $O(1/L^{(d-1)/2})$. Level crossings would occur and perturbations theory would breakdown for Φ of $O(\pi)$. The region in Φ wherein the derivatives are unambiguously defined, therefore shrinks with increasing L in two and higher dimensions.

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

$$\Im m\, \sigma_{xx}(\omega) = \frac{2e^2}{L^d\hbar^2\omega}\left[\frac{1}{2d}\langle -T\rangle - \wp \sum_{\nu\neq 0} \frac{|\langle 0|j_x|\nu\rangle|^2 (E_\nu - E_0)}{(E_\nu - E_0)^2 - \hbar^2\omega^2}\right]. \tag{3}$$

From Eqs. (2) and (3) we see that $\lim_{\omega\to 0} \omega\, \Im m\, \sigma_{xx}(\omega) = (2e^2/\hbar^2)D$, and also $\lim_{\omega\to\infty} \omega\, \Im m\, \sigma_{xx}(\omega) = (e^2/d\hbar^2 L^d)\langle -T\rangle$. The high frequency behaviour of the imaginary part of the conductivity implies for the real part, through the usual dispersion relations, the well known[7] f-sumrule:

$$\int_{-\infty}^{\infty} \Re e\, \sigma_{xx}(\omega) d\omega = \frac{\pi e^2}{d\hbar^2 L^d}\langle -T\rangle. \tag{4}$$

More interesting is the small ω behaviour. From standard dispersion theory we separate the low frequency part and conclude that

$$\Re e\, \sigma_{xx}(\omega) = \frac{2\pi e^2}{\hbar}\left[D\delta(\hbar\omega) + \frac{1}{L^d}\sum_{\nu\neq 0} |\langle 0|j_x|\nu\rangle|^2 \delta((E_\nu - E_0)^2 - \hbar^2\omega^2)\right], \qquad (5)$$

D, the coefficient of $\delta(\hbar\omega)$, if non-zero, implies free acceleration or infinite dc conductivity, which is reasonable here since there is no dissipative mechanism in the model at $T = 0^0$. The coefficient D is essentially the inverse of the effective current carrying mass (for free electrons it is $\pi\rho e^2/m$). Therefore the f-sumrule is satisfied by the *sum of two terms of the same order*, the stiffness D, and the "intraband dipole matrix elements". I would like to remark that Eq. (5) was not written down by Kohn, instead he emphasized the imaginary part of the conductivity (i.e., Eq. (3)), and in fact discussed metals as systems for which the f-sumrule is violated. A slight change of view point is advocated in the Shastry–Sutherland paper,[6] wherein the real part of conductivity, Eq. (5) is explicitly stated, and it is stressed that there is no violation of the f-sumrule, the zero frequency piece, together with the finite frequency piece certainly fulfil it. This point of view makes the charge stiffness D to appear very much like the stiffness in a superfluid or a superconductor.

This is all very nice, but we still need an algorithm to calculate the stiffness. Here Kohn makes the important observation that changing boundary conditions is equivalent to applying the Φ field, we can absorb the Peierls phases by a pseudo gauge-transformation[5,8] and shift the effect of Φ into twisted bc's for the wavefunctions:

$$\Psi(\cdots \mathbf{r} + L\mathbf{x}\cdots) = \exp\{i\Phi\}\Psi(\cdots \mathbf{r}\cdots). \qquad (6)$$

Hence, a calculation of the ground state energy with twisted b.c.'s suffices to give D.

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 Eq. (5) unrenormalized by interactions since $[j_x, H] = 0$ (the first term in Eq. (5) 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 and hence for *interacting lattice fermions* there is the possibility that the two terms in Eq. (2) cancel as some parameter is varied, signalling 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.

We thus see that Kohn's argument is a means of obtaining a "transport coefficient" D, from a calculation of the ground state energy. This is less uncomfortable when we recognize that D is *not* a characteristic of energy dissipation, but rather measures the quantity of freely responsive fluid. In fact it is obvious that the stiffness so defined is precisely the superfluid stiffness in say a superconductor. Thus Kohn's metal is a superconductor as well! True superconductivity may be distinguished

from the Mott–Hubbard–Kohn metal by introducing disorder. True superconductors are insensitive to disorder by the Anderson theorem, whereas the M–H–K metal would become a dirty metal, with a finite resistivity, and with energy dissipation. This brings us to the work of Thouless,[9] who brought a closely related and successful idea to the case of dirty metals, to distinguish between a dirty metal and an insulator, i.e., to study the Anderson transition. Thouless's ideas are worked out in a purely non-interacting limit, where one examines the various one-electron eigenstates of a random potential. The conducting states have a finite curvature with boundary angle, but the curvatures of successive energy levels are typically opposite in sign (since the dirty metal is crudely visualizable as a "periodic" system with a very short period in k-space), whereby a sum over the energy levels would give a thermodynamically negligible stiffness. The insulating states (i.e., localized states) have a vanishing stiffness, typically exponential in system size with a localization length setting the scale. A highly nontrivial part of the Thouless argument concerns the disorder average of the stiffness for the extended states, and relating this to a truly dissipative object, the conductance. This relationship has been explicitized in a recent work by Akkermans and Montamboux.[10]

It is worth noting that the relationship between D and the ground state energy (g.s.e.) is generalizable to finite temperature, with the free energy $F(\Phi)$ replacing the g.s.e. in Eq. (1). This relationship does not seem particularly useful for the Mott problem, since at finite temperatures, D is expected to vanish exponentially with system size since there exists a thermal length scale causing an exponential decay of the one particle correlation function.

I would like to mention a beautiful (if somewhat inaccessible) article on superfluidity by Leggett[11] in 1973, which clarifies the role of twisting boundary conditions in normal fluids, solids and superfluids within the context of rotating bucket like experiments, and illustrates the correspondence between these systems and between metals, insulators and superconductors. Also the work of Fisher *et al.*[12] makes precise the connection between the helicity modulus (i.e., $d^2F(\Phi)/d\Phi^2$) and the superfluid stiffness. A recent paper by Scalapino, White, and Zhang[13] discusses the various limits $\mathbf{q} \to 0$ and $\omega \to 0$, for the electromagnetic response kernel in 2 and higher dimensions, with the object of clarifying the role of the shrinking region of Φ in the Kohn argument alluded to above.

4. 1-d Hubbard Model: Generalities and Curiosities

In this section we specialize to the 1-d Hubbard model, which was solved by Lieb and Wu[4] in 1968. Before discussing the Bethe Ansatz method, we discuss some general ideas concerning the stiffness, and the problem of particles moving in a flux. We pay particular attention to the Jordan–Wigner transformation in this problem, which introduces a certain "flux" of its own, leading to occasionally surprising results. It is convenient, and natural, to convert the model to one involving hard-core bosons. Let us recall the Jordan–Wigner transformation between Pauli matrices σ_n^α, with

$1 \leq n \leq L$ and fermions c_n:

$$\sigma_1^z \cdots \sigma_{n-1}^z \sigma_n^+ = c_n^\dagger , \tag{7}$$

with $\sigma_n^z = 2c_n^\dagger c_n - 1$, and the hermitean conjugate of the Eq. (7). It is straightforward to see that

$$c_n^\dagger c_{n+1} = -\sigma_n^+ \sigma_{n+1}^- \tag{8}$$

and

$$c_L^\dagger c_1 = -(-1)^{\hat{N}-L+1} \sigma_L^+ \sigma_1^- . \tag{9}$$

where $\hat{N} = \sum_i c_i^\dagger c_i$, is the number operator.

We are interested in converting a fermionic hopping Hamiltonian having density dependent interactions, and with a boundary angle (or flux) Φ_f, and with $c_{L+1} = c_1$,

$$H_f = -\sum_{n=1}^{L} (c_n^\dagger c_{n+1} \exp(i\Phi_f/L) + \text{h.c.}) + V_{\text{int}} \tag{10}$$

to a hardcore boson hopping problem with a boundary angle Φ_b, and $\sigma_{L+1} = \sigma_1$,

$$H_b = -\sum_{n=1}^{L} (\sigma_n^+ \sigma_{n+1} \exp(i\Phi_b/L) + \text{h.c.}) + V_{\text{int}} . \tag{11}$$

We can do this in two stages, firstly use the Jordan–Wigner transformation Eq. (7), and next a unitary transformation $U_1 = \sum_n \exp(in\chi/L)$, with an appropriate χ, together this yields

$$\Phi_f = \Phi_b + \pi(\hat{N} - 1); \quad \text{mod } 2\pi . \tag{12}$$

The reason for preferring to work with bosons is that there are no extra phases involved. In fact we can show easily that the boson problem Eq. (11), generalized to any dimensions, and on any lattice, has a preference to having zero flux, i.e.,

$$E_b^0(\Phi) \geq E_b^0(0) , \tag{13}$$

where $E_b^0(\Phi)$ is the ground state energy in the presence of the flux Φ. This *diamagnetic inequality* follows from writing the eigenvalue equation for Eq. (11) in a standard basis, with particles living at various sites, whence the phases make their appearance in the off-diagonal elements of the matrix. We can decrease the ground state energy by increasing the absolute value of the off-diagonal matrix elements by virtue of the Rayleigh–Ritz variational principle. Inequality (13) follows on using $|\cos(\theta)| \leq 1$. Unless the magnetic field is a pure gauge field, we must maximize at least one "bond", and hence Inequality (13), is in general, a strict one and may be regarded as a statement of diamagnetism of bosons. A corresponding theorem for fermions does not exist. In fact Eq. (12) tells us that given the preference of bosons, the fermions like (i.e., the minimizing boundary angle is) to have "happy" phases:

$$\Phi_f^* = 0, \quad \pi \text{ for } \hat{N} = \text{odd, even} . \tag{14}$$

For the Hubbard model, we need a two-component Jordan–Wigner transformation, converting bosons σ_n^α, τ_n^α, to fermions $c_{n,\uparrow}$, $c_{n,\downarrow}$, through

$$\sigma_1^z \cdots \sigma_{n-1}^z \sigma_n^+ = c_{n,\uparrow}^\dagger \tag{15}$$

$$\sigma_1^z \cdots \sigma_L^z \tau_1^z \cdots \tau_{n-1}^z \tau_n^+ = c_{n,\downarrow}^\dagger \tag{16}$$

with $\sigma_n^z = 2c_{n,\uparrow}^\dagger c_{n,\uparrow} - 1$, and $\tau_n^z = 2c_{n,\downarrow}^\dagger c_{n,\downarrow} - 1$. The corresponding phase relations are easily seen to be

$$\Phi_{f,\uparrow} = \Phi_\sigma + \pi(\hat{N}_\uparrow - 1)\,. \tag{17}$$

$$\Phi_{f,\downarrow} = \Phi_\tau + \pi(\hat{N}_\downarrow - 1)\,. \tag{18}$$

with obvious notation. We have thus converted the two fermi component model to one with two hardcore boson species, with given phases. It may appear that the phases of the fermions were completely disposable and not very fundamental. However, at this stage, I would like to inject an essentially elementary digression into the discussion, showing how important the fermi phases really are.

4.1. *Digression: Absence of SU(2) for hard core bosons*

The global SU(2) invariance of the Hubbard model is well known, and together with the particle hole symmetry, gives the model SO(4) symmetry, as recently emphasized by Yang and Zhang.[14] This represents the (maximal) internal symmetry of the system. One may cavalierly expect that the hard core bose representation also possesses SU(2) symmetry. This is not so. An elementary demonstration of this follows from the examination of the commutation relations of the objects:

$$T^z = \sum_1^L (\sigma_i^z - \tau_i^z)/2 \tag{19}$$

$$T^+ = \sum_1^L (\sigma_i^+ \tau_i^-)\,, \tag{20}$$

and its hermitean conjugate. The commutator of T^α and T^β *does not* follow the usual SU(2) relations, and nor do T^α commute with the two-component boson version of the Hubbard Hamiltonian. The SU(2) relations of course follow, if one reinstates the Jordan–Wigner strings. *This is a kind of "spin-statistics" theorem in nonrelativistic physics.*

Getting back to our main theme, we examine the implications of our discussions for the stiffness. The fact that the minimizing flux for fermions is 0 or π implies that we need not necessarily expect a positive definite stiffness D for fermions, in contrast to the bosonic case. In all cases, we should examine the behaviour for an even number of particles closely, since here, the state with flux π is the

minimum. The XXZ model, i.e, the Heisenberg Ising model,[15] can be interpreted as an interacting one-component fermi gas. When the number of particles $\hat{N}$ is even, one has a non-zero momentum in the ground state, i.e., $\langle j_x \rangle \neq 0$. For example think of 2 non-interacting particles in a 6-membered ring, we have a degeneracy with momentum $\pm\pi/3$, and not much can be said about the stiffness in general terms, since the energy shift has a linear term in Φ. An explicit calculation using the Bethe Ansatz was given for the stiffness in this model in Ref. 6, which may be consulted for details. The model has an interesting Metal–Insulator transition, with a crystalline solid phase, and the stiffness has a jump discontinuity at the transition point, very much like the superfluid stiffness jump in the 2-d classical x–y description of a bose fluid.

In the case of the 1-d Hubbard model, the situation is much richer. The method of calculating the stiffness will be discussed in the next section, here one may just assume that numerical calculations have been performed. At half-filling, i.e., $\hat{N}_\uparrow = \hat{N}_\downarrow = L/2$, an interesting phenomenon was first noted by Scalapino and coworkers.[16] They noted that the stiffness D is in fact negative, for $L = 4 * integer$, but is positive for $L = 4 * integer + 2$. The stiffness can be calculated for arbitrary system sizes,[17] and in fact, vanishes exponentially with system size with a characteristic behaviour $D = \exp(-L/\xi)$, with a known ξ, as one would expect for an insulator. An explanation of the sign was provided[17] using the Aharonov–Bohm effect of a hole and a double being created, and transported around the Hubbard ring. A more direct understanding of this result follows from the considerations above. At $L = 4 * integer$, the number of up and down particles is even, and hence the bosons are "unhappy". The state at zero flux is higher in energy than that at flux π, and hence the stiffness is not necessarily positive. The fact that it is negative, does not follow from this (the energy could, for instance, have a local minimum at flux 0), and requires actual calculation. These considerations, turn out to be not as academic and exotic as the reader may suspect. The negative stiffness is in fact known, and has been observed[18] in aromatic organic compounds, which are no longer analogs of Benzene. The compounds are [16]-annulene and [24]-annulene, where NMR shows orbital paramagnetism, and these compounds are essentially the Hubbard model at half-filling for $L = 16, 24$.

Another set of curiosities concern the case when the number of particles is $4 * integer$, away from half-filling, in the Hubbard model. At half-filling, the ground state is a singlet due to a theorem of Lieb.[19] Away from half-filling, however, whenever the number of particles is $4 * integer$, the ground state is a spin-1 state. Figure 2 shows the singlet and the triplet state energies for a ring of 8 sites, with 8, 6 and 4 particles. The noteworthy case of 4 particles has a triplet ground state. For $L > 8$, similar results hold. This result comes about due to an interesting and subtle effect: *the spin zero state has orbital frustration, i.e., unhappy phases in the bosonic representation, which is relieved by partially spin polarizing the system.* The ground state can be easily shown to have $|S_{\rm tot}| \leq 1$, by an argument analogous to that in the Lieb Mattis theorem.[20] We can go to a subplace where the $S_z = 1$, having

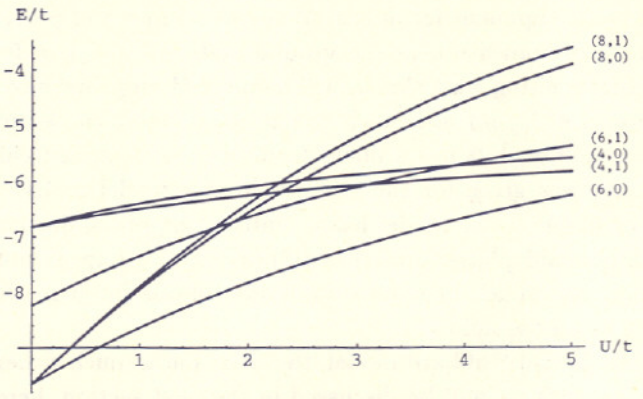

Fig. 2. The spectrum of the Hubbard ring with 8 sites. The numbers (N, S) represent the number of particles and the spin of the state.

an odd number of up and down electrons, and in this sector, there are no frustrating phases, and hence a unique ground state exists. This state cannot be orthogonal to the g.s. of the non-interacting case since the interaction only affects the diagonal matrix elements; for zero U the ground state is degenerate between $S = 0, 1$. Hence the spin of the state could be zero or unity, but no higher. For infinite U, it is readily shown that $S = 1$, from the Bethe equations which become trivial (see Eq. (21)), whereby one expects $S = 1$ for all U. The numerics confirm this. It is fascinating to speculate that this spin polarization, arising from orbital paramagnetism, may be a more widely useful concept.

5. 1-*d* Hubbard: Bethe Equations

We next consider the Bethe Ansatz equations, for the 1-*d* Hubbard model, in the presence of the flux,[6] generalizing the Lieb–Wu equation.[4] Firstly, it is necessary to show that the Bethe Ansatz goes through in the presence of the flux: this is not obvious and should be checked. We checked it, and the details are available.[6] Basically, the fact that the R matrix in the problem conserves the number of particles, is sufficient to guarantee the Bethe solvability. The equations are,

$$Lk_n = 2\pi I_n + \Phi_\uparrow^f + 2\sum_{j=1}^{M} \arctan[4(\Lambda_j - \sin(k_n))/U], \tag{21}$$

and

$$2\sum_{n=1}^{N} \arctan[4(\Lambda_j - \sin(k_n))/U] = 2\pi J_j + (\Phi_\downarrow^f - \Phi_\uparrow^f) + 2\sum_{i=1}^{M} \arctan[2(\Lambda_j - \Lambda_i)/U], \tag{22}$$

where L, N, M are respectively the numbers of sites, particles, and downspin particles. The quantum numbers

$$I_n = \text{integers (1/2 odd integers): M even (odd);} \tag{23}$$

$$J_j = \text{integers (1/2 odd integers): N} - \text{M odd (even)}. \tag{24}$$

The total energy is given by $E_{\text{tot}} = -2\sum \cos(k_n)$.

The case of $\Phi_\uparrow = -\Phi_\downarrow$, gives us the spin-stiffness in the problem, which turns out to be easily computable, and related to the spin susceptibility, by a fairly rigorous calculation.[6] The other case $\Phi_\uparrow = \Phi_\downarrow$, giving the charge stiffness, is not computable with the same rigor, since we note that the energy change due to the twist is not extensive, nor is it $O(1)$, it is in fact $O(1/L)$ in total energy. Moreover, subtle level non-crossing effects can and do happen[21] when the flux is of $O(\pi)$, and one may not be able to continue a solution found at zero flux to a large value of the flux. The usual trick of converting the sums to integrals does not guarantee the accuracy of the result to $O(1/L)$, and the answers obtained by this technique, should be verified by other means, such as numerical studies. Solutions of the integral equations can be found by manipulating the integral equations, assuming that they hold for large enough flux. The justification of these manipulations seem to require at least integrability (which we happen to have for the Hubbard model[22]), and also the avoidance of unfavourable fractions in filling. The theory of handling these transcendental equations is not quite complete at this moment, however the careful work of Woynarovich[23] and others has made a promising start in this direction. Also solutions using ideas from conformal invariance give useful explicit answers.[24] The conclusion is that the stiffness vanishes as we approach half-filling linearly in the departure from half-filling. This implies that the Mott transition is directly visible in the charge stiffness.

Similar ideas can be applied in say 2-dimensions, and interesting work of Millis and Coppersmith,[25] and Poilblanc and Dagotto[26] shows that the 2-d Hubbard model, as well as a t-J model show similar signs of Mott transition. Further applications to a general interacting electron gas have appeared recently.[27] The utility of these calculations in explaining the optical conductivity experiments[28] in High-T_c is noteworthy, and together with the f-sumrule, the charge stiffness gives a good insight into the transfer of optical weight observed, within a one-band Hubbard description.

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References

1. P. W. Anderson, *Science* **235**, 1196 (1987).
2. H. Krishnamurthy, C. Jayprakash, S. Sarker, and W. Wenzel, *Phys. Rev. Lett.* **64**, 950 (1990).
3. B. S. Shastry and B. Sutherland, *Physica* **108B**, 1069 (1981); Proceedings of LT17.
4. E. H. Lieb and F. Y. Wu, *Phys. Rev. Lett.* **20**, 1445 (1968).
5. W. Kohn, *Phys. Rev.* **133A**, 171 (1964).
6. B. S. Shastry and B. Sutherland, *Phys. Rev. Lett.* **65**, 243 (1990).
7. R. Bari, D. Adler, and R. V. Lang, *Phys. Rev.* **B2**, 2898 (1970); I. Sadakata and E. Hanamura, *J. Phys. Soc. Jpn.* **34**, 882 (1973); P. F. Maldague, *Phys. Rev.* **B16**, 2437 (1977).
8. N. Byers and C. N. Yang, *Phys. Rev. Lett.* **7**, 46 (1961).
9. D. J. Thouless, *Phys. Rep.* **C13**, 94 (1974).
10. E. Akkermans and G. Montamboux, *Phys. Rev. Lett.* **68**, 642 (1992).
11. A. J. Leggett, *Phys. Fennica* **8**, 125 (1973).
12. M. E. Fisher, M. N. Barber, and D. Jasnow, *Phys. Rev.* **A8**, 1111 (1973).
13. D. J. Scalapino, S. White, and S. C. Zhang, *Phys. Rev. Lett.* **68**, 2830 (1992).
14. C. N. Yang and S. C. Zhang, *Mod. Phys. Lett.* **B4**, 759 (1990).
15. C. N. Yang and C. P. Yang, *Phys. Rev.* **150**, 321 (1966).
16. R. M. Fye, M. J. Martins, D. J. Scalapino, J. Wagner, and W. Hanke, *Phys. Rev.* **B44**, 6909 (1991).
17. C. Stafford, A. Millis, and B. S. Shastry, *Phys. Rev.* **B43**, 13660 (1991).
18. G. Schroeder and F. J. M. Oth, *Tetrahedron Lett.* **1966**, 4083 (1966); I. C. Calder and F. Sondheimer, *Chem. Comm.* **24**, 904 (1966).
19. E. H. Lieb, *Phys. Rev. Lett.* **62**, 1201 (1989).
20. E. H. Lieb and D. C. Mattis, *Phys. Rev.* **125**, 164 (1962).
21. B. Sutherland and B. S. Shastry, *Phys. Rev. Lett.* **65**, 1833 (1990).
22. B. S. Shastry, *Phys. Rev. Lett.* **56**, 2453 (1986); *J. Stat. Phys.* **50**, 57 (1988).
23. F. Woynarovich and J. Eckle, *J. Phys.* **A20**, L443 (1987).
24. N. Kawakami and S. K. Yang, *Phys. Rev. Lett.* **65**, 3063 (1990).
25. A. J. Millis and S. Coppersmith, *Phys. Rev.* **B42**, 10807 (1990).
26. D. Poilblanc and E. Dagotto, *Phys. Rev.* **B44**, 466 (1991); D. Poilblanc, *Phys. Rev.* **B44**, 9562 (1991).
27. K. Moulopolous and N. W. Ashcroft, *Phys. Rev.* **B45**, 11518 (1992).
28. G. Thomas, in *High Temperature Superconductivity*, ed. D. P. Tunstall and W. Barford (Adam Hilger, England, 1991).