Long Range Dynamics Related to Magnetic Impurity in the 2D Heisenberg Antiferromagnet

O.P. Sushkov
Max-Planck-Institute für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany and School of Physics, University of New South Wales, Sydney 2052, Australia.

We consider a magnetic impurity in the two-dimensional Heisenberg antiferromagnet with long range antiferromagnetic order. At low temperature the impurity magnetic susceptibility has a Curie term ($\propto 1/T$) and a logarithmic correction ($\propto \ln(T)$). We calculate the correction and derive related Ward identity for the impurity-spin-wave vertex.

PACS numbers: 75.10.Jm, 75.30.Ds, 75.30.Hx

I. INTRODUCTION

The problem of magnetic impurities interacting with a system of strongly correlated electrons has attracted much interest recently, mainly due to the experimental discoveries of the high-$T_c$ superconductors and new heavy fermion compounds. In the field of the high-$T_c$ materials, the parent compounds are known to be two-dimensional (2D) antiferromagnetic (AFM) Mott-Hubbard insulators based on CuO$_2$ planes which are driven to a superconducting state by doping (e.g. with holes). Even though the holes can hop, thus destroying the AFM long-range order and causing the development of superconducting pairing, the extreme limit of static holes also has a physical relevance. Systems with static holes have been also realized experimentally in cuprates.

Several theoretical studies have addressed isolated static holes and added spins in 2D Heisenberg antiferromagnets with long range AFM order. A singular logarithmic frequency behavior of the perpendicular magnetic susceptibility at zero temperature has been found in Ref., see also a discussion in Ref. A very interesting problem is a magnetic impurity in 2D Heisenberg antiferromagnet at O(3) quantum critical point. However, this problem is out of the scope of the present paper. The low temperature behavior of the impurity static magnetic susceptibility in a gapped system is trivial, it obeys the simple Curie law, $\delta \chi = \Omega(\Omega+1)/3T$, where $\Omega$ is the impurity spin. However, for 2D systems which possess the long range AFM order at zero temperature, the excitation spectrum is gapless due to Goldstone spin waves and the Curie law is not obvious. A very interesting prediction for such a regime is the classical Curie law, $\delta \chi = \Omega^2/3T$. The behaviour is classical because of alignment of the impurity moment with the local Neel order. This behaviour has been recently confirmed in Monte Carlo simulations for 2D $S = 1/2$ Heisenberg antiferromagnetic clusters with magnetic impurity. Moreover, in these simulations a logarithmic correction, $\propto \ln(T)$, to the classical Curie low has been found. Both the classical Curie low and the logarithmic correction are related to the nontrivial long-range dynamics in the system. In the present work we calculate the logarithmic correction using two different methods, a) Spin-wave perturbation theory, b) Semiclassical non-linear $\sigma$-model. In the leading $1/S$ approximation both methods give the same result. However the results must be identical in all orders in $1/S$ and hence the comparison allows us to derive the Ward identity for the impurity-spin-wave vertex. Value of the logarithmic correction to the magnetic susceptibility is in agreement with Ref.

A crossover from quantum to classical Curie low for a finite AFM cluster with impurity is discussed in Section II. In Section III we derive the impurity susceptibility using the spin-wave perturbation theory, and in Section IV we obtain the same result using the semiclassical non-linear $\sigma$-model and derive the Ward identity.

II. CURIE TERM

The Hamiltonian of the system under consideration is

$$
H = H_0 + H_{\text{int}} + H_B,
$$

$$
H_0 = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,
$$

$$
H_{\text{int}} = J_{\perp} S_0 \cdot \Omega,
$$

$$
H_B = -B \cdot \left( \Omega + \sum_i \mathbf{S}_i \right)
$$

(1)
where $S_i$ is spin 1/2 at the site $i$ of square lattice with antiferromagnetic interaction ($J > 0$), $\Omega$ is the impurity spin coupled to the lattice spin at site 0, and $B$ is magnetic field. To be specific we will assume that $J_x > 0$, but all results are in the end independent of sign of $J_x$. Consider an $L \times L$ cluster ($L \gg 1$ is even) described by the Hamiltonian $H_0$, so no impurities for the beginning. Energy spectrum of the system is known very well\textsuperscript{15,16,17}. Spin of the ground state is 0, and lowest excitations are described by rotational spectrum of the solid top (diatomic molecule with zero projection of spin on axis of the molecule. $K = 0$)

$$E_J = \frac{J(J + 1)}{2I},$$

(2)

where $J = 0, 1, 2...$ is spin of the state ($J = 0$ corresponds to the ground state), $I = L^2\chi_\perp$ is moment of inertia of the top, and $\chi_\perp \approx 0.066/J$ is perpendicular magnetic susceptibility\textsuperscript{18,19}. The spectrum (2) is valid as soon as the rotation is solid, i.e. degrees of freedom of the top are not excited. The first internal excitation is the spin wave with wave length $\lambda = L$ (periodic boundary condition). Energy of this excitation is

$$\Delta_{sw} = 2\pi c/L, \quad c \approx \sqrt{2}J.$$

(3)

There are 8 degenerate spin-wave excitations: $S_z = \pm 1$, $x$ and $y$ directions, and two excitations (cos and sin) in each direction. If we consider $T \ll \Delta_{sw}$ then only rotations are\textsuperscript{(2)} important. A more accurate criterion for solid rotation is: $8 \exp(-\Delta_{sw}/T) \ll 1$, i.e.

$$T \ll T_{sw} \approx \frac{\Delta_{sw}}{\ln(8)}.$$

(4)

In this temperature regime magnetic susceptibility of the cluster is determined by the spectrum (2).

$$\chi_0 = \frac{\partial}{\partial B} \sum_{J,J',s} \frac{J_s e^{-E_s/J_s B}}{E_s} = \frac{1}{3T} \left( \frac{\sum_J (J + 1/2)^3 e^{-((J + 1/2)^2 / 4T^2)} - 1}{\sum_J (J + 1/2)^2 e^{-((J + 1/2)^2 / 4T^2)} - 1} \right),$$

(5)

where summation over $J$ is performed from 0 to $\infty$. If $T \ll T_{rot} = 1/I$ the susceptibility is zero, and if $T_{rot} \ll T \ll T_{sw}$ the evaluation of (5) gives

$$\chi_0 = \frac{1}{3T} \left( 2IT - \frac{1}{3} + \frac{1}{18IT} + ... \right) = \frac{2}{3} L^2 \chi_\perp - \frac{1}{9T} \left( 1 - \frac{T_{rot}}{6T} + ... \right).$$

(6)

The expansion is in integer powers of $T_{rot}/T$.

Now let us put an impurity with spin $\Omega$ which interacts with cluster via $H_{int}$, see Eq. (1). Excitation spectrum of the cluster with impurity is slightly different from (2). Now this is a symmetric top with spin projection on axis of the top $K = \Omega$. This is like a diatomic molecule with uncompensated electron spin and strong spin-axis interaction. Rotational spectrum of such top is\textsuperscript{20}

$$E_J = \frac{J(J + 1) - 2\Omega^2 + <\Omega^2>}{2I},$$

(7)

where $J = \Omega, \Omega + 1, \Omega + 2,...$ is total spin of the cluster, and $<\Omega^2>$ is the average value of $\Omega^2$ in the intrinsic reference frame. Similar to the previous case the spin waves are not excited as soon as the inequality (4) is valid. One can easily check that in this case the magnetic susceptibility of the cluster $\chi_1$ is given by the same Eq. (5), the only difference is that summation over $J$ is performed not from 0 to $\infty$, but from $\Omega$ to $\infty$. If $T \ll T_{rot}$ the cluster susceptibility is $\chi_1 = \Omega(\Omega + 1)/3T$. If $T_{rot} \ll T \ll T_{sw}$ evaluation of (5) gives

$$\chi_1 = \frac{1}{3T} \left( 2IT - \frac{1}{3} + \frac{1 + 3\Omega^2}{18IT} + ... \right) = \frac{2}{3} L^2 \chi_\perp - \frac{1 - 3\Omega^2}{9T} + \frac{1 + 3\Omega^2}{18IT^2} + ...$$

(8)

Hence the impurity susceptibility defined as $\chi_1 - \chi_0$ reads

$$\chi_{imp} = \chi_1 - \chi_0 = \frac{\Omega^2}{3T} \left( 1 + \frac{T_{rot}}{2T} + ... \right)$$

(9)

The expansion goes in integer powers of $T_{rot}/T$. The leading term in (9) agrees with\textsuperscript{18,19}

It is interesting to note that if there are $n$ impurities with spin $\Omega$ on the same sublattice than in Eq. (9) one shall replace $\Omega \rightarrow n\Omega$. The impurities are not independent because the cluster is rigid. In the thermodynamic limit it means that all the impurities within the correlation length are not independent.
III. LOGARITHMIC CORRECTION TO SUSCEPTIBILITY, THE SPIN-WAVE DERIVATION

The above consideration is valid for the case when the inequality (4) is valid and hence there are no real spin-wave excitations. However virtual spin-wave excitations are always there. In the intrinsic reference frame the cluster looks like picture in Fig.1

![FIG. 1: Schematic picture of an AFM cluster with impurity](attachment:image)

The interaction Hamiltonian $H_{int}$, Eq. (1), can be rewritten in terms of spin-wave operators $a$ and $b$ (for review of the spin-wave theory see, e.g. Ref.1)

$$H_{int} = J_\perp \mathbf{S}_0 \rightarrow \frac{1}{2} J_\perp (\Omega_+ S_{0-} + \Omega_- S_{0+}) = \frac{1}{2} J_\perp \left( \Omega_+ b_0 + \Omega_- b_0^\dagger \right)$$

$$= \frac{1}{2} J_\perp \sqrt{\frac{2}{L^2}} \sum_q (\Omega_+ b_q + \Omega_- b_q^\dagger) = \frac{1}{2 \sqrt{2L^2}} J_\perp \sum_q \left( \Omega_+ [u_q \beta_q + v_q \alpha_{-q}^\dagger] + \Omega_- [u_q \beta_q^\dagger + v_q \alpha_{-q}] \right)$$

$$\rightarrow \frac{1}{\sqrt{2L^2}} J_\perp \sum_q Z_\Gamma \left( \Omega_+ [u_q \beta_q + v_q \alpha_{-q}^\dagger] + \Omega_- [u_q \beta_q^\dagger + v_q \alpha_{-q}] \right) . \quad (10)$$

Here $\beta_q^\dagger$ and $\alpha_{-q}^\dagger$ are creation operators for spin waves with spin projection $S_z = \pm 1$ respectively, $u_q$ and $v_q$ are Bogoliubov parameters,

$$u_q^2 = \frac{J}{\omega_q^{(0)}} + \frac{1}{2}, \quad v_q^2 = \frac{J}{\omega_q^{(0)}} - \frac{1}{2} , \quad (11)$$

and $\omega_q^{(0)} = 2J \sqrt{1 - \gamma_q^2} \rightarrow \sqrt{2}Jq$ is the spin wave dispersion in the leading $1/S$ approximation. In (10) we assume that $S = 1/2$. In Eq. (10) the impurity-spin-wave vertex is derived in the leading $1/S$ approximation. However, at the last step we have introduced the vertex renormalization factor $Z_\Gamma$ that takes into account all higher $1/S$ corrections to the vertex. Generally speaking $Z_\Gamma$ depends on $q$, but here we consider only the small $q$ limit, $Z_\Gamma = Z_\Gamma(q = 0)$.

To use perturbation theory we will assume that $J_\perp \ll J$. One loop correction to the impurity energy is given by diagram in Fig.2. The diagram is infrared convergent because it contains the denominator, $\Delta \epsilon = \epsilon_\uparrow - \epsilon_\downarrow = J_\perp < S_z >$,
reads
\[ \delta \epsilon_0 = -\frac{(B/2)^2}{\Delta \epsilon} . \] (13)

The contribution is finite because \( \Delta \epsilon \) is finite. Now let us look at one loop corrections to \( \delta \epsilon_0 \) shown in Fig.4. These corrections are infrared divergent because they contain the energy denominator without spin flip, \( \epsilon_\uparrow - \epsilon_\uparrow \). Using usual Schrödinger perturbation theory one finds the corresponding energy correction
\[ \delta \epsilon_1 = -\left( \frac{\sqrt{2} \Omega}{N} \right) \frac{J^2 \Omega^2}{(\Delta \epsilon)^2} \sum_q \frac{u_q^2 + v_q^2}{\omega_q} \left( \frac{\sqrt{2} \Omega}{\sqrt{2} \Omega} \frac{u_q}{(\Delta \epsilon + \omega_q)^2 \omega_q} + \frac{\sqrt{2} \Omega}{\sqrt{2} \Omega} \frac{v_q}{(\Delta \epsilon)^2 \omega_q} \right) . \] (14)

Here \( \omega_q \rightarrow cq = Z_c \sqrt{2} J q \), where \( Z_c \approx 1.17 \) is the spin-wave velocity renormalization due to higher \( 1/S \) corrections.\(^{1,18,19}\) Keeping only divergent terms we find from (14) the following expression for the susceptibility
\[ \delta \chi_\perp = \frac{J^2 \Omega^2}{Z_c^2} \frac{Z_c^2 \Omega^2}{2 \pi Z_c J < S_z >^2} \int \frac{d^2 q}{q} \int dq , \] (15)

It is interesting that (14) is independent of \( J \). We have to put some lower limit in the integral in (15). At low temperature, when inequality (3) is valid, we have to substitute the spin-wave gap (3) as the lower limit. This gives temperature independent contribution to the impurity susceptibility
\[ \delta \chi_\perp = \frac{2 \Omega^2}{2 \pi Z_c J < S_z >^2} \ln(L) = \frac{2 \Omega^2 Z_c^2}{\pi Z_c Z_s} \ln(L) \] (16)

If \( J \gg T \gg T_{sw} \) one has to put temperature as the lower limit in (15). Hence
\[ \delta \chi_\perp = \frac{2 \Omega^2 Z_c^2}{\pi Z_c Z_s} \ln(J/T) \] (17)

In the leading \( 1/S \) approximation one has to set \( Z_T = Z_c = Z_s = 1 \), hence \( \delta \chi_\perp \rightarrow \frac{2 \Omega^2}{\pi Z_c Z_s} \ln(\ldots) \). This corresponds to the low-frequency susceptibility derived in Ref.\(^{5}\). We have calculated the perpendicular susceptibility (16). (17) in the intrinsic reference frame. The isotropic susceptibility is related to \( \delta \chi_\perp \) by the standard relation, \( \delta \chi = \frac{3}{2} \delta \chi_\perp \).

**IV. NON-LINEAR \( \sigma \)-MODEL DERIVATION OF THE LOG CORRECTION, AND WARD IDENTITY FOR THE IMPURITY SPIN-WAVE VERTEX**

An alternative derivation of (16) and (17) is based on the \( \sigma \)-model. Let us consider a field \( \mathbf{n} \), \( |\mathbf{n}| = 1 \), defined on a disc of radius \( L \). An impurity with spin \( \Omega \) is in the center of the disc. The impurity spin is directed along \( z \) axis (perpendicular to the plane) and due to the magnetic field \( B = B_z \) it is tilted by angle \( \theta \) is x-direction, see Fig. 5. Energy of the medium is
\[ E_\sigma = \frac{1}{2} \rho_s \int (\nabla \mathbf{n})^2 d^2 r , \] (18)
FIG. 5: An impurity (dot) in the center of a disc of radius $L$. The disc carries field $\mathbf{n}$ described by the nonlinear $\sigma$-model. Due to magnetic field $B = B_x$ the impurity spin is tilted in $x$-direction.

where $\rho_s = Z_\rho J^2$ is the spin stiffness. Here $\frac{1}{4}$ is the leading $1/S$ value for the stiffness, and $Z_\rho \approx 0.72$ is the renormalization factor due to higher $1/S$-corrections\textsuperscript{11,18,19}. The field is of the form $\mathbf{n} \approx (n_x, 0, 1)$. Due to the field $n_x$ obeys the usual Poisson equation, solution of the equation is

$$n_x(r) = a \ln(L/r) .$$

(19)

To find the constant $a$ we have to remember that $n_x(r \sim 1) = \theta$, where $\theta$ is tilting angle of the impurity, and $1 = \text{lattice spacing}$. Therefore $a = \theta/\ln(L)$. Substituting (19) in (18) we find the elastic energy

$$E_\sigma = \pi \rho_s \theta^2/\ln(L) .$$

(20)

Minimizing it with respect to $\theta$ we find $\theta = B \Omega \ln(L)/(2\pi \rho_s)$, magnetic moment $M = \Omega \theta$, and the magnetic susceptibility

$$\delta \chi_\perp = \frac{\Omega^2}{2\pi \rho_s \ln(L)} \rightarrow \frac{2\Omega^2}{\pi Z_\rho J} \ln(L) .$$

(21)

At the final step we have substituted $\rho_s = JZ_\rho/4$. In the leading $1/S$ approximation, $Z_\Gamma = Z_c = Z_s = Z_\rho = 1$, hence equation (21) agrees with the spin-wave results\textsuperscript{16} and\textsuperscript{17}. Moreover a comparison of these equations gives a nontrivial Ward identity relating renormalization factors for the spin-wave vertex $Z_\Gamma$, the spin-wave velocity $Z_c$, the staggered magnetization $Z_s$, and the spin stiffness $Z_\rho$

$$\frac{Z_\Gamma^2}{Z_c Z_s^2} = \frac{1}{Z_\rho} .$$

(22)

This gives previously unknown value of $Z_\Gamma$

$$Z_\Gamma = \sqrt{\frac{Z_c Z_s^2}{Z_\rho}} \approx 0.76 .$$

(23)

Similar to\textsuperscript{17} one has to substitute $\ln(J/T)$ instead of $\ln(L)$ in (21) if $J \gg T > T_{sw}$. If the external magnetic field has a nonzero frequency $\omega$, and $\omega > T, T_{sw}$, then $\ln(L) \rightarrow \ln(J/\omega)$. Equations (16), (17), and (21) are in agreement with Ref\textsuperscript{5} and with recent results\textsuperscript{9,21}.

The spin-wave approach in section III assumes that $J_\perp \ll J$. There are numerous two-loop diagrams which are proportional to $(J_\perp/(2\pi)^2 J^2) \ln(L)$ and even to $(J_\perp/(2\pi)^2 J^2) \ln^2(L)$. Some of the diagrams which contain the logarithm squared are shown in Fig. 6. Calculation of all the diagrams is a pretty involved problem. On the other hand the semiclassical derivation based on the $\sigma$-model is independent of $J_\perp/J$. The only assumption in the derivation is that the impurity magnetic moment is localized in the vicinity of the impurity. To check this assumption we have calculated the magnetic cloud around the impurity using the spin-wave theory. We have found that density of the induced magnetization $\delta \mu_z$ drops down faster than $1/r^2$, $\delta \mu_z(r) < 1/r^2$. Therefore, the magnetic moment of the cloud $\mu = \int \delta \mu_z(r) d^2r$ is convergent at large distances, and it means that the above assumption is valid. This implies that all higher order in $J_\perp$ infrared divergent diagrams must cancel out. This is a highly unusual situation and it would be interesting to check the cancellation by a direct calculation.
FIG. 6: Two loop double logarithmic contributions to $\delta\chi_\perp$ proportional to $J_\perp/J^2$.

V. CONCLUSIONS

We have analyzed excitation spectrum of a finite antiferromagnetic cluster with magnetic impurity, and considered a crossover between quantum and classical Curie law for the impurity magnetic susceptibility. We have also derived a logarithmic correction to the impurity magnetic susceptibility. Dependent on the parameters this can be logarithm of system size, temperature, or frequency of the external magnetic field. Using the results for the logarithmic correction we have derived the Ward identity for the impurity-spin-wave vertex.

VI. ACKNOWLEDGMENTS

I am very grateful to A. W. Sandvik and G. Khaliullin for important discussions. I am also very grateful to K. H. Höglund, A. W. Sandvik, and S. Sachdev for communicating me their results prior publication.

* Electronic address: sushkov@newt.phys.unsw.edu.au

1 E. Manousakis, Rev. Mod. Phys. 63, 1 (1991).
2 E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).
3 S. -W. Cheong et al., Phys. Rev. B 44, 9739 (1991); S. T. Ting et al., *ibid.* 46, 11772 (1992); M. Corti et al., *ibid.* 52, 4226 (1995); P. Carretta, A. Rigamonti, and R. Sala, *ibid.* 55, 3734 (1997).
4 O. P. Vajk, P. K. M. Ng, M. Greven, P. M. Gehring, and J. W. Lynn, Science 295, 1691 (2002).
5 N. Nagaosa, Y. Hatsugai, and M. Imada, J. Phys. Soc. Jpn. 58, 978 (1989); N. Nagaosa and T. -K. Ng, Phys. Rev. B 51, 15588 (1995).
6 N. Bulut, D. Hone, D. J. Scalapino, and E. Y. Loh, Phys. Rev. Lett. 62, 2192 (1989).
7 A. W. Sandvik, E. Dagotto, and D. J. Scalapino, Phys. Rev. B 56, 11701 (1997).
8 S. Sachdev, C. Buragohain, and M. Vojta, Science 286, 2479 (1999); M. Vojta, C. Buragohain, and S. Sachdev, Phys. Rev. B 61, 15152 (2000).
9 K. H. Höglund and A. W. Sandvik, cond-mat/0302273.
10 J. Igarashi, K. Murayama, and P. Fulde, Phys. Rev. B 52, 15966 (1995); K. Murayama and J. Igarashi, J. Phys. Soc. Jpn. 66, 1157 (1997).
11 V. N. Kotov, J. Oitmaa, and O. P. Sushkov, Phys. Rev. B 58, 8495 (1998).
12 A. L. Chernyshev, Y. C. Chen, and A. H. Castro Neto, Phys. Rev. B 65, 104407 (2002).
13 O. P. Sushkov, Phys. Rev. B 62, 12135 (2000).
14 M. Troyer, Prog. Theor. Phys. Suppl. 145, 326 (2002).
15 H. Neuberger and T. Ziman, Phys. Rev. B 39, 2608 (1989).
16 K. J. Runge, Phys. Rev. B 45, 12292 (1992).
17 P. Hasenfratz and F. Niedermayer, Z. Phys. B 92, 91 (1993).
18 R. R. P. Singh, Phys. Rev. B 39, 9760 (1989).
19 Zheng Weihong, J. Oitmaa, and C. J. Hamer, Phys. Rev B 43, 8321 (1991).
20 L. D. Landau and E. M. Lifshitz, Quantum Mechanics: non-relativistic theory. Oxford, New York, Pergamon Press, 1977.
21 S. Sachdev, M. Vojta, cond-mat/0303001.