

PERTURBATION THEORY FOR THE SPIN $\frac{1}{2}$ HEISENBERG FERROMAGNET

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The analogue to the Wick theorem for Pauli operators is given and by summation of the simplest diagrams the energy of a spin wave excitation is obtained.

There are two different schemes to get an approximate expression for a Green function: 1) One writes down the equation of motion for the Green function under consideration and breaks off the chain of equations by a certain decoupling procedure for the higher Green functions [1]. This decoupling is a methodically necessary step but physically not well understood. 2) One applies quantum field theoretic perturbation theory [2]. In problems of the theory of magnetism the perturbation theory has to overcome the difficulties arising from the peculiar commutation relations of the spin operators. There have been done different perturbation theoretic approaches to the problem of magnetic impurities in metals [3, 4] for arbitrary values of spin.

We intend to develop a perturbation theory for spin $\frac{1}{2}$ only with the hope to find a rather simple structure of it. The essential point is the proof of the Wick theorem for Pauli operators. There have been several papers on this subject. Mills et al. [5] and Wang et al. [6] interpret the Pauli operators as Bose operators when acting at different lattice sites and as Fermi operators when acting at the same lattice site. Taking into account the properties of the unperturbed states they can formulate the Wick theorem in the usual form. If we accept this point of view, defining the free Green function as in the Fermi case, then we do not get a physically acceptable spin wave energy from the summation of the simplest diagrams and we cannot find corrections which make the result better. Tyablikov and Moskalev-

ko [7] have given complicated expressions for an analogue to the Wick theorem for Pauli operators. These authors do not use all the algebraic properties of the Pauli operators and do not refer to traces over special states. We want to write down the analogue to the Wick theorem adequate to the perturbation theory for the Heisenberg ferromagnet with the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where $\mathcal{H}_0 = \epsilon_0 \sum_f b_f^\dagger b_f$ ($\epsilon_0 = J(0) + mH$) and

$$\mathcal{H}_1 = -\sum_{f,g} J_{fg} b_f^\dagger b_g - \sum_{f,g} J_{fg} b_f^\dagger b_f b_g^\dagger b_g. \quad (1)$$

J_{fg} is the exchange integral, no intra-atomic exchange is present: $J_{ff} = 0$; $J(0) = \sum_g J_{fg}$, f, g

labelling the lattice sites. The Pauli operators obey the commutation relations $[b_g, b_f^\dagger] = \delta_{fg}(1 - 2b_f^\dagger b_f)$. We wish to calculate the two-point Green function in the Matsubara formalism [2]

$$G_{lm}(\tau_l - \tau_m) = - \langle T_\tau (b_l(\tau_l) b_m^\dagger(\tau_m)) S \rangle_0 / \langle S \rangle_0 \quad (2)$$

where S is the S -operator (T_τ is the exponential of the integral over $-\mathcal{H}_1$ from 0 to $1/T$).

The brackets mean the trace over the eigenstates of \mathcal{H}_0 , the density operator ρ_0 contains \mathcal{H}_0 . T_τ stands for the usual T -product with respect to τ . We look at the Pauli operators as at Bose operators with q -number commutation relations. Expanding the S -operator we get a series for the Green function (2) containing traces of more and more Pauli operators.

Using the identity [1]

$$[a_1, a_2 \dots a_n] = [a_1 a_2] a_3 \dots a_n + \dots + a_2 \dots a_{n-1} [a_1, a_n] \quad (3)$$

and the relation $a \rho_0 = \rho_0 a \gamma$, $\gamma = \exp\{\pm(\epsilon_0 - \mu)/T\}$ (upper sign, if a is a creation operator, lower sign, if a is an annihilation operator) we obtain

$$\langle a_1 \dots a_n \rangle_0 = (1-\gamma)^{-1} (\langle [a_1, a_2] a_3 \dots a_n \rangle_0 + \dots). \quad (4)$$

Here we cannot put the commutators outside the brackets, because they are q -numbers. This fact is an expression of the so-called "kinematic interaction". As an example we write down the zeroth order Green function. In the case $\tau_l > \tau_m$ we have

$$G_{lm}^0(\tau_l - \tau_m) = - (1-\gamma)^{-1} \sigma_0 \delta_{lm} \exp\{-(\tau_l - \tau_m)(\epsilon_0 - \mu)\}, \quad (5)$$

where $\sigma_0 = \langle 1 - 2b_f^\dagger b_f \rangle_0 = 1 - 2\bar{n}_0$ is the mean magnetization per lattice site. Comparing with $G_{lm}^0 = -(1-\bar{n}_0) \exp\{-(\tau_l - \tau_m)(\epsilon_0 - \mu)\}$ we find the Fermi distribution function for \bar{n}_0 . The Fourier transform $G_{lm}^0(\omega)$ is the one of Bose operators with an additional factor σ_0 . Computing the traces over products of more than two Pauli operators we take into account that the traces over an odd number of operators vanish. In this way we can reduce all the traces appearing in the perturbation series to products of free Green functions G_{lm}^0 and after that we may introduce diagrams for the terms in the series. The simplest diagrams are the usual ones.

$$\text{---}, \text{---} \rightarrow \text{---} \text{---} \text{---}, \text{---} \text{---} \text{---} \text{---}, \text{---} \text{---} \text{---} \text{---} \text{---}, \dots \quad (6)$$

The point indicates the 2-interaction (first term in eq. (1)), the square stands for the 4-interaction (second term in eq. (1)). Summing all the diagrams indicated in (6) we find the energy of a spin wave excitation $\epsilon(\mathbf{k}) = mH + \sigma_0 \times [J(0) - J(\mathbf{k})]$. This expression differs from that one obtained by the "equation of motion" in the RPA decoupling by the fact, that the trace for σ_0 is taken with respect to the free Hamiltonian instead of the full Hamiltonian. So we do not get terms proportional to T^3 , T^4 etc. in the magnetization. We could obtain the result of the "equation of motion method" for the magnetization [1] requiring self-consistency of the equation determining σ at an intermediate step of the calculations. Higher order contributions to the mass operator will give corrections to the above expression for the spin wave energy and will alter the "renormalization factor". Work about that is in progress. The perturbation parameter will be \bar{n}_0 , the number of flipped spins.

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