Understanding quantum spin chains: KIAS-SNU winter camp

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We know from experiences over the past century of quantum mechanics that one of the best ways to make progress in theoretical physics is to write down a very good model and to try to solve it in as many different ways as one can. The Ising model published in 1925 (same year as quantum mechanics) has prompted ideas of mean-field theory, duality, a whole field of mathematical statistical physics, Monte Carlo simulation, correspondence of statistical models to quantum models in one lower dimensionality, and of course, the very renormalization group. In a word, Ising model is the most powerful and fruitful model of *classical many-body system*.

There is a quantum many-body model with a long-lasting impact that spans almost a century. This is the one-dimensional spin chain Hamiltonian

$$H = \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \tag{1}$$

representing anti-ferromagnetic exchange interaction between neighboring spins of size $(\boldsymbol{S}_i)^2 = S(S+1)$. The model has enjoyed early success due to Bethe, who wrote down the exact many-body ground state wave function for this Hamiltonian in 1931 when he was only 25 years old. Bethe's solution is historically known as the Bethe's ansatz (Bethe's guess), but this is a misleading statement of Bethe's accomplishment. He really wrote down the exact wave function, and since in many-body physics the only way to find the correct wave function is by guesswork, it is referred to as Bethe's "guess". The same is also true of Laughlin's wave function for fractional quantum Hall state, which was a guess built upon his numerical simulation for small systems.

Bethe's solution apparently had a lasting impact on the way that the field of spin chain physics was developed for the subsequent half a century. It was only in the 70s that other creative ideas, particularly that of bosonization, has infiltrated the spin chain problem. The idea here was to work with some continuum, low-energy Hamiltonian instead of the bare, lattice Hamiltonian as given in Eq. (1). Both the lattice and the continuum Hamiltonian are, after all, Hamiltonians, and one follows the protocol of diagonalizing the model and carrying out some correlation function calculations and so forth, which yields a wealth of information about the behavior of the model.

We know that Feynman's remarkable insight was to re-visualize quantum mechanics away from Schrodinger's view, and to turn it into a spacetime view, or the Lagrangian view in place of the Hamiltonian view. We know that this

marked something of a phase transition in the way we view and solve quantum-mechanical problems. A revolutionary change in our understanding of quantum spin chain problem has taken place exactly in this way, when Haldane first tried to look at the problem with a spacetime, Lagrangian perspective. Partly of the citation for Haldane's 2016 Nobel prize is to his contribution for action approach to spin chains and the identification of topological term in defining the gap in the spin chain.

The story I want to share with you over the next three lectures is a survey of the developments of ideas built around the quantum spin chain Hamiltonian. Lecture 1 will discuss the classical approach initiated by Bethe and focuses on the wave function aspect. Lecture 2 will show how the continuum version of the low-energy dynamics can be obtained by a method of Jordan-Wigner transformation followed by bosonization techniques. Lecture 3 will review Haldane's mapping of the spin Hamiltonian to an action form using the coherent state basis and how the topological term arises naturally in the process. Exercise problems are at the end.

1 Bethe's approach to quantum spin chain

Let's express the spin-1/2 antiferromagnetic spin exchange Hamiltonian in one dimension as

$$H = \frac{1}{2}\sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}. \tag{2}$$

This model can come in many disguises. For a pair of particles one can define a permutation operator as doing the swapping between them. If there are two spin states the permutation operator acts on them as $P|\sigma_1, \sigma_2\rangle = |\sigma_2, \sigma_1\rangle$, $\sigma_{1,2} = \pm 1$. Interestingly the Pauli product $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$ does exactly the same thing, as one can verify by

$$P_{ij}|\sigma_i, \sigma_j\rangle = |\sigma_j, \sigma_i\rangle = \frac{1}{2}(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 1)|\sigma_i, \sigma_j\rangle. \tag{3}$$

It means the Heisenberg Hamiltlnian becomes $H = \sum_i P_{i,i+1}$ up to an overall constant. The Heisenberg interaction $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1}$ comes from the exchange part of the Coulomb interaction. That's why it was called the "exchange interaction" in the first place. By some accident, it also turns out to be identical to the true "exchange operation" of the two spins.

A second, very useful way to express the Heisenberg Hamiltonian is to view the spin-up state $|\uparrow\rangle$ as an equivalent of an empty particle state $|0\rangle$, and the spin-down state $|\downarrow\rangle$ as an equivalent of a single-particle state $|1\rangle = b^\dagger|0\rangle = S^-|\uparrow\rangle$. In this picture the spin operators are identified with boson operators by

$$S_i^+ = b_i,\ S_i^- = b_i^\dagger,\ S_i^z = \frac{1}{2} - b_i^\dagger b_i. \tag{4}$$

To inherit the commutation properties of the spin operators, the b-particles must be regarded as bosons, $[b_i, b_j] = 0$, for different sites $i \neq j$. On the other same

the same-site commutation must be fermionic, $b_i^\dagger b_i + b_i b_i^\dagger = 1$, $(b_i^\dagger)^2 = (b_i)^2 = 0$, ensuring that each site can have either zero or one boson, but no more. Using the boson language the Heisenberg Hamiltonian (2) becomes

$$H = \sum_i \left(b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger + 2 n_i n_{i+1} \right), \; n_i = b_i^\dagger b_i. \tag{5}$$

Apart from any practical usage, this kind of boson mapping is useful in visualizing an otherwise very abstract spin problem. There are many examples of many-body models that can be written in various equivalent ways. Each way provides a unique perspective in visualizing the problem.

The total spin along the z-direction $S^z = \frac{1}{2}\sum_i \sigma_i^z$ commutes with the Hamiltonian. Each eigenstate of H is also an eigenstate of S^z. The highest-weight state is obviously the ferromagnetic one, $|\mathrm{FM}\rangle = |\uparrow, \cdots, \uparrow\rangle$ corresponding to no boson occupation over the entire lattice. A single-boson state, with one spin down, can be written

$$\sum_i \psi_i S_i^- |\mathrm{FM}\rangle = \sum_i \psi_i b_i^\dagger |0\rangle. \tag{6}$$

When there is only one boson in the whole system, the interaction term $n_i n_{i+1}$ in Eq. (24) is always zero. The leftover piece is just the tight-binding model, for which we know the exact solution by way of Bloch's theorem:

$$|1\mathrm{boson}\rangle = \sum_i e^{ikx_i} b_i^\dagger |0\rangle. \tag{7}$$

In other words the eigenstate with single spin down has the exact form $|1\mathrm{down}\rangle = \sum_i e^{ikx_i} S_i^- |\mathrm{FM}\rangle$.

Encouraged by the ease with which a single boson (single spin-flip) solution has been found, we move to find the two-boson solution in the form

$$|2\mathrm{boson}\rangle = \sum_{i<j} \psi(i,j) b_i^\dagger b_j^\dagger |0\rangle = \sum_{i<j} \psi(i,j) S_i^- S_j^- |\mathrm{FM}\rangle. \tag{8}$$

From the commutation of two boson operators we also conclude $\psi(j,i) = \psi(i,j)$. The i,j sites are the locations of two bosons. The equation one gets when i,j are adjacent, $j = i+1$, is different from the one for i,j further than one lattice spacing apart. The latter case makes the density term $n_i n_{i+1}$ inoperative, and just gives

$$\psi(i+1,j) + \psi(i-1,j) + \psi(i,j+1) + \psi(i,j-1) = E\psi(i,j). \tag{9}$$

E is the energy eigenvalue of the two-boson eigenstate. For $j = i+1$,

$$\psi(i+1,i+1) + \psi(i-1,i+1) + \psi(i,i+2) + \psi(i,i) + 2\psi(i,i+1) = E\psi(i,i+1). \tag{10}$$

In fact, one must set $\psi(i,i) = \psi(i+1,i+1) = 0$ since there can't be two bosons sitting at the same site. Bethe was clever enough to see that the first of these equations, (9), is solved by the ansatz (hence "Bethe ansatz")

$$\psi(i,j) = Ae^{ik_1 n_i + ik_2 n_j} + Be^{ik_2 n_i + ik_1 n_j}. \tag{11}$$

Substitution into Eq. (9) gives

$$\begin{aligned} &2(\cos k_1 + \cos k_2)(A\cos k_1 e^{ik_1 n_i + ik_2 n_j} + B\cos k_2 e^{ik_2 n_i + ik_1 n_j}) \\ &= E(Ae^{ik_1 n_i + ik_2 n_j} + Be^{ik_2 n_i + ik_1 n_j}). \end{aligned} \tag{12}$$

That is, $E = 2(\cos k_1 + \cos k_2)$. The second equation (10) gives the ratio

$$\frac{B}{A} = -\frac{e^{ik_1+ik_2} - 2e^{ik_2} + 1}{e^{ik_1+ik_2} - 2e^{ik_1} + 1} = e^{-i\phi_{12}}. \tag{13}$$

The ratio is just a phase, so we assign half of it to each:

$$\psi(i,j) = e^{ik_1 n_i + ik_2 n_j + i\phi_{12}/2} + e^{ik_2 n_i + ik_1 n_j - i\phi_{12}/2}. \tag{14}$$

The final step is the quantization of k_1, k_2 by imposing periodic boundary conditions: $\psi(i+N,j) = \psi(i,j+N) = \psi(i,j)$. Please keep in mind that $\psi(i+N,j)$ should be written $\psi(j,i+N)$ as we promised to keep the larger-valued coordinate to the right.

$$\begin{aligned} \psi(j,i+N) &= e^{ik_1 N} e^{ik_2 n_j + ik_1 n_i - i\phi_{12}/2} + e^{ik_2 N} e^{ik_1 n_j + ik_2 n_i + i\phi_{12}/2} = \\ \psi(i,j) &= e^{ik_1 n_i + ik_2 n_j + i\phi_{12}/2} + e^{ik_1 N} e^{ik_2 n_i + ik_1 n_j - i\phi_{12}/2} \end{aligned} \tag{15}$$

The first and the second terms from each line must match:

$$e^{ik_1 N - i\phi_{12}} = 1 = e^{ik_2 N + i\phi_{12}}. \tag{16}$$

This would have led to the usual quantization $k_1 N = I_1$, $k_2 N = I_2$, with $1 \le I_1, I_2 \le N$ integers. We obtain the quantization condition on k_1, k_2:

$$k_1 = \frac{2\pi}{N} I_1 + \frac{\phi_{12}}{N}, k_2 = \frac{2\pi}{N} I_2 - \frac{\phi_{12}}{N}. \tag{17}$$

This is the usual quantization condition on the wave number plus a "tiny" phase shift $\pm\phi_{12}/N$ that vanishes in the thermodynamic limit $N \to \infty$. This is not surprising as placing two particles in an infinitely long chain would give them very little chance of interacting with each other. The phase ϕ_{12} depends implicitly on k_1, k_2 through Eq. (13). The quantization condition we derived in Eq. (17) gives a highly non-linear relations between k_1, k_2, that can only be solved exactly by a computer. (So much for the "exact" solution...)

Having come this far, you can probably "guess" (=ansatz in German) the form of the general solution with M spins down, or M bosons in the lattice of

length N. This will be a plane-wave solution with permutations of M momenta among M particles, $\exp(ik_{P(1)}n_1 + ik_{P(2)}n_2 + \cdots + ik_{P(M)}n_M)$, with an extra factor to account for phase shifts between any pair of particles: $\exp(i\phi_{P(i),P(j)})$. The general solution with bosons placed at $(n_1, \cdots n_M)$ is

$$\psi(n_1, \cdots, n_M) = \sum_P e^{i\sum_i k_{P(i)}n_i} e^{\frac{i}{2}\sum_{i<j}\phi(P(i),P(j))}. \tag{18}$$

There are N different momenta k_i $(1 \leq i \leq N)$ and $N(N-1)/2$ different phase angles $\phi(i,j)$ to solve for. A particular set $\{k_i, \phi(i,j)\}$ will be one eigenstate of the Heisenberg Hamiltonian with M spins down. In a chain of length N there are $C_M^N = N!/(N-M)!M!$ ways of arranging M down spins, hence there are as many different eigenstates, or as many different choices of the set $\{k_i, \phi(i,j)\}$.

The ground state of the antiferromagnetic spin chain of even length N will have $M = N/2$ down spins. Among the $N!/[(N/2)!]^2$ eigenstates the one with the lowest energy E will be the ground state. Finding this state is a challenge. As an exercise problem I am asking you to solve the $N = 4, M = 2$ problem by Bethe ansatz techniques. The final stage of the solution must be done with computer. You have probably learned enough about the Bethe ansatz to feel that the method, powerful as it may be, is really geared to finding solutions near the ferromagnetic limit, whereas the most interesting stuff may be happening far, far away from that limit around $M = N/2$. Working out the correlation functions and the excitation spectrum is hard, too. We need a simplified approach that is more geared toward the antiferromagnetic ground state and the small number of excitations around such ground state. The continuum approach in the following section provides such method.

For the curious readers I am attaching Hans Bethe's original 1031 paper (translated in English). You will be amazed by how modern the language he uses is. Nothing in his original paper requires much modification for today's readers. The other side, though, is that the method has hardly been improved upon over the past 85 years. What Bethe found is here to stay. Progress had to come from completely new ways of thinking about the antiferromagnetic chain problem.

2 Continuum approach to quantum spin chain

In the previous section we learned that spin-1/2 operators can equally well be written in terms of boson operators. There is a famous rule in one dimension that allows the transformation of boson operator into a fermion operator:

$$f_i^\dagger = b_i^\dagger e^{i\pi\sum_{j<i} b_j^\dagger b_j}, \quad f_i = b_i e^{-i\pi\sum_{j<i} b_j^\dagger b_j}. \tag{19}$$

Let's see what happens if we multiply two f's at different sites $i < i'$:

$$f_i f_{i'} = b_i e^{-i\pi\sum_{j<i} b_j^\dagger b_j} b_{i'} e^{-i\pi\sum_{j'<i'} b_{j'}^\dagger b_{j'}}. \tag{20}$$

The string factor $e^{-i\pi\sum_{j'<i'} b_{j'}^\dagger b_{j'}}$ can be divided into three pieces:

$$e^{-i\pi\sum_{j'<i'} b^\dagger_{j'}b_{j'}} = e^{-i\pi\sum_{j'<i} b^\dagger_{j'}b_{j'}} e^{-i\pi b^\dagger_i b_i} e^{-i\pi\sum_{i<j'<i'} b^\dagger_{j'}b_{j'}}. \quad (21)$$

After some algebra, $f_i f_{i'}$ becomes

$$e^{-2i\pi\sum_{j<i} b^\dagger_j b_j} e^{-i\pi\sum_{i<j'<i'} b^\dagger_{j'}b_{j'}} b_{i'} b_i e^{-i\pi b^\dagger_i b_i} = e^{-i\pi\sum_{i<j'<i'} b^\dagger_{j'}b_{j'}} b_{i'} b_i e^{-i\pi b^\dagger_i b_i}. \quad (22)$$

Since hard-core bosons can only have occupations 0 or 1, the first factor $e^{-2i\pi\sum_{j<i} b^\dagger_j b_j}$ is equal to one. If the factor $b_i e^{-i\pi b^\dagger_i b_i}$ acts on a zero-boson state one gets zero. If it acts on a one boson state one gets $-b_i|1\rangle = -|0\rangle$. In other words, it is equal to $-e^{-i\pi b^\dagger_i b_i} b_i$, with a minus sign. Due to this minus sign, one can show $f_i f_{i'} = -f_{i'} f_i$, which is the anti-commutation property of the fermion! In one dimension one cannot really distinguish between a hard-core boson and a fermion. They are just different ways of expressing the same particle. Depending on the problem at hand and how one wishes to approach the problem, sometimes fermion representations are better, sometimes worse. Due to the one-to-one correspondence between hard-boson bosons and Pauli operators, there also exists a one-to-one relation between spin-1/2 and fermions. All three representations are connected by well-defined mappings.

$$\begin{aligned} S^-_i &= b^\dagger_i = f^\dagger_i e^{-i\pi\sum_{j<i} f^\dagger_j f_j}, \\ S^+_i &= b_i = f_i e^{i\pi\sum_{j<i} f^\dagger_j f_j}, \\ S^z_i &= \frac{1}{2} - b^\dagger_i b_i = \frac{1}{2} - f^\dagger_i f_i. \end{aligned} \quad (23)$$

One should not be very surprised that the fermion representation of the Heisenberg Hamiltonian looks very similar to the boson representation (24):

$$H = \sum_i \left(-f^\dagger_i f_{i+1} - f_i f^\dagger_{i+1} - 2n_i + 2\lambda n_i n_{i+1} \right), \; n_i = f^\dagger_i f_i. \quad (24)$$

Note that a previously unknown factor λ has sneaked into the formula. For the isotropic Heisenberg model this factor should have been $\lambda = 1$. Oftentimes progress in theoretical physics is made by pretending that the real problem, which is hard, shares most of the key features with another problem, which is much easier to handle. This is usually the case as long as there is no (quantum) phase transition as the small parameter is tuned from zero to its full value. Supposing that this is indeed the case, we have the fermionized Hamiltonian for $\lambda = 0$ in Fourier space:

$$H = -2\sum_k \cos k f^\dagger_k f_k. \quad (25)$$

At absolute zero temperature all the states with energies $\varepsilon_k = -2\cos k$ up to the chemical potential will be filled. The filling factor (average fermion number) is decided by the condition $S^z_i = 1/2 - f^\dagger_i f_i$, or $m = 1/2 - n$. The average

magnetization m is zero for the antiferromagnetic ground state, so we arrive at the half-filled fermion band $n = 1/2$. The antiferromagnetic ground state becomes (at least when we ignore the $\sigma_i^z \sigma_{i+1}^z$ term) equivalent to the half-filled fermi sea! The fermi picture also gives an idea of the low-energy excitations as the fermi particles excited from below to above the Fermi level. Such excitation, after properly translated back to the spin language, will describe excitations around the antiferromagnetic ground state.

The role of the fermion interaction must not be neglected. Ways to treat the interaction effect in one-dimensional fermion system have developed over the years, culminating in the bosonization techniques of the 70s. We skip this important topic due to the time constraint. Let me just emphasize that while bosonization is an extremely important and powerful idea, it is also entirely a Hamiltonian idea. It gives you the correct low-energy Hamiltonian description of the antiferromagnetic spin chain. It does not tell you what the low-energy Lagrangian of the same model is. For that we go to the early 80s.

3 Spacetime approach to quantum spin chain

Methods discussed in the previous section gave a simple way to understand excitations around the antiferromagnetic ground state. The method, like Bethe's ansatz, is engineered to work for $S = 1/2$, but not for any other spins. If you know something about the group theory, you will know that Pauli operators are two-dimensional representations (i.e. 2×2 matrix representations) of the SU(2) algebra. One can also have SU(2) representations in terms of 3×3, 4×4 matrices corresponding to spin-1, spin-3/2, and so on. The spin-1 chain Hamiltonian will look the same as the Heisenberg model, $H = \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$, except that $\mathbf{S}$ are spin-1 operators with $S^z = \mathrm{diag}(1, 0, -1)$, etc.

Spin-1 chain was not really looked into at all until the beginning of 80s. First of all none of the well-known, well-established techniques for spin-1/2 chain carried over to spin-1. One can do, in principle, brute-force exact diagonalization of the spin-1 chain on a small system size. It was only in the beginning of the early 80s that people had enough computing power to try the exact diagonalization for spin chains. But it was the genius of Haldane that brought in the necessary insight to figure out what's going on with spin-1 chain that's distinctly different from spin-1/2 chain. This year's Nobel prize is in part in recognition of Haldane's breakthrough theory of spin chains. Haldane's view on spin chain problem is largely associated with his derivation of the famous Berry phase action for spin chains. It has the beautiful, Wess-Zumino-Witten form for a single spin, a skyrmion form for an antiferromagnetic chain with the prefactor proportional to the spin size S. The only catch here is that none of these "derivations" in fact appears in Haldane's original paper published between 1981-1983. What Haldane in fact did was to derive the equation of motion for the low-energy excitations of the spin chain. As we know, equation of motion follows from variations of the action. So, Haldane's derivation of the equation of motion is implicitly equivalent to the derivation of the action, although it's not so manifest if you were to just pick up his papers and read them. Anyway, all modern descriptions of Haldane's breakthrough theory are in terms of the action.

One can begin with a very simple question: What is the action (path integral) for spins? As a simplest example take the Zeeman Hamiltonian

$$H = -\mathbf{B}\cdot\mathbf{S}. \tag{26}$$

As I said, the orthodox derivation is to have the time evolution operator sliced up into infinitesimal pieces and insert intermediate states for each time slice.

$$\begin{aligned}\langle f|e^{-itH}|i\rangle \quad &= \int dI_N dI_{N-1}\cdot dI_1\ \langle f|e^{-i\Delta tH}|I_{N-1}\rangle\langle I_{N-1}|e^{-i\Delta tH}|I_{N-2}\rangle\langle I|_{N-2}\\ &\quad \cdots\langle I_1|e^{-i\Delta tH}|i\rangle.\end{aligned} \tag{27}$$

The popular choice for spin problem is the coherent state basis defined by the SU(2) rotation of the highest-weight state:

$$|\mathbf{n}\rangle = e^{-i\phi J_z}e^{-i\theta J_y}\mathbf{n}_0,\ \mathbf{n}_0 = \begin{pmatrix}1\\0\end{pmatrix}. \tag{28}$$

Since $\mathbf{J} = (1/2)\boldsymbol{\sigma}$ one readily finds $\mathbf{n} = \begin{pmatrix}\cos\theta/2\\ e^{i\phi}\sin\theta/2\end{pmatrix}$. Working through the usual Feynman path integral algebra gives the path integral

$$\int \mathcal{D}\mathbf{n}e^{iS\int dt(\cos\theta-1)\dot{\phi}+S\mathbf{B}\cdot\mathbf{n}} \tag{29}$$

with $S = 1/2$ since we are presently dealing with spin-1/2 particle. The first term, which comes from working out $\langle\mathbf{n}|\dot{\mathbf{n}}\rangle$, is the famous Berry's phase of a single spin. Michael Berry wrote this term down in his 1984 epic paper using the purely first-quantized formalism, i.e. using wave functions alone. In the path integral language this is done by inserting the coherent states as we just saw. The idea generalizes quickly to higher spin $S > 1/2$. For instance $S = 1$ coherent state is found to be

$$e^{-i\phi J_z}e^{-i\theta J_y}\begin{pmatrix}1\\0\\0\end{pmatrix} = \begin{pmatrix}e^{-i\phi}\cos^2(\theta/2)\\ (1/\sqrt{2})\sin\theta\\ e^{i\phi}\sin^2(\theta/2)\end{pmatrix}. \tag{30}$$

Working out $\langle\mathbf{n}|\dot{\mathbf{n}}\rangle$ once again gives $iS(\cos\theta-1)\dot{\phi}$ with $S = 1$.

We have just worked out a very general structure of the Lagrangian for the spin problem. It is the "Berry phase" term $S(\cos\theta-1)\dot{\phi}$ minus the Hamiltonian, obtained by replacing the spin operator $\mathbf{S}$ in the Hamiltonian language with the space-time dependent classical vector $S\vec{n}$ of size S. The Lagrangian counterpart to the Zeeman Hamiltonian is

$$L = S(\cos\theta-1)\dot{\phi} + S\mathbf{B}\cdot\mathbf{n}. \tag{31}$$

Equation of motion for spin follows, as usual, by the variational procedure leading to the Euler-Lagrange equation for θ and ϕ. Recall that $\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$.

The resulting equations must also be in terms of θ and ϕ, so it will look unfamiliar at first. On the other hand, we could have started with the Hamiltonian itself, $H = -\mathbf{B} \cdot \mathbf{S}$, and simply applied the commutator algebra $[S^\alpha, S^\beta] = i\varepsilon^{\alpha\beta\gamma} S^\gamma$ together with the Heisenberg equation of motion $\dot{A} = i[H, A]$, to recover the "operator" equation of motion

$$\frac{d\mathbf{S}}{dt} = \mathbf{S} \times \mathbf{B}. \tag{32}$$

Now go back to the two equations you got from the classical Euler-Lagrange equations. You will sooner or later figure out that they are nothing but the two independent components of the operator equation we just derived, provided we replace $\mathbf{S} \to S\mathbf{n}$ in Eq. (32). In this way, we can be confident that the Lagrangian we just derived in the path integral formalism using the coherent state basis is a good one, since it gives the correct equation of motion in the semi-classical limit $\mathbf{S} \to \langle \mathbf{S} \rangle = S\mathbf{n}$.

Can we generalize to multi-spin system? Of course. In some sense the answer is trivially out there. All we need is to bring in the extra index i for each i-th spin and write $\mathbf{S}_i \to S\mathbf{n}_i$ in the Hamiltonian-to-Lagrangian transition, and to introduce a whole bunch of Berry phase terms: $\sum_i iS(\cos\theta_i - 1)\dot{\phi}_i$. If we stopped here though we wouldn't be looking at the low-energy theory of any microscopic spin Hamiltonian. It would just be a re-writing of the same physics from Hamiltonian to Lagrangian form. The nice feature of the Lagrangian approach is that all variables are classical, so it's much easier to do various manipulations to the bare expressions. Let's take another look at the one-dimensional antiferromagnetic Hamiltonian $H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$. For the bare Lagrangian we should just have

$$L = iS \sum_i (\cos\theta_i - 1)\dot{\phi}_i - S^2 \sum_i \mathbf{n}_i \cdot \mathbf{n}_{i+1}. \tag{33}$$

Within the Lagrangian formalism we can try to make the semi-classical approach. This is to assume that $\mathbf{n}_i$ is oscillating fairly mildly around the classical configuration, which in this case would be the alternating up-and-down spin configuration like $(-1)^i \hat{z}$. So an obvious attempt is to re-write the $\mathbf{n}$ vector as $\mathbf{n}_i = (-1)^i \hat{z} + \delta\mathbf{n}_i$, delegating all the fluctuation effects to $\delta\mathbf{n}_i$ part. A theory-savvy person will then recognize a problem with such expansion, because the form explicitly breaks the rotational symmetry of the spin space. Although we know that the classical ground state of the antiferromagnetic Hamiltonian must break the spin rotation symmetry, we do not know which direction it will break into. The earlier decomposition simply supposed that the spins align in the $\pm\hat{z}$ direction, but that's not quite general enough.

A more careful approach is to build in the alternating nature explicitly by re-expressing $\mathbf{n}_i$ as $(-1)^i \mathbf{n}_i$, and then further following up with the decomposition into the slow ($\mathbf{s}_i$) and fast ($\mathbf{f}_i$) components as

$$\mathbf{n}_i \to (-1)^i \mathbf{s}_i (1 - \mathbf{f}_i^2)^{1/2} + \mathbf{f}_i. \tag{34}$$

To ensure that the new expression for the local spin remains of unit magnitude we require $\mathbf{s}_i \cdot \mathbf{f}_i = 0$ for the slow and fast vectors. One can view $\mathbf{s}_i$ as the

slow precession of the spin vector, and $\mathbf{f}_i$ as the fast wobble around $\mathbf{s}_i$. There is another complicated step to follow, but if you did that properly (this is why you need hard training in math to do important work in theoretical physics!), the true effective, low-energy action $A = \int Ldt$ in Lagrangian form for the antiferromagnetic chain emerges beautifully.

$$A = \frac{S}{2}\int dxdt\mathbf{n}\cdot\left(\frac{\partial\mathbf{n}}{\partial x}\times\frac{\partial\mathbf{n}}{\partial t}\right) + \int dxdt\ \left[(\partial_t\mathbf{n})^2 - (\boldsymbol{\nabla}\mathbf{n})^2\right]. \tag{35}$$

The first term in the action is topological. One way to see it is that it remains invariant under the coordinate change $x \to ax, t \to bt$. The other way is to invoke some topological theorem that says that

$$\frac{1}{4\pi}\int dxdt\mathbf{n}\cdot\left(\frac{\partial\mathbf{n}}{\partial x}\times\frac{\partial\mathbf{n}}{\partial t}\right) \tag{36}$$

is an integer no matter what the configuration $\mathbf{n}$ is. Calling this integer N, the path integral e^{iA} gives $e^{i2\pi NS}$. If the spin size is half-integer this number oscillates between +1 and -1 depending on the topological number N. If the spin size is an integer it would be +1 no matter what we choose for N. So apparently the size of the spin S decides whether the path integral of the antiferromagnetic spin chain depends sensitively on the proliferation of topological defects called skyrmions.

When we just try to "solve" the antiferromagnetic spin chain problem in the Hamiltonian framework such topological terms are never manifest. When the problem is re-cast as a path integral, the topological term just pops up.

4 Modern approaches to spin chain

Techniques and ideas keep evolving around the spin chain problem. The latest and hottest way to attack the spin chain and other quantum spin problems in low dimensions is the tensor network theory. This is too much material to cover for this school and I hope there will be another lecture in a few years to talk about the tensor network theory. Let me say that some knowledge in the tensor network theory will be as much a must as the coherent-state-based Lagrangian formulation of the spin chain problem has been for generations of upstart physicists over the past 20-30 years. Let me just give you the gist of the idea. Any many-body wave function of the spin chain problem will be written, as already discussed in Sec. II,

$$\sum_{\{\sigma_i\}}\psi(\sigma_1,\cdots,\sigma_N)|\sigma_1,\cdots,\sigma_N\rangle. \tag{37}$$

The ansatz of the tensor network theory is that the amplitude function $\psi(\sigma_1,\cdots,\sigma_N)$ can be written as a tensor product form

$$\psi(\sigma_1,\cdots,\sigma_N) = A^{\sigma_1}_{l_1r_1}\delta_{r_1l_2}A^{\sigma_2}_{l_2r_2}\cdots A^{\sigma_N}_{l_Nr_N}\delta_{r_Nl_1}. \tag{38}$$

Taking a fixed spin configuration $\{\sigma_i\}$ gives a fixed configuration of matrices A^{σ_i} for each site i. These matrices are then to be multiplied in the usual matrix multiplication manner. The ground state of the spin-1 antiferromagnetic chain (nowadays called the Haldane chain) can be written in this manner with extremely good accuracy using a very simple 2×2 matrix A^σ for each spin orientation $\sigma = +1, 0, -1$. For spin-1/2 chain one can also do this, but the matrix has to be bigger if a faithful representation of the true ground state is to be obtained. In fact the larger matrix we use for A^σ the better is the tensor network wave function to the true ground state. This is essentially a variational idea. The revelation that writing the many-body wave function of spin liquid states in this way is an extremely efficient variational approach has proved both powerful and useful.

5 Problems for spin chain lecture

You don't have to do all three problems. I think picking one problem that you like will be good enough.

1. Define the spin-1 exchange operator $P_{ij}|\sigma_i, \sigma_j\rangle = |\sigma_j, \sigma_i\rangle$, where $\sigma_{i,j} = +1, 0, -1$ run over the three spin states of $S = 1$. Can you find a matrix representation that does the same thing? You will find that up to some constants and prefactors the answer is $\mathbf{\Lambda}_i \cdot \mathbf{\Lambda}_j$, wehre $\Lambda = (\Lambda_1, \cdots \Lambda_8)$ is a collection of eight, 3×3 matrices called the Gell-Mann matrices. If you know something about the Lie group, you should know that Pauli matrices are generators of the group SU(2), and Gell-Mann matrices those of the group SU(3).

2. Find the Bethe ansatz solution of the $S = 1/2$ Heisenberg spin chain with $N = 4, M = 2$. Pick the one with the lowest energy, which is the ground state of the $N = 6$ antiferromagnetic Heisenberg chain.

3. Can you derive $\langle \mathbf{n}|\dot{\mathbf{n}}\rangle = S(\cos\theta - 1)\dot{\phi}$ for arbitrary spin S? With any spin size the coherent state is always defined by

$$|\mathbf{n}\rangle = e^{-i\phi J_z} e^{-i\theta J_z} \mathbf{n}_0 \tag{39}$$

with $\mathbf{n}_0 = (1, 0, \cdots, 0)^T$.

On the Theory of Metals, I.
Eigenvalues and Eigenfunctions of a Linear Chain of Atoms

H. Bethe in Rome
(Zeit. f. Physik **71**, 205 (1931))

A method is given whereby the zero-order eigenfunctions and first-order eigenvalues (in the sense of the London-Heitler approximation scheme) are calculated for a one-dimensional "metal" consisting of a linear chain of a very large number of atoms, each of which has a single s-electron with spin, outside closed shells. In addition to the spin waves of Bloch, bound states are found, in which parallel spins are predominantly on nearest neighbor atoms; these features may be important for the theory of ferromagnetism.

71.10.-w

I. INTRODUCTION

Until now, the theory of metals has for some time been limited to the investigation of the motion of individual conduction electrons in the potential field of the metal atoms (Sommerfeld, Bloch). The interaction of electrons with one another has been ignored, at least insofar as the electronic-interaction potentials are concerned. Although this procedure has been very fruitful in problems of metallic conductivity (with the exception of superconductivity), it did not allow for a deeper penetration into the problem of ferromagnetism [1] and for example, it rendered the calculation of the cohesive forces in metals a completely hopeless undertaking: exchange forces among the conduction electrons dominate first order perturbation theory and have the same order of magnitude as the zero-point energy of the electron gas (the energy in zeroth-order perturbation theory). Accordingly, one estimates that the second-order approximation will again be of the same order of magnitude, and so on. Under such circumstances, one should be skeptical of an approximation in which the motional energy of the electrons (kinetic zero-point energy) is considered to be overwhelmingly more important than their interaction energy (exchange energy).

It is for such reasons that Slater [2] and Bloch [3] have recently tried to approximate the problem from another angle, that is assuming the atomic structures to be given and their interactions to be the perturbation, in accordance with the London-Heitler approximation for molecules. Slater was mainly interested in the cohesive energy of non-ferromagnetic materials, in which the London-Heitler exchange integral is generally negative [4] [1], and gave an interesting method for the approximate calculation of the ground state energy of such metals when the total spin vanishes. In the case of ferromagnetism, Bloch calculated approximately the leading terms in the opposite case $J > 0$ [2] in a systematic fashion, but obtained too many eigenvalues by his method. It is the aim of the present work first, to give a procedure for the case of a linear chain of atoms, which allows the calculation of every eigenvalue of this one-dimensional crystal to arbitrary within the context of the first approximation of the London-Heitler method, such that the problem will be at exactly the same stage as the hydrogen molecule H_2 in the London and Heitler work. And in addition, to obtain other types of solutions differing from the (somewhat modified) Bloch [3] solutions, ensuring that the total number of eigenvalues turns out exactly correct.

II. FORMULATION

Our problem can be stated as follows: Given a linear chain composed of a large number (N) of like atoms where each atom has a single valence electron in an s-orbit outside closed shells occupying a known atomic eigenfunction, what are the zeroth-order eigenfunctions and first-order eigenvalues of the entire system when the interaction among the individual atoms is taken into account?

As long as one neglects the interaction energies, there are two states of equal energy for each atom-the spin of the valence electron can point either right or left. The energy eigenvalue of the chain is therefore 2^N-fold degenerate in zeroth approximation. Each of these states of the chain can be specified by enumerating the atoms which carry a right-handed spin; assume this to be the case for atoms $m_1, m_2, \ldots, m_r$. The corresponding totally antisymmetric eigenfunction of the chain is

[1] Here, $J < 0$ implies "antiferromagnetic" couplings
[2] Here, $J > 0$ implies "ferromagnetic" couplings

$\varphi(m_1, m_2, \ldots, m_r)$. The correct zeroth-order eigenfunctions therefore assume the form

$$\Psi = \sum_{m_1, m_2, \ldots, m_r} a(m_1, m_2, \ldots, m_r)\varphi(m_1, m_2, \ldots, m_r)$$

where each of the integers $m_1, m_2, \ldots, m_r$ runs from 1 to N. We specialize to $m_1 < m_2 < \ldots < m_r$.

One calculates matrix elements of the interaction energy using these states, each specified by its spin distribution $m_1, m_2, \ldots, m_r$, obtaining: [3]

Diagonal Elements: If in the spin distribution $m_1, m_2, \ldots, m_r$ these are N' nearest neighbor pairs of parallel spins, then

$$W_{m_1, m_2, \ldots, m_r} = E_0 - N'J.$$

E_0 is the electrostatic interaction energy of the atoms are neglected, as they fall off exponentially with distance.

Nondiagonal Elements occur between any two states which differ merely by a single perturbation of a pair of adjacent antiparallel spins as, for example, between $m_1, \ldots, m_i, \ldots, m_r$ (where we suppose $m_i + 1$ to be a left-handed spin and therefore missing from the enumeration) and $m_1, \ldots, m_i+1, \ldots, m_r$, (with m_i missing). All such off-diagonal matrix elements have a value $-J$.

With the aid of the interaction matrix elements, one obtains the following equations among the coefficients $a(m_1, m_2, \ldots, m_r)$ of the eigenstate Ψ which we are seeking:

$$2\varepsilon a(m_1, \ldots, m_r) + \sum \{a(m_1', \ldots, m_r') - a(m_1, \ldots, m_r)\} = 0 \tag{1}$$

Here,

$$2\varepsilon J = e - E_0 + NJ \tag{2}$$

and e is the total first-order perturbation energy. The summation is over all sets $m_1', m_2', \ldots, m_r'$ which differ from $m_1, m_2, \ldots, m_r$ by a single permutation of nearest-neighbor antiparallel spins. [3]

In addition to Eqs.(1), the a's must satisfy periodic boundary conditions:

$$a(m_1, \ldots, m_i, \ldots, m_r) = a(m_1, \ldots, m_i + N, \ldots, m_r) \tag{3}$$

III. REAL SOLUTIONS

For $r = 1$ the solution of (1) is

$$\begin{array}{c} a(m) = e^{ikm} \\ \varepsilon = 1 - \cos k \\ k = \frac{2\pi\lambda}{N}, \lambda = integer \end{array} .$$

For $r = 2$, two cases are to be distinguished: either the two right-handed spins are separated, in which case

$$\begin{array}{c} -2\varepsilon a(m_1, m_2) = a(m_1 + 1, m_2) + a(m_1 - 1, m_2) + \\ a(m_1, m_2 + 1) + a(m_1, m_2 - 1) - 4a(m_1, m_2) \end{array} \tag{4a}$$

with $m_2 \neq m_1 + 1$, or else they are adjacent, and:

$$\begin{array}{c} -2\varepsilon a(m_1, m_1 + 1) = a(m_1 - 1, m_1 + 1) \\ +a(m_1, m_1 + 2) - 2a(m_1, m_1 + 1). \end{array} \tag{4b}$$

The first set of equations are rigorously solved by an ansatz,

$$\begin{array}{c} a(m_1, m_2) = c_1 e^{i(f_1 m_1 + f_2 m_2)} + c_2 e^{i(f_2 m_1 + f_1 m_2)}, \\ \varepsilon = 1 - \cos f_1 + 1 - \cos f_2, \end{array} \tag{5}$$

in which c_1, c_2, f_1, f_2 are as yet undetermined by all this.

The second set can be satisfied by selecting c_1 and c_2 so as to satisfy

$$0 = a(m_1, m_1) + a(m_1 + 1, m_1 + 1) - 2a(m_1, m_1 + 1). \tag{6}$$

Here, $a(m_1, m_1)$ has no physical meaning but, rather, is to be defined by (5). Obviously, by adding (6) to (4b) we bring it to the form (4a), and we have already satisfied equations of this type. Inserting (5) into (6) yields:

$$\begin{array}{c} e^{i(f_1 + f_2)m_1}[c_1(1 + e^{i(f_1 + f_2)} - 2e^{if_2}) \\ +c_2(1 + e^{i(f_1 + f_2)} - 2e^{if_1})] = 0, \end{array} \tag{7}$$

$$\frac{c_1}{c_2} = -\frac{\cos\frac{f_1+f_2}{2} - e^{i(\frac{f_1-f_2}{2})}}{\cos\frac{f_1+f_2}{2} - e^{-i(\frac{f_1-f_2}{2})}} = \frac{\sin\frac{f_1-f_2}{2} + ic_{12}}{\sin\frac{f_1-f_2}{2} - ic_{12}}$$

with $c_{12} = \cos\frac{f_1+f_2}{2} - \cos\frac{f_1-f_2}{2}$ [$= -2\sin\frac{f_1}{2}\sin\frac{f_2}{2}$.] [Editor's note: $|c_1/c_2| = 1$, therefore we just seek a phase factor.] Set $c_1 = e^{i\frac{\varphi}{2}}$, $c_2 = e^{-i\frac{\varphi}{2}}$, so that

$$\begin{array}{c} \cot\frac{\varphi}{2} = \frac{\sin\frac{f_1-f_2}{2}}{c_{12}}, \\ 2\cot\frac{\varphi}{2} = \cot\frac{f_1}{2} - \cot\frac{f_2}{2}. \end{array} \tag{8}$$

Thus, one obtains

$$a(m_1, m_2) = e^{i(f_1 m_1 + f_2 m_2 + \frac{\varphi}{2})} + e^{i(f_2 m_1 + f_1 m_2 - \frac{\varphi}{2})}. \tag{9}$$

Additionally, it is assumed that m_1 and m_2 lie in the fundamental period of the chain, i.e., $1 \leq m_1 < m_2 \leq N$. Periodic boundary conditions require:

$$a(m_1, m_2) = a(m_2, m_1 + N). \tag{10}$$

[3] Eq.(1) is more extensively derived by Bloch in Eq.(5) of Ref.3, where he labels atoms f_i instead of m_i, and instead of $2\varepsilon J$, simply writes as ε.

[The notation $a(m_2, m_1+N)$ is explained by our convention of listing the m_i in the order of increasing magnitude, see above.] Inserting (9) into (10):

$$e^{i(f_1 m_1 + f_2 m_2 + \frac{\varphi}{2})} + e^{i(f_2 m_1 + f_1 m_2 - \frac{\varphi}{2})}$$

$$= e^{i(f_1 m_2 + f_2 (m_1+N) + \frac{\varphi}{2})} + e^{i(f_2 m_2 + f_1 (m_1+N) - \frac{\varphi}{2})}.$$

As these must hold for all m_1 and m_2, the first term on the left must be equal to the second term on the right, as they have the same dependence on m_1 and m_2, and conversely, so that

$$N f_1 - \varphi = 2\pi\lambda_1, N f_2 + \varphi = 2\pi\lambda_2, \tag{11}$$

and $\lambda_1, \lambda_2 = 0, 1, 2, \ldots, N-1$. Although, individually, the f_1 and f_2 do not have the usual form $\frac{2\pi\lambda}{N}$, their sum,

$$k = f_1 + f_2 = \frac{2\pi(\lambda_1 + \lambda_2)}{N}, \tag{12}$$

is a true constant of the motion of the problem; the coefficient $a(m_1, m_2)$ is multiplied by e^{ik} if both the right-handed spins are displaced by one atomic position to the right, a translation which obviously does not affect any physical properties [by translation invariance].

We now discuss the behavior of the phase φ as a function of f_1 and f_2, for which we specify that

$$-\pi \leq \varphi \leq \pi. \tag{13}$$

If one interchanges f_1 and f_2, then clearly φ changes sign and the coefficients remain unchanged, according to (9). If f_2 is held fixed and f_1 is allowed to increase from zero, then $\cot\frac{\varphi}{2}$ falls from $+\infty$ to smaller positive values, finally reaching zero for $f_1 = f_2$; thus, φ ranges from 0 to π. If f_1 becomes slightly greater than f_2, φ jumps from π to $-\pi$, gradually increasing back to zero as f_1 increases to 2π. If $f_1 = f_2$, then either

$$\varphi = +\pi, \lambda_1 = \lambda_2 - 1 = \frac{N f_1}{2\pi} - \frac{1}{2},$$

or

$$\varphi = -\pi, \lambda_1 = \lambda_2 + 1 = \frac{N f_1}{2\pi} + \frac{1}{2}.$$

In either instance, according to (9) for all m_1, m_2, $a(m_1, m_2)$ becomes

$$a(m_1, m_2) = e^{i f_1 (m_1+m_2)}(e^{i\frac{\pi}{2}} + e^{-i\frac{\pi}{2}}) \equiv 0.$$

This means that $f_1 = f_2$ [4] does not lead to a meaningful solution of the problem, and if λ_2 is specified, λ_1 can take on only the values

$$\lambda_1 = 0, 1, 2, \ldots, \lambda_2 - 2, \lambda_2 + 2, \ldots, N-1.$$

As f_1, f_2 and f_2, f_1 yield the same eigenfunction, we can specify $f_1 < f_2$ without loss of generality. Thus, for fixed λ_2, there are $\lambda_2 - 1$ solutions $\lambda_1 = 0, 1, \ldots, \lambda_2 - 2$ and λ_2 goes from 2 to $N-1$, so that the total number becomes:

$$\sum_{\lambda_2=2}^{N-1} (\lambda_2 - 1) = \begin{pmatrix} N-1 \\ 2 \end{pmatrix} \equiv \frac{(N-1)!}{2!(N-3)!}$$

a binomial coefficient. Clearly, there must be as many solutions as there are distinct configurations for m_1 and m_2, namely $\begin{pmatrix} N \\ 2 \end{pmatrix} = \frac{N!}{2!(N-2)!}$. So in fact the foregoing exact analysis yields an *insufficient number* of solutions, whereas Bloch [3] believed that the method yields too many, namely $\begin{pmatrix} N+1 \\ 2 \end{pmatrix} = \frac{(N+1)}{2!(N-1)!}$.

IV. ADDITIONAL IMAGINARY SOLUTIONS

There must exist $N-1$ additional solutions. These are obtained by allowing the wave numbers f_1 and f_2 to take on complex-conjugate values. In fact we shall find that for each, arbitrary, value of $k = f_1 + f_2$ there is found precisely one pair of complex conjugate solutions to Eqs.(8) and (11) [5]. Let

$$\begin{aligned} f_1 &= u + iv, \\ f_2 &= u - iv, \end{aligned} \tag{14}$$

then

$$\cot\frac{f_1}{2} = \frac{\cos\frac{u}{2}\cosh\frac{v}{2} - i\sin\frac{u}{2}\sinh\frac{v}{2}}{\sin\frac{u}{2}\cosh\frac{v}{2} + i\cos\frac{u}{2}\sinh\frac{v}{2}}$$

$$= \frac{\sin u - i\sinh v}{\cosh v - \cos u}. \tag{15}$$

By (11),

$$\begin{aligned} N(f_1 - f_2) = 2Niv &= 2\pi(\lambda_1 - \lambda_2) + 2\varphi, \\ \varphi &= \psi + i\chi, \\ \psi &= \pi(\lambda_2 - \lambda_1), \\ \chi &= Nv. \end{aligned} \tag{16}$$

If v is finite, then χ must be very large, such that

$$\cot\frac{\varphi}{2} \approx \frac{\sin\psi - i\frac{1}{2}e^{\chi}}{\frac{1}{2}e^{\chi} - \cos\psi} = -i + 2e^{-\chi}(\sin\psi - i\cos\psi),$$

[4] $\lambda_1 = \lambda_2 \pm 1$

[5] the "bound-state"

$$\cot\frac{\varphi}{2} = -i(1+2e^{-\chi+i\psi}). \tag{17}$$

In *first* approximation, the following holds:

$$2\cot\frac{\varphi}{2} = \cot\frac{f_1}{2} - \cot\frac{f_2}{2} = -2i$$

$$= \frac{\sin u - i\sinh v}{\cosh v - \cos u} - \frac{\sin u + i\sinh v}{\cosh v - \cos u},$$

$$\sinh v = \cosh v - \cos u,$$

$$e^{-v} = \cos u \tag{18}$$

and

$$\varepsilon = 2 - \cos(u+iv) - \cos(u-iv)$$

$$= 2 - 2\cos u\cosh v = 2 - \cos u(\cos u + \frac{1}{\cos u}),$$

$$\varepsilon = \sin^2 u = \frac{1}{2}(1-\cos 2u). \tag{19}$$

Clearly, $\cos u$ has to be ≥ 0, that is $-\frac{\pi}{2} \leq u \leq \frac{\pi}{2}$. If then $k = 2u + 2n\pi$ (n an integer) is between 0 and π, then

$$u = \frac{k}{2},$$

if between π and 2π, then

$$u = \frac{k}{2} + \pi.$$

In a *second* approximation we set

$$v = v_0 + \varepsilon, \tag{20}$$

where v_0 is value obtained in the first approximation. Then,

$$2\cot\frac{\varphi}{2} = -2i - 4ie^{-\chi+i\psi} = -2i\frac{\sinh v}{\cosh v - \cos u}$$

$$= -2i\frac{\sinh v_0}{\cosh v_0 - \cos u}\left[1 + \varepsilon\left(\frac{\cosh v_0}{\sinh v_0} - \frac{\sinh v_0}{\cosh v_0 - \cos u}\right)\right]$$

$$= -2i\cdot 1\cdot\left[1 + \varepsilon\cdot\left(\frac{1+\cos^2 u}{1-\cos^2 u} - 1\right)\right] = -2i(1+2\varepsilon\cot^2 u),$$

$$\varepsilon = (\tan^2 u)e^{-\chi+i\psi}.$$

As ε is in general very small, Nv_0 can be written for χ. ψ is now adjusted according to the prescribed value of k:

If $\frac{Nk}{2\pi} = \lambda_1 + \lambda_2 = \lambda$ is even and smaller than $\frac{N}{2}$, we can set

$$\lambda_1 = \lambda_2 = \frac{\lambda}{2}, \psi = 0.$$

Likewise, for $\lambda \geq \frac{N}{2}$, $N+\lambda$ even:

$$\lambda_1 = \lambda_2 = \frac{N+\lambda}{2}, \psi = 0.$$

If either λ or $N+\lambda$ is odd, then we must write:

$$\lambda_2 = \lambda_1 + 1, \psi = \pi.$$

From this,

$$\varepsilon = \pm\tan^2 u e^{-Nv_0}. \tag{21}$$

For even λ (or $N+\lambda$), $v > v_0$. If in the next approximation v_0 is replaced by v then resulting ε is smaller than that of the second approximation. The procedure for the determination of v always converges, indeed very rapidly. On the other hand, if a negative sign be chosen (odd λ or $N+\lambda$) then $v < v_0$ and absolute value of ϵ increases in higher approximations. This makes no difference so long as v_0 is finite, as then the correction to ε is infinitesimal. But if u is small and therefore $\cos u \approx 1$, then v_0 is also small, and to sufficient accuracy

$$v_0 = -\log\cos u = 1 - \cos u = \frac{u^2}{2}.$$

If u is small of order $\frac{1}{\sqrt{N}}$, then Nv_0 is finite and

$$\varepsilon = -u^2 e^{-Nv_0}$$

is larger than v_0 in absolute value so long as $Nv_0 < \log 2 \approx 0.7$, $u^2 < \frac{1.4}{N}$. For $u < \sqrt{\frac{1.4}{N}}$ and odd λ, then $v_1 = v_0 + \varepsilon$ will be negative, the process diverges, and no solution with two complex conjugate wave numbers can be found. [6]

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In its place, there occurs an additional solution with two real wave numbers. We again consider k as given and $f_2 = k - f_1$. Earlier in the discussions of real solutions it was tacitly assumed that with increasing f_1, $F = Nf_1 - \varphi$

[6] In fact, this occurs already for $u < \frac{2}{\sqrt{N}}$, despite that in the second approximation v is positive, because higher approximations push it down to negative values.

increased monotonically. This might seem obvious, insofar as f_1 is multiplied by a very large factor N and φ is $o(1)$. Nevertheless, this assumption is invalid at small k. Looking at (8) in some greater detail, we obtain

$$\frac{dF}{df_1} = N - 2\frac{A}{D},$$

where

$$A \equiv \frac{1}{4\sin^2\frac{f_1}{2}} + \frac{1}{4\sin^2\frac{k-f_1}{2}}$$

and

$$D \equiv 1 + [\frac{1}{2}\cot\frac{f_1}{2} - \frac{1}{2}\cot\frac{k-f_1}{2}]^2;$$

setting $f_1 = f_2 = \frac{k}{2}$, then clearly

$$\frac{dF}{df_1} = N - \frac{1}{\sin^2\frac{f_1}{2}}$$

is positive only so long as $\sin\frac{f_1}{2} > \frac{1}{\sqrt{N}}$. For $k < 4\sin^{-1}(\frac{1}{\sqrt{N}}) \approx \frac{4}{\sqrt{N}}$ the increase of $F = Nf_1 - \varphi$ as function of f_1 is broken off by a decrease in the vicinity of $f_1 = \frac{k}{2}$. If $\frac{Nk}{2\pi} = \lambda$ is odd, then

$$\frac{Nk}{2} - \pi = 2\pi\lambda_1 = 2\pi\frac{\lambda-1}{2}$$

where λ_1 is an integer, and for $\lambda_1 = \frac{\lambda-1}{2}$, $\lambda_2 = \frac{\lambda+1}{2}$, there are two [7] solutions of the system of equations (8) and (11): besides $f_1 = f_2$, $\varphi = \pi$, there exists a solution $f_1 < f_2$, $\varphi \neq \pi$, for which the coefficients (9) remain finite in contrast to the first solution.

To actually find this solution, we put $f_1 = f - 2\frac{\varepsilon}{N}$ and throughout and use $\sin f = f$, $\cos f = 1$, $\cot f = \frac{1}{f}$, valid for small f. Then,

$$2\cot\frac{\varphi}{2} = \frac{2}{f - 2\frac{\varepsilon}{N}} - \frac{2}{f + 2\frac{\varepsilon}{N}} = \frac{8\varepsilon}{Nf^2} \qquad (8a)$$

$$2\varphi = 2\pi(\lambda_2 - \lambda_1) - N(f_2 - f_1) = 2\pi - 4\varepsilon \qquad (11a)$$

$$\cot\frac{\varphi}{2} = \tan\varepsilon,$$

$$\frac{\tan\varepsilon}{\varepsilon} = \frac{4}{Nf^2}. \qquad (22)$$

From this, ε is determined, ε is $< \frac{\pi}{2}$, therefore $\varphi > 0$ and $Nf_1 > 2\pi\lambda_1$.

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With this, we have determined an additional solution, with real or complex wave number, at each value of λ. The largest allowed value of λ is obviously $N-2$ with $\lambda_1 = \lambda_2 = N-1$; for $\lambda = N-1$ on the other hand, $\lambda_2 = N$, outside the permissible interval [8]. Thus, we find $N-1$ solutions $\lambda = 0, 1, 2, \ldots, N-2$, precisely the required number.

According to Eqs.(9), (12), (16a), the coefficients $a(m_1, m_2)$ of our complex solutions are

$$a(m_1, m_2) = e^{iu(m_1+m_2)}(e^{v(m_1-m_2+\frac{N}{2})} \pm e^{-v(m_1-m_2+\frac{N}{2})}),$$

$$a(m_1, m_2) = e^{iu(m_1+m_2)} \left\{ \begin{array}{c} \cosh \\ \sinh \end{array} \right\} v\left(\frac{N}{2} - (m_2 - m_1)\right) \qquad (23)$$

with cosh or sinh applying according to whether λ (or $N+\lambda$ for $\lambda > \frac{N}{2}$) is even or odd. For our solutions it is most probable that both right-handed spins lie as close together as possible, as the probability $|a(m_1, m_2)|^2$ falls off exponentially with distance $m_2 - m_1$. The extreme case occurs for the solution with $\lambda = \frac{N}{2}$, $u = \frac{\pi}{2}$ and $v = \infty$. Here, after appropriate normalization,

$$a(m_1, m_2) = \left\{ \begin{array}{cc} 0 & \text{for } m_2 \neq m_1 + 1 \\ (-1)^{m_1} & \text{for } m_2 = m_1 + 1 \end{array} \right. ,$$

and both spins are always precisely adjacent.

Every eigenvalue ε for a solution with two complex conjugate wave numbers is *smaller* than any eigenvalue with the same total wave number k and real wave numbers, as we shall now show. According to (2) then, the corresponding energy e in the first approximation is *lower* than all the solutions with real wave numbers if the exchange integral J is positive (for ferromagnetism) or higher, if J is negative (the usual case).

For the complex solution we have, specifically,

$$\varepsilon_k = \sin^2 u, \qquad (19)$$

whereas for the real,

$$\varepsilon_r = 1 - \cos f_1 + 1 - \cos(k - f_1), \qquad (5)$$

(5) reaches its minimum for

$$f_1 = \left\{ \begin{array}{cc} \frac{k}{2} & \text{for } 0 \leq k \leq \pi \\ \frac{k}{2} + \pi & \text{for } \pi \leq k \leq 2\pi \end{array} \right. ,$$

[7] One can show that F can assume no other integer value more than once (for odd λ) and none at all for even λ.

[8] The solution $\lambda_1 = N-1$, $\lambda_2 = N$ has, in fact, already been counted once, in the form $\lambda_2 = 0$, $\lambda_1 = N-1$.

that is, generally for $f_1 = f_2 = u$. The minimum is

$$\varepsilon_{min} = 2(1 - \cos u),$$

so that

$$\frac{\varepsilon_k}{\varepsilon_{min}} = \frac{1 + \cos u}{2} \leq 1, \tag{24}$$

where the equal sign applies only at $u = 0$ [9]. QED.

V. GENERAL CASE

We turn now to the general case of r right-handed spins. Eqs.(1) again fall into two types: If none of the r designated spins $m_1, \ldots, m_r$ are adjacent, then

$$-2\varepsilon a(m_1, \ldots, m_i, \ldots, m_r) = \sum_{r=1}^{r} [a(m_1, \ldots, m_i+1, \ldots, m_r)$$

$$+a(m_1, \ldots, m_i - 1, \ldots, m_r) - 2a(m_1, \ldots, m_i, \ldots, m_r)]. \tag{24a}$$

If instead, two are adjacent, say $m_{k+1} = m_k + 1$, then,

$$-2\varepsilon a(m_1, \ldots, m_i, \ldots, m_k, m_k + 1, \ldots, m_r)$$

$$= a(\ldots, m_k - 1, m_k + 1, \ldots) + a(\ldots, m_k, m_k + 2, \ldots)$$

$$-2a(\ldots, m_k, m_k + 1, \ldots) + \sum_{i \neq k, k+1}^{r} [a(\ldots, m_i + 1, \ldots)$$

$$+a(\ldots, m_i - 1, \ldots) - 2a(\ldots, m_i, \ldots)] \tag{24b}$$

and analogously for any larger number of adjacent right-handed spins.

We next suppose [10]

$$a(m_1, \ldots, m_i, \ldots, m_r) = \sum_{P=1}^{r!} e^{i[\sum_{k=1}^{r} f_{P_k} m_k + \frac{1}{2} \sum \varphi_{P_k, P_n}]}, \tag{25}$$

$$\varepsilon = \sum_{k=1}^{r} (1 - \cos f_k). \tag{26}$$

P is any permutation of the r numbers $1, 2, \ldots, r$, and P_k is the number which replaces k under this permutation. The ansatz satisfies the first set of equations (24a) by inspection. The remaining equations are satisfied by requiring that

$$2a(\ldots, m_k, m_k + 1, \ldots)$$

$$= a(\ldots, m_k, m_k, \ldots) + a(\ldots, m_k + 1, m_k + 1, \ldots) \tag{27}$$

in which the [11] amplitudes on the right are to be *defined* according to (25). Eq.(27) must hold for any arbitrary set of $m_1, m_2, \ldots, m_r$ of which an arbitrary number can be nearest-neighbors, provided only $m_1 < m_2 < \ldots < m_r$. All the relations (24b) are simultaneously satisfied by this device, including cases in which the $m_1, m_2, \ldots, m_r$ involve more than one pair of adjacent parallel spins; all equations are reduced to the type (24a), which have already been solved. Eq.(27) itself is satisfied by requiring the phase φ to satisfy the relations,

$$2 \cot \frac{\varphi_{kn}}{2} = \cot \frac{f_k}{2} - \cot \frac{f_n}{2}; \tag{28}$$

$-\pi \leq \varphi_{kn} \leq \pi$.

There remain the periodic boundary conditions,

$$a(m_1, m_2, \ldots, m_r) = a(m_2, \ldots, m_r, m_1 + N),$$

$$\sum_P e^{i[\sum_{k=1}^{r} f_{P_k} m_k + \frac{1}{2} \sum \varphi_{P_k, P_n}]}$$

$$= \sum_{P'} e^{i[\sum_{k=2}^{r} f_{P'_{k-1}} m_k + f_{P'_r}(m_1 + N) + \frac{1}{2} \sum_{k<n} \varphi_{P'_k, P'_n}]}.$$

This holds for all $m_1, m_2, \ldots, m_r$; therefore terms on the left-hand and right-hand sides of the equation which have the same dependence on m_k must be precisely equal. For example, consider a term P on the left and P'' on the right, with P'' defined by

$$P''_{k-1} = P_k (k = 2, \ldots, r), P''_r = P_1.$$

These results

$$N f_{P''_r} + \frac{1}{2} \sum_{k<n} \varphi_{P''_k, P''_n} - \frac{1}{2} \sum_{k<n} \varphi_{P_k, P_n} = 2\pi\lambda$$

$$= N f_{P_1} + \frac{1}{2} \sum_{k<n \leq r-1} \varphi_{P_{k+1}, P_{n+1}} + \frac{1}{2} \sum_{k=1}^{r-1} \varphi_{P_{k+1}, P_1}$$

[9] As f_1 is never exactly equal to f_2 (cf. Sec.III), in fact the inequality always applies.

[10] "Bethe ansatz"

[11] "unphysical"

$$-\frac{1}{2}\sum_{2<k\leq n}\varphi_{P_k,P_n}-\frac{1}{2}\sum_{2}^{r}\varphi_{P_1,P_k}$$

$$=Nf_{P_1}-\sum_{k=2}^{r}\varphi_{P_1P_k},$$

making use of $\varphi_{kn}=-\varphi_{nk}$. Since this relation holds for every P, it follows that

$$Nf_i=2\pi\lambda_i+\sum_{k\neq i}\varphi_{ik} \tag{29}$$

for all $i=1,\ldots,r$.

In complete analogy with Sec.III, one further can show that two f_i's can never coincide, otherwise all the coefficients vanish, and therefore for real f_i two succeeding λ_i's must differ by at least 2. The number of solutions with real f's is thus

$$\left(\begin{array}{c}N-r+1\\ r\end{array}\right),$$

far fewer than

$$\left(\begin{array}{c}N\\ r\end{array}\right),$$

the number of solutions we seek.

VI. COMPLEX SOLUTIONS

If $f_k=u_k+iv_k$ is a complex wave number, then it follows from

$$Nf_k=2\pi\lambda_k+\sum_{n\neq k}\varphi_{kn}$$

that at least one of the φ_{kn}'s has to have a very large imaginary part of $O(N)$. That means in first approximation (cf. Sec.IV)

$$2\cot\frac{\varphi_{kn}}{2}=\cot\frac{f_k}{2}-\cot\frac{f_n}{2}=-2i.$$

That is, there must be an f_n such that the real part of $\cot\frac{f_n}{2}$ must agree with that of $\cot\frac{f_k}{2}$, while their imaginary parts differ by 2 (to $O(e^{-N})$). One is led to the following solution, which we shall denote a *wavecomplex* [12]: n wave numbers are defined by the equations:

$$\cot\frac{f_\kappa}{2}=a-i\kappa;\kappa=-(n-1),-(n-3),\ldots,(n-3),(n-1) \tag{30}$$

in which a is a constant for all n wave numbers. Clearly,

$$\varphi_{\kappa,\kappa\pm2}=\psi-(\pm)i\infty$$

where the remaining φ's have finite imaginary parts. ψ remains undetermined. Applying (15) one obtains

$$\frac{\sin u_\kappa}{\cosh v_\kappa-\cos u_\kappa}=a,$$

$$\frac{\sinh v_\kappa}{\cosh v_\kappa-\cos u_\kappa}=\kappa,$$

for which the solutions are

$$u_\kappa=\tan^{-1}\frac{2a}{a^2+\kappa^2-1}=\cot^{-1}\frac{a}{\kappa+1}-\cot^{-1}\frac{a}{\kappa-1}, \tag{31}$$

$$\tanh v_\kappa=\frac{2\kappa}{a^2+\kappa^2+1},$$

$$e^{2v_\kappa}=\frac{(\kappa+1)^2+a^2}{(\kappa-1)^2+a^2}, \tag{32}$$

and $\sin u$ has therefore the sign of a.

We assert that a can be expressed using the total wave number of our wavecomplex,

$$k=\sum_{\kappa=-(n-1)}^{(n-1)}f_\kappa=\sum_{\kappa}u_\kappa \tag{33}$$

which, in simplest form, is

$$a=n\cot\frac{k}{2}. \tag{34}$$

For $n=1$ this is evident, for $n=2$ it follows by inserting the solution obtained earlier (Eq.(18), Sec.IV)

$$e^{-v}=\cos u, u=\frac{k}{2}\ \ (\text{or }\tfrac{k}{2}+\pi),$$

$$a=\frac{\sin u}{\cosh v-\cos u}=\frac{\sin u}{\frac{\frac{1}{\cos u}+\cos u}{2}-\cos u}$$

$$=2\cot u=2\cot\frac{k}{2}.$$

On the other hand, at fixed a, the wave numbers for a complex of n waves are exactly the same as for a complex

[12] a many-spin bound state, i.e., a "soliton"

of only $n-2$ waves, there are only two new wave numbers $u_{n-1} = u_{-(n-1)}$ to be added, so that

$$\frac{k_n}{2} = \frac{k_{n-2}}{2} + u_{n-1}. \qquad (33a)$$

Now taking (34) for $n-2$ as proven, then

$$\frac{k_n}{2} = \cot^{-1}\frac{a}{n-2} + \cot^{-1}\frac{a}{n} - \cot^{-1}\frac{a}{n-2} = \cot^{-1}\frac{a}{n}.$$

We further assert that our wavecomplex has eigenvalue

$$\varepsilon_n = \frac{1-\cos k}{n}. \qquad (35)$$

This is also evident for $n = 1$, and for $n = 2$ proved in (19). In general,

$$\varepsilon_n = \sum_{\kappa=-(n-1)}^{n-1} (1 - \cos(u_\kappa - iv_\kappa))$$

$$= \varepsilon_{n-2} + 2 - \cos(u_{n-1} + iv_{n-1}) - \cos(u_{n-1} - iv_{n-1})$$

$$= \varepsilon_{n-2} + 2(1 - \cos u_{n-1}\cosh v_{n-1})$$

$$= \varepsilon_{n-2} + 2\left(1 - \frac{[a^2+(n-1)^2-1][a^2+(n-1)^2+1]}{[a^2+(n-1)^2+1]^2 - 4(n-1)^2}\right)$$

$$= \varepsilon_{n-2} + 4\frac{a^2 - n(n-2)}{(a^2+n^2)(a^2+(n-2)^2)}$$

using (31), (32). We now assume (35) to be valid for $n-2$ and use (34), from which it follows that

$$\frac{\varepsilon_n}{2} = \frac{1}{(n-2)(1+\frac{a^2}{(n-2)^2})} + 2\frac{a^2-n(n-2)}{(a^2+n^2)(a^2+(n-2)^2)}$$

$$= \frac{(n-2)(a^2+n^2) + 2(a^2-n(n-2))}{(a^2+n^2)(a^2+(n-2)^2)}$$

$$= \frac{n}{a^2+n^2} = \frac{1-\cos k}{2n}$$

Finally, by analogy with Sec.IV, we establish the following: if the number of right-handed spins r and the total wave number k of all spin waves is given, then one obtains the smallest eigenvalue ε when one combines all r spin waves into a single wavecomplex of eigenvalue

$$\varepsilon_r = \frac{1-\cos k}{r}.$$

For if one has *two* wavecomplexes with n and $p = r-n$ waves, then

$$\varepsilon_{p+n} = \frac{1-\cos k_1}{n} + \frac{1-\cos(k-k_1)}{p}.$$

The minimum of this expression is at

$$\frac{\sin k_1}{n} = \frac{\sin(k-k_1)}{p},$$

$$\sin k_1 = \frac{n\sin k}{\sqrt{n^2+2np\cos k+p^2}},$$

and is

$$\varepsilon_{min} = \frac{n+p-\sqrt{n^2+2np\cos k+p^2}}{np}.$$

Certainly,

$$(n+p)\sqrt{n^2+2np\cos k+p^2} < (n+p)^2 - np(1-\cos k)$$

as immediately seen by squaring both sides. From this it follows directly that

$$\varepsilon_r < \varepsilon_{min}. \qquad (36)$$

If the spin waves are composed of more than two wavecomplexes, naturally ε is still larger. The state of lowest energy for r right-handed spins is then, for $J > 0$ (ferromagnetic case), a single wavecomplex of r spins; or, if $J < 0$ (the more usual case), r individual waves with real wave numbers. In the latter instance, of course, the lowest energy state has not yet been fixed by this expedient.

It is easy to compute the second approximation for the wave numbers in a wavecomplex, by using the u and v of formulas (31), (32), altering them slightly in order to satisfy the actual periodic boundary conditions (29). The solution proceeds analogously to Sec.IV; one finds that in general for finite k one solution in the immediate vicinity of (31), (32) is allowed, while for small k of $O(\frac{1}{\sqrt{N}})$, the nature of the solution changes if $\frac{Nk}{2\pi} = \lambda$ is indivisible by n. Instead of a complex of three spin waves there would occur, for example, a pair of conjugate complex waves as were already analyzed in Sec.IV for even λ, together with a single wave of almost the same, but real, wave number. The number of solutions is unaffected by this change of appearance. There is one solution for $\lambda = 0, 1, 2, \ldots, N-n$; the last value corresponds to $\lambda_{-(n-1)} = \lambda_{-(n-3)} = \cdots = \lambda_{n-1} = N-1$. For $\lambda > N-n$, one or more λ_κ would $= N$, which is not allowed.

From now on we shall also exclude $\lambda_i = 0$ in general. We immediately gain in symmetry from this, and automatically distinguish those solutions for which the left-handed component of total spin $M = \frac{N}{2} - r = S_{tot}$, the total spin, from all those others with the same value of M which belong to a higher value of S_{tot}. The latter are just those states in which one or more of the r wave numbers are zero. After eliminating them, there remain only $N-2n+1$ wavecomplex solutions of n spin waves: $\lambda = n, n+1, \ldots, N-n$.

VII. THE NUMBER OF SOLUTIONS

We assume that *two* complexes of $p\ (>n)$ spin waves are available, and ask about the number of solutions that can be obtained by means of the ansatz. This leads us to discuss the phases φ. If the wave numbers in the first complex are given by

$$\cot\frac{f_\kappa}{2}=a-i\kappa,\quad \kappa=-(n-1),(n-3),\ldots,n-1$$

$$a=n\cot\frac{k_1}{2},\quad k_1=\sum_\kappa f_\kappa \tag{37a}$$

and in the second by

$$\cot\frac{f_\mu}{2}=b-i\mu,\quad \mu=-(p-1),(p-3),\ldots,p-1$$

$$b=p\cot\frac{k_2}{2},\quad k_2=\sum_\mu f_\mu \tag{37b}$$

then by (28), (29), (31)

$$Nk_1=2\pi\lambda_1+\sum_\kappa\sum_\mu\varphi_{\kappa\mu},$$

$$Nk_2=2\pi\lambda_2-\sum_\kappa\sum_\mu\varphi_{\kappa\mu},$$

$$\cot\frac{\varphi_{\kappa\mu}}{2}=\cot\left(\frac{\psi_{\kappa\mu}}{2}+i\frac{\chi_{\kappa\mu}}{2}\right)=\frac{a-b}{2}-i\frac{\kappa-\mu}{2},$$

$$\tan\psi_{\kappa\mu}=\frac{a-b}{(\frac{a-b}{2})^2+(\frac{\kappa-\mu}{2})^2-1}. \tag{38}$$

The sign of $\psi_{\kappa\mu}=$ sign of $a-b$, and $\sum_\kappa\sum_\mu\chi_{\kappa\mu}=0$, because the f_κ and f_μ come in ordered complex conjugate pairs.

The $\psi_{\kappa\mu}$ are zero if k_1 is very small, a very large, and then with increasing k_1 they become positive as long as $a>b$. We are interested most of all in their for the case where a approaches b very closely and ultimately becomes smaller than b, in order to determine the number of forbidden integers λ_1, λ_2. For this we fix [13] $\lambda_0=\frac{Nk_2}{2\pi}$ and define λ' through

$$n\cot\frac{\pi\lambda'}{N}>p\cot\frac{\pi\lambda_0}{N}>n\cot\frac{\pi(\lambda'+1)}{N}. \tag{39}$$

For $Nk_1=2\pi\lambda'$, $a-b$ will be evidently be positive and small, of $O(\frac{1}{N})$. Then, $\psi_{\kappa\mu}$ is small and positive if $|\kappa-\mu|>2$; small and negative if $|\kappa-\mu|<2$ and very large and positive if $|\kappa-\mu|\approx 2$.

The last is a consequence of the κ and μ differing from integers only by quantities $O(e^{-N})\ll\frac{1}{N^2}$ (cf. Sec.IV), such that $(\frac{\kappa-\mu}{2})^2-1\ll(a-b)^2$ as soon as $|\kappa-\mu|$ lies in the vicinity of 2. Up to quantities $O(\frac{1}{N})$:

$$\psi_{\kappa\mu}=\begin{cases}0 & \text{for } |\kappa-\mu|>2\\ \pi & \text{for } |\kappa-\mu|<2\\ \frac{\pi}{2} & \text{for } |\kappa-\mu|=2\end{cases} \tag{40}$$

Next, assume $p-n$ is *odd*. Then for a given κ there are just two values $\mu=\kappa+1$ and $\mu=\kappa-1$ for which $\psi_{\kappa\mu}$ does not vanish, but has the value π. This yields

$$\sum_\kappa\sum_\mu\psi_{\kappa\mu}=2\pi n. \tag{41}$$

$p-n$ is *even*. For each κ there are 3 μ's for which $\psi_{\kappa\mu}\neq 0$:

$$\mu=\kappa,\psi_{\kappa\mu}=\pi,$$
$$\mu=\kappa+2,\psi_{\kappa\mu}=\tfrac{\pi}{2},$$
$$\mu=\kappa-2,\psi_{\kappa\mu}=\tfrac{\pi}{2}.$$

Together, this yields once again

$$\sum_\kappa\sum_\mu\psi_{\kappa\mu}=2\pi n.$$

So,

$$\lambda_1=\frac{Nk_1}{2\pi}-n=\lambda'-n,\lambda_2=\lambda_0+n. \tag{42a}$$

Corresponding for $Nk_1=2\pi(\lambda'+1)$:

$$\sum_\kappa\sum_\mu\psi_{\kappa\mu}=-2\pi n,$$

$$\lambda_1=\lambda'+1+n,\lambda_2=\lambda_0-n. \tag{42b}$$

Thus λ_1 ranges over the values,

$$\lambda_1=n,n+1,\ldots,\lambda'-n,\lambda'+n+1,\ldots,N-n. \tag{42c}$$

The $2n$ values $\lambda'-n+1,\ldots,\lambda'+n$ are forbidden by the presence of the other spin complexes. Thus, we see that if λ_0 is small, then in general $b>a$, thus $\lambda_2=\lambda_0-n$. However, λ_2 must be at least equal to p (see end of preceding paragraph) and therefore, $\lambda_0\geq p+n$. Likewise

[13] We shall see later that for $a\approx b$, k_1 and k_2 in fact have the form $\frac{2\pi}{N}\times$ integer, and that therefore $\lambda_0=$ integer.

$\lambda_0 \leq N - p - n$, from which it follows that if the other spin complex were not present. It is important in both cases that n be the number of waves of the *smaller* of the two spin complexes. The total number of solutions is, then,

$$(N - 2n - 2p + 1)(N - 4n + 1).$$

The case $n = p$ remains to be investigated. Here for $\kappa = n - 1$, the single partner, $\mu = \kappa + 2$, which earlier gave $\psi_{\kappa\mu} = \frac{\pi}{2}$, is missing, and for $\kappa = -(n-1)$, the partner $\mu = \kappa - 2$ is missing, so now

$$\sum_\kappa \sum_\mu \psi_{\kappa\mu} = (2n-1)\pi. \tag{43}$$

In addition, there is now a λ', so that $n \cot \frac{\pi\lambda'}{N} = p \cot \frac{\pi\lambda_0}{N}$ and, simply, $\lambda' = \lambda_0$. But this does not lead to a solution because whenever $f_k = f_\mu$, $\kappa = \mu$, and the eigenfunction has already been seen to vanish if two wave numbers are equal. That is, k_1 is at most

$$Nk_1 = 2\pi(\lambda_0 - 1),$$

which yields

$$\lambda_1 = \lambda_0 - \frac{1}{2} - n, \lambda_2 = \lambda_0 - \frac{1}{2} + n;$$

just as, for $Nk_1 = 2\pi(\lambda_0 + 1)$,

$$\sum_\kappa \sum_\mu \psi_{\kappa\mu} = -(2n-1)\pi,$$

$$\lambda_1 = \lambda_0 + \frac{1}{2} + n, \lambda_2 = \lambda_0 + \frac{1}{2} - n.$$

λ_0 is therefore, obviously, a half integer. Over the range of λ_1, once again $2n$ numbers are missing: $\lambda_0 - n + \frac{1}{2}, \ldots, \lambda_0 + n - \frac{1}{2}$, but only $2n-1$ in the range of λ_0, so λ_0 must equal or exceed $2n - \frac{1}{2}$ ($\lambda_2 = n$), while it is at most equal to $N - 2n + \frac{1}{2}$ ($\lambda_2 = N - 3n + 1$), that is, λ_0 possesses $N - 4n + 2$ values instead of the $N - 2n + 1$ which are allowed when only a single complex of n waves is present. As interchange of λ_1 and λ_2 does not affect the solution, the total number of solutions is

$$\frac{1}{2}(N - 4n + 2)(N - 4n + 1).$$

The situation will perhaps become clearer if, for the moment, we normalized the ψ differently. Let ψ' be defined such that, for very large a it coincides with a, but for $a = b$ it remains constant. Then (in the case of two complexes with n waves,) $\sum_\kappa \sum_\mu \psi'_{\kappa\mu}$ grows from zero to $(2n-1)2\pi$, while k_1, with k_2 fixed, goes from $\frac{2\pi n}{N}$ to $\frac{2\pi(N-n)}{N}$. If

$$2\pi\lambda'_1 = Nk_1 - \sum_\kappa \sum_\mu \psi'_{\kappa\mu},$$

then λ'_1 clearly takes on all values from n to $N - 3n + 1$, that is $N - 4n + 2$ values; this also applies to λ_2, with the one restriction, a prohibition against the value which corresponds to $k_2 = k_1$.

Now, in general we assume q_n complexes each with n waves, that is q_1 single waves with real wave numbers, q_2 pairs with complex conjugate wave numbers, and so on. The constant λ_1 of the first of the n wave complexes could assume any of the values $n, n+1, \ldots, N-n$, i.e. take on $N - 2n + 1$ possible values if there were no other wave-complex present. For each complex with $p > n$ waves, $2n$ numbers are lost, as we have seen; for each complex of $p < n$, only $2p$; finally, for each of the remaining $q_n - 1$ complexes with n waves, $2n - 1$ numbers. Thus, these are

$$Q'_n = N - 2n + 1 - 2\sum_{p<n} pq_p - 2\sum_{p>n} nq_p - (2n-1)(q_n - 1)$$

remaining values all allowed for λ_1. The constant λ_2 of the second complex of n waves may not allow k_2 to coincide with k_1, that is, it has one fewer possibilities; finally, the constant λ_{q_n} of the last complex of n waves can take on only

$$Q'_n - (q_n - 1) = Q_n + 1$$

distinct values, where

$$Q_n(N, q_1, q_2, \ldots) = N - 2\sum_{p<n} pq_p - 2\sum_{p\geq n} nq_p. \tag{44}$$

Finally, considering that interchange of the λ's of the various wavecomplexes with equal numbers of waves n does not lead to new solutions, one finds for the total number of solutions

$$Z(N, q_1, q_2, \ldots) = \prod_{n=1}^{\infty} \frac{(Q_n + q_n) \cdots (Q_n + 1)}{q_n!}$$

$$= \prod_n \binom{Q_n + q_n}{q_n} \tag{45}$$

where the Q_n are defined by (44).

VIII. IMPORTANT IDENTITY

We shall prove now that we have obtained the correct number of solutions. It is known that the number of eigenvalues $Z(N,r)$ for a fixed value of total spin $S_{tot} = \frac{N}{2} - r$ equals the number of eigenvalues

with $M = S_{tot}$ left-handed spins, less the number for $M = S_{tot} + 1$, i.e. [1]

$$Z(N,r) = \begin{pmatrix} N \\ r \end{pmatrix} - \begin{pmatrix} N \\ r-1 \end{pmatrix} = \frac{N-2r+1}{N-r+1} \begin{pmatrix} N \\ r \end{pmatrix}. \tag{46}$$

The following must also hold true

$$\sum_{q_1,q_2,\cdots} Z(N,q_1,q_2,\ldots) = Z(N,r) \tag{47}$$

the sums being over all values spanned by $q_1, q_2, \ldots$ for which the total number of spin waves equals r, that is

$$q_1 + 2q_2 + 3q_3 + \cdots = \sum_n n q_n = r.$$

In other words, one sums over all the "partitions" of r; q_n gives the number of times the summand n appears in the particular partition.

We introduce the *total index* of the spin complex

$$q = \sum_n q_n \tag{48}$$

and rewrite (44) as

$$Q_n(N,q_1,q_2,\ldots) = N - 2q - 2\sum_{p<n}(p-1)q_p - 2\sum_{p\geq n}(n-1)q_p$$

$$= Q_{n-1}(N-2q, q_2, q_3, \ldots). \tag{49}$$

Especially,

$$Q_1(N,q_1,q_2,\ldots) = N - 2q. \tag{49a}$$

By E.(45),

$$Z(N,q_1,q_2,\ldots) = \begin{pmatrix} N-2q+q_1 \\ q_1 \end{pmatrix} Z(N-2q, q_2, q_3, \ldots). \tag{50}$$

On the right, next to the binomial coefficient, is the number of allowed solutions with q_2 single spin waves, and generally, q_n complexes each with $n-1$ waves in a chain of $N-2q$ sites. This corresponds to a total of

$$r' = \sum_n q_n(n-1) = r - q \tag{50a}$$

right-handed spins arranged in

$$q' = \sum_{n\geq 2} q_n = q - q_1 \tag{50b}$$

wavecomplexes.

Now we introduce the number of all these solutions, for which r right-handed spins are arranged in precisely q wavecomplexes, without distinguishing how many waves each individual complex contains

$$Z(N,r,q) = \sum_{\substack{q_1+q_2+q_3+\cdots = q \\ q_1+2q_2+3q_3+\cdots = r}} Z(N,q_1,q_2,\ldots) \tag{51}$$

It follows then from (50), (50a), (50b) that

$$Z(N,r,q) = \sum_{q_1=0}^{q-1} \begin{pmatrix} N-2q+q_1 \\ q_1 \end{pmatrix} Z(N-2q, r-q, q-q_1) \tag{52}$$

and

$$Z(N,r) = \sum_{q=0}^{r} Z(N,r,q). \tag{53}$$

From here on we treat the problem by complete induction. We assume

$$Z(N,r,q) = \frac{N-2r+1}{N-r+1} \begin{pmatrix} N-r+1 \\ q \end{pmatrix} \begin{pmatrix} r-1 \\ q-1 \end{pmatrix}. \tag{54}$$

For $q = 1$ this is certainly correct– we have a single complex of r waves whose wave numbers can take on $N-2r+1$ values. Likewise, (54) is correct for $q = r$; then $q_1 = r$ and $q_n = 0$ for $n > 1$ inserted into (45) transforms it into (54). Let us take (54) as proven for $N-2q$, $r-q$, $q-q_1$ and by (52) have

$$Z(N,r,q) = \sum_{q_1=0}^{q-1} \begin{pmatrix} N-2q+q_1 \\ q_1 \end{pmatrix} \begin{pmatrix} N-r-q+1 \\ q-q_1 \end{pmatrix}$$

$$\times \begin{pmatrix} r-q-1 \\ q-q_1-1 \end{pmatrix} \frac{N-2r+1}{N-r-q+1}.$$

Then,

$$\begin{pmatrix} N-2q+q_1 \\ q_1 \end{pmatrix} = \sum_{s=0}^{q_1} \begin{pmatrix} r-1 \\ s \end{pmatrix} \begin{pmatrix} N-2q+q_1+1-r \\ q_1-s \end{pmatrix},$$

$$Z(N,r,q) = \sum_{q_1=0}^{q-1} \sum_{s=0}^{q_1} \frac{(N-r-q+1)!}{(q-q_1)!(N-r-2q+q_1+1)!}$$

$$\times \frac{(N-r-2q+q_1+1)!}{(q_1-s)!(N-r-2q+s+1)!} \frac{N-2r+1}{N-r-q+1}$$

$$\times \begin{pmatrix} r-1 \\ s \end{pmatrix} \begin{pmatrix} r-q-1 \\ q-q_1+1 \end{pmatrix}$$

$$= \frac{N-2r+1}{N-r-q+1} \sum_{s=0}^{q-1} \begin{pmatrix} r-1 \\ s \end{pmatrix} \begin{pmatrix} N-r-q+1 \\ q-s \end{pmatrix}$$

$$\times \sum_{q_1=s}^{q-1} \binom{q-s}{q_1-s} \binom{r-q-1}{q-q_1-1}$$

$$= \frac{N-2r+1}{N-r-q+1} \sum_s \binom{N-r-q+1}{q-s}$$

$$\times \frac{(r-1)!}{s!(r-s-1)!} \frac{(r-s-1)!}{(q-s-1)!(r-q)!}$$

$$= \frac{N-2r+1}{N-r-q+1} \binom{r-1}{q-1} \sum_s \binom{q-1}{s} \binom{N-r-q+1}{q-s}$$

$$= \frac{N-2r+1}{N-r-q+1} \binom{r-1}{q-1} \binom{N-r}{q}$$

identical with (54). Since (54) holds for $q = 1$ and for $q = 2$, $r = 3$ and 4, then for $q = 2$ and $r = 3, 4$, then for $q = 2$ and greater values of r, and finally for $q = 3, 4$, etc. Inserting (54) in (53) yields

$$Z(N,r) = \frac{N-2r+1}{N-r+1} \sum_{q=1}^{r} \binom{N-r+1}{q} \binom{r-1}{r-q}$$

$$= \frac{N-2r+1}{N-r+1} \binom{N}{r}$$

in agreement with the number of solutions which we were seeking, Eq.(46). *Therefore, our method yields all the solutions of this problem.*

In a future paper, this method will be extended to space [14] lattices, and its physical implications for cohesion, ferromagnetism and electrical conductivity, will be derived. [15]

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[2] J. C. Slater, Phys. Rev. **35** 509 (1930).
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[14] three-dimensional
[15] This rash promise has apparently not been kept.