On the relationship between the ground-state wave function of a magnet and its static structure factor

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We state and prove two theorems about the ground state of magnetic systems described by very general Heisenberg-type models. The first theorem states that the relationship between the Hamiltonian and the ground-state correlators is invertible. The second theorem states that the relationship between the wave function and the correlators is also invertible. We discuss the implications of these theorems for neutron scattering. We propose, in particular, a variational approach to quantum magnets where a representation of the wave function (held, for instance, in a neural network or in the qubit register of a quantum processor) is optimised to fit experimental neutron-scattering data directly, without the involvement of a model Hamiltonian.

The Rayleigh-Ritz variational principle states that the ground state wave function of a quantum system is an absolute minimum of the energy. It provides the theoretical underpinning of many successful approaches to the quantum many-body problem including Density Functional Theory (DFT) [1], Variational Monte Carlo methods [2], the BCS theory of superconductors [3] and the Laughlin theory of the fractional quantum Hall effect [4] to name a few cases. More recently it has been used to find optimal representations of wave functions using quantum computers [5, 6] and neural networks [7]. Such theories start with a model Hamiltonian $\hat{H}$ and proceed by minimising the energy $\left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle$ to obtain the wave function Ψ. The Rayleigh-Ritz variational principle ensures that no wave function can yield a lower value of the energy than the system's true ground state.

Once the wave function is known, it is is straightforward to predict expectation values of observables. Very often, however, $\hat{H}$ is not known *a priori*. In such instances $\hat{H}$ has to be found first from experimental data. That involves a laborious and ill-posed inverse problem: multiple candidate Hamiltonians must be studied until one is found that predicts the experimentally-determined value of a set of observables. In general there is no guarantee of uniqueness of $\hat{H}$ or Ψ for a given data set. Here we consider the inverse problem for the magnetic structure factor of a magnetic insulator (in particular, one described by an anisotropic Heisenberg model, which covers a vast range of real materials). We show that, for systems described by a Heisenberg model, there is a one-to-one correspondence between the structure factors, the model Hamiltonian and the ground state wave function.

Our results have several direct implications for the study of magnetic insulators using neutron scattering. Firstly, they put the inverse problem on a firmer footing and will help the design of efficient solutions, for instance ones exploiting machine learning [8]. Secondly, they suggest new variational methods where the wave function is optimised to describe the experimental data, obviating the need to minimise the energy of a model Hamiltonian. This provides an alternative to methods based on neural-network [7] or quantum-processor [5] representations that are based on minimising the energy for a given model Hamiltonian. The new methods will be appropriate when the model is not yet known but experimental structure factor information is available. In analogy with the Rayleigh-Ritz variational principle, our theorem guarantees that no wave function other than the true ground-state wave function of the system under investigation can yield a better fit to the data. Finally, our results imply that every ground-state property of the system is contained in the structure factors. This has important implications for efforts to quantify quantum entanglement from experimental neutron scattering data [9, 10].

Our starting point is the anisotropic Heisenberg model:

$$\hat{H} = \sum_{i,j} \sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta} \hat{S}_i^{\alpha} \hat{S}_j^{\beta}. \tag{1}$$

Here $i, j = 1, 2, \ldots, N$ represent atomic sites, whose positions $\mathbf{R}_i, \mathbf{R}_j$ we assume to be known. $\hat{S}_i^{\alpha}$ represents the $\alpha^{\underline{\text{th}}}$ component of the spin operator for the magnetic moment at the $i^{\underline{\text{th}}}$ atomic site ($\alpha = x, y, z$; we assume each spin component is defined with reference to some local axes defined on each site). We assume the spin quantum number at each site is $S = 1/2$ in what follows but the results can be generalised to arbitrary S straight-forwardly. $J_{i,j}^{\alpha,\beta}$ is an exchange constant describing the interaction between the $\alpha^{\underline{\text{th}}}$ component of the spin at the $i^{\underline{\text{th}}}$ site of a given lattice and the β component of the spin in the j site. The terms with $i = j$ describe site anisotropy (easy planes or easy axes). The dependence of $J_{i,j}^{\alpha,\beta}$ on i, j, α, and β is entirely arbitrary. The model of Eq. (1) can thus describe a very broad range of magnetic models in arbitrary dimensions with and without translational invariance, including among others the Ising model [11], XY model [12], and Kitaev model to name but a few [13]. Models of this type are believed to describe well the physics of many materials from single-molecule magnets [14] through infinite-chain compounds [10] to three-dimensional quantum spin ices [15] and other spin liquids [16]. The observable quantity of interest is the two-point

magnetic correlator

$$\rho_{i,j}^{\alpha,\beta}\left[\Psi\right] \equiv \left\langle \Psi \left| \hat{S}_i^{\alpha} \hat{S}_j^{\beta} \right| \Psi \right\rangle. \tag{2}$$

The correlator is a single-valued functional of the wave function Ψ, as indicated.

We wish to prove two closely related theorems:

Theorem 1: The exchange constants in Eq. (1) are single-valued functionals $J_{i,j}^{\alpha,\beta}\left[\rho\right]$ of the correlators.

Theorem 2: The ground state wave function Ψ_0 is also uniquely determined by the correlators (we write this $\Psi_0\left[\rho\right]$).

Our approach is inspired by the DFT formalism Heisenberg models developed by Líbero and Capelle [17]. Our aims, however, are quite different. The latter work (like other DFT formalisms for lattice models [17–19]) is an energy-minimisation variational theory closely modelled on the original DFT for electrons in solids [1]. In Density Functional Theories generally, the aim is to show that the energy is a functional of a density-like quantity (in the case of Ref. [17], the local magnetisation). One then splits the energy into two parts, one that is "universal" and the other that depends on local fields. In order to be useful, it is necessary to have exact results for the universal function and motivated approximations for the field-dependent contribution. Here our primary quantity is not a density but a correlator, and we are not interested in splitting the energy into one contribution that is known and another that is to be approximated. Instead we treat the energy as a single unit and are interested in proving that only one "universal" Hamiltonian is compatible with a given set of correlators. In practice, applications of our approach involve the optimisation of the match to experimental data, rather than the minimisation of the energy. Moreover, we will work in the absence of a known model Hamiltonian, rather than using knowledge of one model (e.g. a translationally-invariant Heisenberg model) to approximately solve another (e.g. the same model but with an impurity potential).

Proof of Theorem 1.- Inspired by the original proof of the Hohenberg-Kohn theorem of DFT, we will proceed by *redutio ad absurdum*. Suppose there are two distinct Hamiltonians $\hat{H}$ and $\hat{H}'$, with different exchange interaction functions $J_{i,j}^{\alpha,\beta}$ and $J'^{\alpha,\beta}_{i,j}$, respectively, that give the same correlator $\rho_{i,j}^{\alpha,\beta}$. In other words, if Ψ_0 and Ψ_0' represent the respective ground states, then

$$\rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] = \rho_{i,j}^{\alpha,\beta}\left[\Psi_0'\right] \text{ for all } i,j,\alpha,\beta. \tag{3}$$

In this case the ground-state energy obtained from the first Hamiltonian is

$$E_0 = \left\langle \Psi_0 \left| \hat{H} \right| \Psi_0 \right\rangle < \left\langle \Psi_0' \left| \hat{H} \right| \Psi_0' \right\rangle \tag{4}$$

$$= \left\langle \Psi_0' \left| \hat{H} - \hat{H}' \right| \Psi_0' \right\rangle + \left\langle \Psi_0' \left| \hat{H}' \right| \Psi_0' \right\rangle \tag{5}$$

$$= \sum_{i,j} \sum_{\alpha,\beta} \left(J_{i,j}^{\alpha,\beta} - J'^{\alpha,\beta}_{i,j} \right) \rho_{i,j}^{\alpha,\beta}\left[\Psi_0'\right] + E_0' \tag{6}$$

where the inequality due to the Rayleigh-Ritz variational principle. Similarly the ground state energy obtained from the second Hamiltonian is

$$E_0' = \left\langle \Psi_0' \left| \hat{H}' \right| \Psi_0' \right\rangle < \left\langle \Psi_0 \left| \hat{H}' \right| \Psi_0 \right\rangle \tag{7}$$

$$= \left\langle \Psi_0 \left| \hat{H}' - \hat{H} \right| \Psi_0 \right\rangle + \left\langle \Psi_0 \left| \hat{H} \right| \Psi_0 \right\rangle \tag{8}$$

$$= \sum_{i,j} \sum_{\alpha,\beta} \left(J'^{\alpha,\beta}_{i,j} - J_{i,j}^{\alpha,\beta} \right) \rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] + E_0, \tag{9}$$

Adding the two inequalities we obtain

$$E_0' + E_0 < \sum_{i,j} \sum_{\alpha,\beta} \left(J'^{\alpha,\beta}_{i,j} - J_{i,j}^{\alpha,\beta} \right) \times \left\{ \rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] - \rho_{i,j}^{\alpha,\beta}\left[\Psi_0'\right] \right\} + E_0 + E_0'.$$

Using now our assumption (3) this reduces to

$$E_0' + E_0 < E_0 + E_0' \tag{10}$$

which is absurd. Thus our initial assumption must be incorrect: two Heisenberg-type Hamiltonians with different exchange interaction constants can never give the same correlator. In other words, the exchange interaction function is a single-valued functional $J_{i,j}^{\alpha,\beta}\left[\rho\right]$ of the correlator $\rho_{i,j}^{\alpha,\beta}$.

Our result implies that the inverse problem of deducing the Hamiltonian from the correlators is indeed well-defined, as long as we know that the material under investigation is described by a model of the form in Eq. (1). That could explain the success of a recent machine learning based approach to this problem [8]. In that reference an auto-encoder was trained using simulations of the neutron scattering function $S_{\alpha,\beta}\left(\mathbf{q}\right)$ obtained for a family of candidate Hamiltonians [for completeness, we have offered a proof of the equivalence between knowledge of $S_{\alpha,\beta}\left(\mathbf{q}\right)$ and of $\rho_{i,j}^{\alpha,\beta}$ in the Appendix. The auto-encoder thus trained can be used to generate a low-dimensional latent space on which experimental data can be projected, effectively finding an optimal model Hamiltonian. Our formal result guarantees that this is possible. We note that the work in Ref. [8] dealt with classical models however similar dimensionality-reduction has been shown for quantum models using closely-related Principal Component Analysis [20].

In the above paragraph we have implicitly assumed that the ground states of $\hat{H}$ and $\hat{H}'$ are non-degenerate. Let us now see what happens when we relax that assumption. Let us first consider the case when the ground state of one of the Hamitonians (which we take to be $\hat{H}$ without loss of generality) is degenerate, while that of the other Hamiltonian remains non-degenerate. Then the first of the above two inequalities (4,7) is not strict, as there is always the possibility that $|\Psi_0'\rangle$ happens to be a ground state of $\hat{H}$ as well as of being a ground state of $\hat{H}'$. Barring that possibility, the arguments above hold, so we only need to consider that special case. In the special case we have

$$E_0 = \sum_{i,j}\sum_{\alpha,\beta}\left(J_{i,j}^{\alpha,\beta} - J'^{\alpha,\beta}_{i,j}\right)\rho_{i,j}^{\alpha,\beta}\left[\Psi_0'\right] + E_0' \qquad (11)$$

and

$$E_0' < \sum_{i,j}\sum_{\alpha,\beta}\left(J'^{\alpha,\beta}_{i,j} - J_{i,j}^{\alpha,\beta}\right)\rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] + E_0 \qquad (12)$$

When we add the equality (11) to this inequality (12) we still arrive at the same contradiction as before, (10).

Let us now consider the case when *both* Hamiltonians have ground-state degeneracy. Then there is a new possibility, namely that $|\Psi_0\rangle$ is a ground state of $\hat{H}'$ *and* $|\Psi_0'\rangle$ is a ground state of $\hat{H}$ (all other possibilities have already been covered above). In that case all the above inequalities become equalities and we do not arrive at a contradiction. Therefore, this is a special case when Theorem 1 does not apply. Note, however, that in this case the two Hamiltonians must share *all* their degenerate ground states as a single ground state of one which is not also a ground state in the other suffices to generate a contradiction. Hence, this is a trivial case: if two Hamiltonians share the ground state, then of course they also must have the same ground-state correlators, since those are single-valued functionals of the ground state wave function. An example of this would be two spin-1/2 ferromagnetic Ising models differing only by an overall multiplicative factor. In both cases, the ground state is a classical state where all the spins are pointing along the positive or negative direction of the quantisation axis. The correlators are therefore identical in the ground state (although differences would emerge at finite temperatures) [21]. Moreover this exception to Theorem 1 does not affect Theorem 2, below.

Proof of Theorem 2.- In the preceding paragraphs we proved that the exchange constants $J_{i,j}^{\alpha,\beta}$ are single-valued functionals of the correlators $\rho_{i,j}^{\alpha,\beta}$ (with the caveat mentioned above). Since obviously the ground state $|\Psi_0\rangle$ is in turn fixed by the choice of $J_{i,j}^{\alpha,\beta}$ this also proves that $|\Psi_0\rangle$ is uniquely determined by $\rho_{i,j}^{\alpha,\beta}$, within the constraint that $|\Psi_0\rangle$ must be the ground state of a Heisenberg-type Hamiltonian of the form give by Eq. (1). To prove Theorem 2 we need to show that the result holds even without that constraint. Again, we proceed by *reductio ad absurdum.* Let us assume that there is a state $|\tilde{\Psi}\rangle$ that gives the same correlator as $|\Psi_0\rangle$:

$$\rho_{i,j}^{\alpha,\beta}\left[\tilde{\Psi}\right] = \rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] \text{ for all } i,j,\alpha,\beta. \qquad (13)$$

Let us further assume that $|\tilde{\Psi}\rangle$ is *not* the ground state of $\hat{H}$. There are two possibilities: either it is the ground state of some other Heisenberg-type Hamiltonian or it is not the ground state of a Heisenberg Hamiltonian at all. Below we will not assume either case, so our proof will cover both instances. By the Rayleigh-Ritz variational principle, we know that $|\Psi_0\rangle$ gives the absolute minimum of the energy, which implies

$$E_0 \equiv \left\langle \Psi_0 \left| \hat{H} \right| \Psi_0 \right\rangle \leq \left\langle \tilde{\Psi} \left| \hat{H} \right| \tilde{\Psi} \right\rangle. \qquad (14)$$

Using Eqs. (1) and (2) we can write this as

$$E_0 \equiv \sum_{i,j}\sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta}\rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] \leq \sum_{i,j}\sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta}\rho_{i,j}^{\alpha,\beta}\left[\tilde{\Psi}\right].$$

Let us now consider separately the two cases when the two expectation values of $\hat{H}$ in Eq. (14) are different (a) and when they are equal (b). Let us first consider the case when they are different (a):

$$E_0 \equiv \left\langle \Psi_0 \left| \hat{H} \right| \Psi_0 \right\rangle < \left\langle \tilde{\Psi} \left| \hat{H} \right| \tilde{\Psi} \right\rangle.$$

Then we have

$$\sum_{i,j}\sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta}\rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] < \sum_{i,j}\sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta}\rho_{i,j}^{\alpha,\beta}\left[\tilde{\Psi}\right]. \qquad (15)$$

and from our assumption (13) this reduces to

$$\sum_{i,j}\sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta}\rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] < \sum_{i,j}\sum_{\alpha,\beta} J_{i,j}^{\alpha,\beta}\rho_{i,j}^{\alpha,\beta}\left[\Psi_0\right] \qquad (16)$$

which is a contradiction. Therefore, the only possibility is that the two expectation values are equal (b):

$$E_0 \equiv \left\langle \Psi_0 \left| \hat{H} \right| \Psi_0 \right\rangle = \left\langle \tilde{\Psi} \left| \hat{H} \right| \tilde{\Psi} \right\rangle.$$

However in that case $\left\langle \tilde{\Psi} \left| \hat{H} \right| \tilde{\Psi} \right\rangle$ is the absolute miminum E_0 and therefore $|\tilde{\Psi}\rangle$ is a ground state of $\hat{H}$, which contradicts our starting assumption. Thus we conclude that the only state that reproduces the ground-state correlator of $\hat{H}$ is the actual ground state of $\hat{H}$ (or one of its ground states, if the ground state of $\hat{H}$ happens to be degenerate), *quod erat demonstrandum.* We note that this is true even when we include candidate wave functions that are not derived from any Hamiltonian of the form (1) so Theorem 2 is stronger than just a corollary of Theorem 1. We note also that our proof of Theorem 2 does not rely on having proved Theorem 1.

Note that our result implies that the correlator completely determines the ground state wave function is general, in particular it applies to wave functions which are not ground states of any Heisenberg-type Hamiltonian. This means that unconstrained searches in wave function space are guaranteed to be able to find the true ground state, which may be relevant for instance for quantum processor-based evolutionary searches [6].

Our last result offers the possibility to study systems for which experimental magnetic neutron scattering data is available by working directly with the wave function, without the need for a model Hamiltonian. Compared to the machine learning based approaches commented on above [8, 20] the process here would be much swifter as rather than multiple optimisations carried out for different model Hamiltonians a single optimisation loop would be required. For instance, one could encode the wave function in a neural network, trained once to reproduce the experimental data. Alternatively, a quantum circuit could be optimised to place the qubits in quantum processor in a state that reproduces the measurements. Both neural networks and quantum circuits can, in principle, generate any wave function. Our theorem implies that any general-purpose optimisation algorithm will converge towards the right ground state, because there are no wave functions that can describe the data and are not solutions to the physical problem at hand. This is akin to the guarantee offered by the Rayleigh-Ritz variational principle that no wave function can give an energy lowerg than the true ground state wave function.

To conclude we note some limitations of Theorem 2. Firstly, it relies on the assumption that the physical system under investigation is described by a Hamiltonian of the form in Eq. (1). Systems with itinerant electrons or with interaction terms involving three or more spins at a time are therefore excluded. The generalisation of our results to such systems is left for subsequent work. Secondly, Theorem 2 establishes the existence of a fitness peak at Ψ_0 but says nothing about its steepness. The peak could be almost a plateau in some cases, which would complicate practical applications. Investigating this for different models provides another focus for future research. Finally, our theorems refer only to the ground state. Generalisations to states of thermodynamic equilibrium and to excited states are left for future work.

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Appendix A: Equivalence between correlators and the spin structure factor

Here we show that the correlators $\rho_{ij}^{\alpha,\beta}$ are unique functionals of the diffuse magnetic neutron scattering function, or static spin structure factor, $S_{\alpha,\beta}(\mathbf{q})$, which can be determined experimentally and is given by

$$S_{\alpha,\beta}(\mathbf{q}) \equiv \frac{1}{N\hbar}\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\left\langle \hat{S}_i^{\alpha}\hat{S}_j^{\beta}\right\rangle. \tag{A1}$$

This is not quite the same as a Fourier transform, in which case we could say straightaway there is a 1-2-1 correspondence between $S_{\alpha,\beta}(\mathbf{q})$ and $\left\langle \hat{S}_i^{\alpha}\hat{S}_j^{\beta}\right\rangle$, but almost. Again, let us proceed by *redutio ad absurdum*. First, we assume that there are two different correlation functions that give the same scattering function. Let us designate these two correlation functions as $\rho_{i,j}^{\alpha,\beta}$ and $\tilde{\rho}_{i,j}^{\alpha,\beta}$, respectively. Our assumption is that the difference $\Delta_{i,j}^{\alpha,\beta} \equiv \rho_{i,j}^{\alpha,\beta} - \tilde{\rho}_{i,j}^{\alpha,\beta} \neq 0$. Since they give the same scattering function we have

$$\begin{aligned} S_{\alpha,\beta}(\mathbf{q}) &= \frac{1}{N\hbar}\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\rho_{i,j}^{\alpha,\beta} \\ &= \frac{1}{N\hbar}\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\tilde{\rho}_{i,j}^{\alpha,\beta} \end{aligned}$$

for all $\mathbf{q}, \alpha, \beta$. The last equality implies that

$$\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\Delta_{i,j}^{\alpha,\beta} = 0 \text{ for all } \mathbf{q}, \alpha, \beta. \tag{A2}$$

Suppose that all magnetic sites are equivalent. Then the function $\Delta_{i,j}^{\alpha,\beta} = \Delta^{\alpha,\beta}(\mathbf{R}_i - \mathbf{R}_j)$ and (A2) becomes

$$\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}}\Delta^{\alpha,\beta}(\mathbf{R}) = 0 \text{ for all } \mathbf{q}, \alpha, \beta$$

which evidently implies $\Delta^{\alpha,\beta}(\mathbf{R}) = 0$ for all $\mathbf{R}$ as the Fourier transform of a null function is a null function which contradicts our original assumption, concluding our argument.

Suppose now that the magnetic sites are not equivalent. Nevertheless, as long as we are dealing with a crystal, the function $\rho_{i,j}^{\alpha,\beta}$ will have to be periodic. This periodicity can be established experimentally (for instance, by magnetic neutron crystallography) and it is also straight-forward to impose it on the wave function therefore we can restrict ourselves to the assumption that $\tilde{\rho}_{i,j}^{\alpha,\beta}$ (and therefore, also $\Delta_{i,j}^{\alpha,\beta}$) has the same periodicity [22]. In practice this means that we can write the LHS

of Eq. (A2) in the following form:

$$\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\Delta_{i,j}^{\alpha,\beta} = \mathcal{N}\sum_{i=1}^{M\times\mathcal{N}}\sum_{j=1}^{M} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\Delta_{j}^{\alpha,\beta}(\mathbf{R}_i)$$
$$= \mathcal{N}\sum_{j=1}^{M} e^{-i\mathbf{q}\cdot\mathbf{R}_j} f_j(\mathbf{q})$$

with

$$f_j(\mathbf{q}) = \sum_{i=1}^{M\times\mathcal{N}} e^{i\mathbf{q}\cdot\mathbf{R}_i}\Delta_{j}^{\alpha,\beta}(\mathbf{R}_i).$$

Here $\mathcal{N}$ is the number of magnetic unit cells (repeating units) and M is the number of sites within a unit cell and the sum. Thus the sum over j runs over all the sites in the first unit cell while the sum over i runs over all the other sites in the lattice. For the expression $\sum_{j=1}^{M} e^{-i\mathbf{q}\cdot\mathbf{R}_j} f_j(\mathbf{q})$ to vanish for all $\mathbf{q}$ we must have each of the $f_j(\mathbf{q})$ for $j = 1, 2, \ldots, M$ vanish independently. But $f_j(\mathbf{q})$ is the Fourier transform of $\Delta_j^{\alpha,\beta}(\mathbf{R}_i)$ therefore $\Delta_j^{\alpha,\beta}(\mathbf{R}_i)$ must vanish too for each $j = 1, 2, \ldots, M$. This means $\Delta_{i,j}^{\alpha,\beta}$ is identically zero, contradicting again our starting assumption.

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[21] We also note that for this special case to invalidate our proof we require *all* the ground states of the two Hamiltonians to coincide as any degenerate ground state of one Hamiltonian that is not a ground state of the other would could still be used to produce a contradiction. We thank Tymoteusz Tula for pointing this out. .
[22] This is the basis for expressing the neutron scattering cross-section in terms of the static structure factor $S(\mathbf{q})$ in the case of crystals with lowered periodicity, see Zaliznyak, Igor A. and Lee, Seung-Hun, "Magnetic Neutron Scattering", *Spin* **5**, 1 (2004) [see in particular the discussion in Section 3.5].