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Magnetization process from Chern-Simons theory and its application to $\text{SrCu}_2(\text{BO}_3)_2$

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In two-dimensional systems, it is possible to transmute bosons into fermions by use of a Chern-Simons gauge field. Such a mapping is used to compute magnetization processes of two-dimensional magnets. The calculation of the magnetization curve then involves the structure of the Hofstadter problem for the lattice under consideration. Certain features of the Hofstadter butterfly are shown to imply the appearance of magnetization plateaus. While not always successful, this approach leads to interesting results when applied to the 2D AF magnet $\text{SrCu}_2(\text{BO}_3)_2$.

§1. Introduction

Among the accidents that may happen to the magnetization curve of a magnet, the formation of a plateau has been observed already in a variety of physical situations. In antiferromagnets with a triangular lattice, a plateau at $M/M_{sat}=1/3$ has been discovered in C_6Eu , CsCuCl_3 and $\text{RbFe}(\text{MoO}_4)_2$. On the theoretical side, there is such a plateau at $M/M_{sat}=1/3$ for the two-dimensional Heisenberg antiferromagnet on the triangular lattice¹⁾. This plateau has a semiclassical explanation : it is due to the stabilization of a collinear $\uparrow\uparrow\downarrow$ state. In a similar vein, there is a plateau at $M/M_{sat}=1/2$ in a model with a four-spin exchange which is due to stability of a $\uparrow\uparrow\uparrow\downarrow$ state²⁾.

Plateau formation also happens in a series of one-dimensional systems, both experimentally and theoretically. In some cases, they can be explained by a limit in which one has a dimerized system, i.e. this happens for the alternating $S=1$ spin chain. When, say, odd bonds are much stronger than even bonds then we have a set of essentially decoupled dimers and if we apply a magnetic field upon such a set of dimers there is a two-step magnetization process. If we now add perturbatively a coupling between the dimers, the plateau will of course survive at least for a finite range of parameters. There are also plateaus that can be understood in terms of a band filling picture. This happens for the alternating ferro-antiferro $S=1/2$ spin chain. In the XY limit it is a system of free fermions by the Jordan-Wigner mapping. These fermions have a 1D band structure with gaps due to the modulation of hopping from the alternating F-AF pattern. These gaps then naturally

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corresponds to magnetization plateaus.

If we consider now again 2D systems, then similarly some of the plateaus that are known may be explained via a dimerized structure. It is tempting to speculate that some others may be due to nontrivial band-filling effects for fermions living on the lattice defining the magnet. The most intriguing 2D magnet with plateaus in $M(H)$ is, up to now, the compound³⁾ $\text{SrCu}_2(\text{BO}_3)_2$. It is a 2D antiferromagnet with localized spins $S=1/2$, a spin gap⁴⁾ and its magnetization curve has plateaus⁵⁾ $M/M_{\text{sat}}=1/3, 1/4, 1/8$. These plateaus are observed by using fields as high as 57 T. There may be even more plateaus waiting for us in this system. The magnetic ions Cu^{2+} have a peculiar lattice structure which is shown in Fig. 1. This is the so-called Shastry-Sutherland lattice, a model system that was invented theoretically many years ago⁶⁾. This system is a square lattice with AF exchange J' and there are additional bonds on some of diagonals that we note J . It is easy to guess that when J is large enough the system will be dimerized but in fact the Shastry-Sutherland lattice has the remarkable peculiarity that the direct product of local dimers on the J bonds is an *exact* eigenstate of the Hamiltonian. This is true for all values of the couplings and due to the fact that the coupling involves only triangles of spins. This dimerized state is the ground state when J is large enough. For J' smaller than $\sim 0.7 J$ ⁷⁾, the system has dimer long-range order and for larger J' it has conventional Néel long-range AF order since when $J=0$ we find the known square lattice AF magnet. There may be additional phases inbetween like a plaquette singlet phase⁸⁾ but they are probably not realized in $\text{SrCu}_2(\text{BO}_3)_2$ where J'/J estimated to be smaller than 0.65^{9), 10)}. In fact, susceptibility data as well as specific heat pointed to a value $J'/J=0.68$ but taking into account three-dimensional couplings leads to a revised estimate⁹⁾ $J'/J=0.635$.

Fig. 1. Shastry-Sutherland lattice. Full (resp. dotted) lines denote the coupling J (J').

If we concentrate on the dimerized phase, then it naturally explains the appearance of a spin gap. The first excited state will be a triplet state formed by breaking a dimer and this triplet will move on the lattice and form a band. In fact, due to the

peculiar triangular coupling which is responsible for the exact eigenstate property, the motion of the triplet arises only at high order in perturbation theory. As a consequence the dispersion of the triplet band is very weak. This fact has been confirmed by direct neutron inelastic scattering¹¹⁾. Curiously, the two-triplet states are on the contrary strong dispersions. The slow motion of the elementary triplet has led to the hypothesis that they may form some kind of crystal states when they are present at a finite density which means finite magnetization. A first line of attack has used an effective theory in which only the lowest-lying member of the triplet is kept (since there is Zeeman splitting) and it is treated as an effective hard-core boson. This has led to the prediction of the $1/3$ plateau¹²⁾ which has been then discovered experimentally. In fact the effective bosonic particles may display a variety of quantum phases¹³⁾. There is also a related exactly solvable model with plateaus¹⁴⁾. So far there is no microscopic probe of the nature of plateau states.

If we want to investigate the possibility that band-filling effects have something to do with the plateaus of $\text{SrCu}_2(\text{BO}_3)_2$, we first have to formulate the spin model in terms of fermions. This is done in Section II. Then in section III, we explain how to derive the magnetization curve in this mean-field approach. Results for various lattices including the Shastry-Sutherland lattice are given in section IV. Finally some conclusions and open problems are discussed in section V.

§2. Chern-Simons statistics transmutation

The Hamiltonian for the AF Heisenberg model on the Shastry-Sutherland lattice is :

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j - B \sum_i S_i^z, \quad (2.1)$$

where \vec{S}_i are spin-1/2 operators, the exchange couplings J_{ij} are equal to J' when i, j are nearest-neighbors on the square lattice and equal to J when i, j are related by a diagonal bond ($J, J' > 0$) and the external magnetic field B is applied along the z -axis. We then use the standard mapping of the spin operators to hard-core boson operators :

$$H = H_{XY} + H_Z, \quad (2.2)$$

$$H_{XY} = \frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} (b_i^\dagger b_j + b_j^\dagger b_i), \quad (2.3)$$

$$H_Z = \sum_{\langle i,j \rangle} J_{ij}^z (n_i - 1/2)(n_j - 1/2) - B \sum_i (n_i - 1/2), \quad (2.4)$$

where $n_i \equiv S_i^z + 1/2$ is the occupation number of site i . The problem is now a lattice boson system. To map it onto fermions, one has to generalize the well-known Jordan-Wigner transformation to two space dimensions. The corresponding recipe is well-known in the continuum limit. One has to attach a flux tube onto each fermion and tune the flux to exactly one flux quantum ϕ_0 . If we call $\varrho(r)$ the fermion density, we have to require :

$$\nabla \times a = \phi_0 \varrho(r) \hat{z}. \quad (2.5)$$

The vector potential $a(r)$ can be computed if we take a density which is a sum of delta functions :

$$a(r_i) = \frac{\phi_0}{2\pi} \sum_{j \neq i} \nabla_i \arctan \left(\frac{y_j - y_i}{x_j - x_i} \right). \quad (2.6)$$

There is now a nontrivial phase :

$$\alpha_{ij} = \arctan \left(\frac{y_j - y_i}{x_j - x_i} \right) \equiv \alpha(r_i - r_j), \quad (2.7)$$

which maps fermionic wavefunctions onto bosonic wavefunctions through the following unitary operator :

$$U = \exp \left[i \sum_{i < j} \alpha_{ij} \right]. \quad (2.8)$$

Indeed if ϕ is bosonic then Ψ given by :

$$\Psi(r_1, \dots, r_N) = U \phi(r_1, \dots, r_N) \quad (2.9)$$

is a fermion wavefunction which has the same eigenvalue as the bosonic problem provided one adds the gauge field a in the Hamiltonian. This is due to the fact that the following identity is true :

$$U p_i U^{-1} = p_i - e a(r_i). \quad (2.10)$$

Here e appears because $\phi_0 = 2\pi/e$. The fake gauge field a has to obey Eq.(2.5) and this can be enforced through a very special Lagrangian which is permissible only in two space dimensions :

$$L_{CS} = \int d^2r \quad a_0 \left(\frac{e}{\phi_0} \varepsilon_{\alpha\beta} \partial_\alpha a_\beta - e \varrho \right). \quad (2.11)$$

The time component of the gauge field a_0 is a Lagrange multiplier. This is the so-called Chern-Simons Lagrangian. It is at the heart of a very interesting mean-field theory for the fractional quantum hall effect. For a detailed exposition we refer to the book by Nagaosa¹⁵⁾.

If we want to perform the same kind of trick^{16),17)} on the lattice Bose model, then there is a part of the method which is straightforward. It is the coupling of the gauge fields. These fields live naturally on the bonds of the lattice so they enter only the expression of H_{XY} :

$$H_{XY} = \frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) \equiv \frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \left(c_i^\dagger e^{ia_{ij}} c_j + c_j^\dagger e^{-ia_{ij}} c_i \right) \quad (2.12)$$

The part H_Z is unchanged since only a phase relates bosons and fermions, hence $b^\dagger b = c^\dagger c$. The relation between flux and density is not as simple as in the continuum formulation. This is because gauge fields are living on bonds while matter (fermions) is living on sites. The correct prescription is to attach the flux of a site x onto only

one plaquette which touches the site, say the upper right plaquette on a square lattice. This is discussed at length in the work of Eliezer and Semenoff¹⁸⁾. This is of no importance for the results we discuss because we next perform a mean-field approximation. Also the lattice version of the Chern-Simons Lagrangian is quite complicated but is of no concern here. The only thing that matter is that density is tied to flux by $\Phi = 2\pi\rho(x)$ where $\rho(x)$ is the fermion density at site x and Φ is the flux piercing the "corresponding" (say upper right) plaquette *of the square lattice*. This mapping is exact in the sense that it involves no approximations (even if it is probably not rigorous : the Eliezer-Semenoff construction has been done for the square lattice only, so far). To use this mapping one has to perform a mean-field treatment^{19),20)} which is detailed in the next section.

It is important to note that the fake magnetic field piercing the plaquettes has nothing to do with the externally applied real magnetic field. Indeed the applied field is a chemical potential for the system of bosons as well as for the system of fermions.

§3. Mean-field treatment of the magnetization process

To compute physical quantities with the lattice fermion model coupled to the Chern-Simons gauge field, we perform the so-called "average flux approximation". It amounts to replace the gauge field a static uniform gauge field whose average flux is defined by the average particle number on any site :

$$\Phi \equiv 2\pi\langle\varrho\rangle. \quad (3.1)$$

In addition we have to treat the Ising term H_Z in Eq.(2.1). This is done by the simplest mean-field decoupling. As a consequence the fermionic problem is now reduced to a one-body problem. This is the problem of fermions on a lattice pierced by a uniform flux. This very old problem has been investigated by many people including Wannier, Azbel and Hofstadter²¹⁾.

We first discuss the procedure for the square lattice. The tight-binding Hamiltonian on the square lattice with nearest-neighbor hopping only has a single band in the absence of flux. If the flux is rational, $\Phi/2\pi = p/q$ then this single band disintegrates into q magnetic subbands. This leads to an infinitely complicated pattern of bands as a function of the flux, the celebrated Hofstadter butterfly²¹⁾. If we now consider a state of given magnetization for the fermion system, then this leads to a given flux since we have :

$$\frac{\Phi}{2\pi} = \langle\varrho\rangle = (\langle S^z \rangle + \frac{1}{2}) = M + \frac{1}{2}. \quad (3.2)$$

For example if $M = 0$ then we have flux $\Phi = \pi$ and the system is half-filled. This is the case $q = 2$ hence there are two subbands and we obtain the ground state by filling the lower band with the available fermions. In the case of the square lattice these two subbands do touch (but without overlapping). If we consider the state for which $M/M_{sat}=1/3$ then we have $M=1/6$ and $\Phi/2\pi = 2/3$ there are three subbands and since $\langle\varrho\rangle$ is also $2/3$ the ground state is then obtained by filling the lowest

two subbands. By adding the energies of the occupied states we get the energy of the fermion system. If we perform such a calculation, we do not obtain directly the energy as a function of the applied field but we obtain in fact the Legendre transform of the energy as a function of the magnetization $E(M) - BM$ (see Eq.(2.4)). So M as a function of B can be obtained by minimizing this quantity. A plateau in the magnetization curve is a point on the $E(M)$ curve at which there is a discontinuity in the *slope*. It may also happen that a given slope (a B value) is realized at *two* points, this leads to a metamagnetic jump in the magnetization curve. All these phenomena in fact do happen in the Chern-Simons mean-field theory for antiferromagnets.

It is straightforward to get $E(M)$ numerically because this is only a one-body problem. One has to diagonalize a tight-binding problem with flux and fill the bands accordingly. The Legendre transform is then also performed numerically. We discuss the results of this approach²²⁾ for various lattices in the next section.

§4. Results for various lattices

We first discuss the case of the square lattice. From the Hofstadter paper, it is clear that there is always a huge fermionic gap just above the highest occupied state for all magnetizations. The highest occupied state never jumps across the gap even if it follows a fractal curve with the flux. As a consequence the energy as a function of flux (hence magnetization) is *smooth*. The magnetization curve of the square lattice is then featureless. This is the left curve of Fig. 6. Since the density of fermions is uniform, this is of course not a valid description of a magnet with Néel order. This can be improved by using a mean-field generalized to allow for two sublattices. The difference of fermion densities is then found by imposing self-consistency. Such an approach was pioneered by Lopez, Rojo and Fradkin²⁰⁾. The results are given in Fig. 2. As a function of Ising-type anisotropy, one sees the appearance of Néel order. The correct value of the transition to Néel order $J^z = 1$ is not correctly recovered but the phase structure is correct.

Fig. 2. Magnetization curve for the square lattice model with use of a self-consistent mean-field with two-sublattices. From left to right: $J^z = 0, 0.39$ and 1 . Néel long-range order appears at $J^z \simeq 0.39$ (Lopez *et al.*), for higher values an Ising gap opens at $M = 0$.

In the case of the triangular lattice, we formulate the Chern-Simons gauge theory by deciding that there is flux $\Phi/2$ piercing each triangular plaquette. If we use a uniform mean-field then the resulting magnetization curve is strongly irregular :

it has many plateaus as can be seen in Fig. 3. There is also a prominent zero-field gap¹⁹⁾. It is widely believed that, instead, this spin system is gapless and its magnetization process shows only a single plateau at $M/M_{sat} = 1/3$. To improve these results, we allow the mean-field to have a three-sublattice structure: one introduces three fermion densities n_A, n_B, n_C and numerically search for a self-consistent solution where the flux ϕ_α matches the density n_α on each sublattice. For $M = 0$ the self-consistent solution remains uniform. However, for non-zero magnetization the translation symmetry is broken. This non-uniform mean-field solution leads to a magnetization curve shown Fig. 3 which is much closer to the truth albeit the zero-field ground state remains unrealistic. The $1/3$ plateau has a semiclassical origin : it derives from the uud state that appears in the Ising limit $J^z \gg J$.

Fig. 3. Magnetization curve of the triangular lattice. Full line: mean-field with three-sublattices. Dashed line: uniform mean-field.

We now discuss the Shastry-Sutherland lattice. The Hofstadter butterfly for $J = J'$ is given in Fig. 4. It is clear that there are jumps of the Fermi energy as a function of M . This leads to discontinuity of the slope of the function $E(M)$ and thus these jumps corresponds to plateaus in the magnetization curve. The appearance of the plateaus is coded into the delicate structure of the Hofstadter butterfly. It is interesting to note that when there is an integer number of filled subbands, then one has a well-defined quantized Hall conductance. There is a recipe to compute this Hall conductance in the case of the square lattice²³⁾ : one has to solve a simple Diophantine equation. We have computed some of the Hall conductances for the Shastry-Sutherland lattice by continuity arguments (as integers of topological origin, they can only be changed by gap closure). These conductances are given in Fig. 4.

When the Fermi level follows smoothly the lower part of an "eye" in the butterfly, we observe that the Hall conductance is $+1$. This is due to the Streda formula. Indeed if we add one flux quantum to the system we also add one fermion. If this fermion is going to fill exactly one extra state at the bottom of the "eye" it means that there should be exactly one extra state coming across the gap from the upper states. This change of the number of states is equal to the Hall conductance as shown by the Streda formula. Changing the Hall conductance imply closing a gap and this is exactly when there is a jump of the Fermi level. In this case we see a plateau in the magnetization process. The domain of stability of plateaus are given in Fig. 5.

If we try to reproduce the qualitative shape of the experimental curve for

Fig. 4. The Hofstadter butterfly for the Shastry-Sutherland lattice. Some hall conductances are given in the corresponding gaps. The lower thick line is the highest occupied state.

Fig. 5. Regions of appearance of the magnetization plateaux as a function of J/J' for $M/M_{\text{sat}} = \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$ and $\frac{1}{5}$. Additional plateaux at fractions $\frac{1}{n}$ for $n > 5$ also exist in the vicinity of $J/J' = 1.5$.

Fig. 6. Magnetization curves for the Shastry-Sutherland lattice as a function of J'/J . From left to right $J = 0$ (dashed) , 0.75 (full), 1.5(dashed), 2.5 (full), 3.5 (dashed) and 5 (full) ($J' = 1$).

$\text{SrCu}_2(\text{BO}_3)_2$, it is best to use $J' = 29.5\text{K}$ and $J = 74\text{K}$, the resulting fit is shown in Fig. 7. These values do not lead to a satisfactory spin gap : 13K instead of 34K, but the roundings close to the plateaus are in good agreement with the experiment. This approximation predicts prominent plateaus at $1/3$ and $1/2$ and no other plateaus till full saturation. There are also small metamagnetic jumps just below saturation, the most prominent one being at $3/4$. We note that at $1/4$ there is in fact an avoided plateau : the value of J'/J is just outside the range of stability of the $1/4$ plateau (see Fig. 5).

Fig. 7. Best fit of the experimental magnetization curve of $\text{SrCu}_2(\text{BO}_3)_2$.

§5. Conclusions

In the Chern-Simons mean-field approach, magnetization plateaus appear as a manifestation of the integer quantum Hall effect for fermions living on a lattice. These plateaus presumably survive beyond mean-field. Indeed Gaussian fluctuations¹⁹⁾ of the gauge field are massive provided that the TKNN integer σ describing the quantized Hall coefficient of the fermions on the frustrated lattice differs from the continuum value of *unity*. The plateaus are not suppressed since we find $\sigma = -3$, -2 and -1 respectively for $\frac{1}{4}$, $\frac{1}{3}$ and $\frac{1}{2}$. At $M/M_{sat} = 0$ we have $\sigma = -1$ (resp 0) for $J/J' < \sqrt{2}$ (resp $J/J' > \sqrt{2}$).

This approach has at least some qualitative success in the case of $\text{SrCu}_2(\text{BO}_3)_2$. It is important to note that a consequence of these non-trivial quantized Hall coefficients is that the spin state is chiral and exhibits a ‘spin quantum Hall effect’²⁴⁾.

Finally we note that higher-field experiments should be able to test the prediction for the magnetization curve of $\text{SrCu}_2(\text{BO}_3)_2$.

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