# Impurity-pinned vortices contribution to the response function in randomly diluted easy-plane ferromagnet on a square lattice

Fagner M. Paula, Afranio R. Pereira
*Departamento de Física, Universidade Federal de Viçosa, Viçosa, 36570-000, Minas Gerais, Brazil*

Gary M. Wysin
*Department of Physics, Kansas State University, Manhattan, KS 66506-2601*

Using spin dynamics techniques we determine the neutron scattering function $S_{xx}(\vec{q}, \omega)$ of the two-dimensional classical XY-model on a square lattice containing a percentage of nonmagnetic impurities on the magnetic sites. Dilution substantially transforms the shape and the position of the central and spin wave peaks. Besides the spin wave peak, an additional inelastic peak arises. We argue that the causes of this rich structure are vortex-vacancy interactions.

PACS numbers: 75.10.Hk; 75.30.Hx; 75.40.Mg

Magnetic vortices and other nonlinear magnetization distributions have attracted much attention in physics of low dimensional magnetism. The direct experimental visualization of these structures in nanomagnetism has given new impulses to investigate not only the physical relevance but also the technological importance of nonlinear excitations in magnetic materials [1–4]. Now, even a delicate phenomenon like a shift of the vortex center position from the center of a nanodot can be observed experimentally. However, although there is a large class of layered insulators that has been shown to exhibit the experimental characteristic of two-dimensional (2D) magnetism, it is not so easy to get a direct observation of vortices in these materials. In such systems, the vortex or soliton signature may be found in the dynamical correlation functions via vortex motion or vortex-magnon (or soliton-magnon) interactions. In fact, vortex motion may cause a central peak in the spin-spin dynamical structure factor [5, 6] while vortices or solitons interacting with magnons may contribute to the electron-paramagnetic-resonance (EPR) linewidth [7–9], which is the temporal integral of the four-spin-correlation function. Surprisingly, some Monte Carlo calculations indicate that a single vortex very seldom moves freely over a larger distance. Normally the vortex travels only one or two lattice spacings until it annihilates with the antivortex of a pair which meanwhile appeared spontaneously in the neighborhood [10, 11]. This result would be in contrast to the phenomenological theories that predict the vortex contribution to the central peak, but as pointed out by Mertens and Bishop [12], probably only the effective vortex motion is important for the dynamic correlation function. This would mean that it does not matter if a vortex is annihilated with the antivortex of a pair in the considered time interval $[0, t]$, because the vortex of that pair has a motion similar to that of the original vortex. Only effective lifetimes are seriously affected.

On the other hand, to the authors' knowledge, there are no experiments in easy-plane magnets to explicitly determine the vortex signature using the EPR techniques (EPR linewidth measurements have provided an important indirect method to experimentally detect solitons in two-dimensional isotropic magnetic materials [7, 8, 13]). Therefore, since the interpretation of the central peak in the spin-spin correlation function is not at all clear, vortices are still objects that need to be observed (direct or indirectly) in 2D easy-plane magnetic materials. Perhaps, the inclusion of external factors in the system may help vortices to manifest themselves more clearly. For example, the introduction of an amount of nonmagnetic impurities into the magnetic sites of a classical magnet may create conditions that affect the vortex dynamics. Really, recent works [14–17] have shown that vortices are attracted and pinned by nonmagnetic impurities. A bound state vortex-impurity with the vortex center around the impurity is then formed [14] and as a first consequence, the mean vortex mobility should decrease. Hence, if vortex motion is the cause of the central peak, this peak should be considerably modified in diluted systems. Following this idea, other possibilities could also appear. For instance, it was shown that vortices can develop an oscillatory motion[17] around a vacancy and this motion could also contribute to the spin dynamics. For these and many other motivations, it should be important to study the spin dynamics in doped layered magnetic materials. In fact, the site dilution problem is an important subject in modern condensed matter physics. In this letter we develop some arguments based on numerical and analytical calculations that vortex-vacancy interactions may play a crucial role in the spin dynamics.

We consider the classical 2D XY model with a fraction of nonmagnetic impurities to study the behavior of the system dynamics using combined Monte-Carlo (MC) and Spin Dynamics (SD) simulations. The spin model under consideration may also have relevance to the study of superconductivity, in particular, to the interaction between vortices and spatial inhomogeneities. It is described by the following Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \left( S_i^x S_j^x + S_i^y S_j^y \right), \quad (1)$$

where $J$ is the ferromagnetic exchange coupling, $\langle i,j \rangle$ indicates nearest neighbor sites of an $L \times L$ square lattice and the quenched dilution factors $\{\sigma_i\}$ independently take the values 1 or 0 depending on whether the associated site is occupied by a spin or vacant. The classical spins $\vec{S}_i$ have three components $S_i^2 = (S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = 1$. The behavior of the dynamics was analyzed considering several values for the impurity concentration $\rho_v$ and temperature $T$. The critical temperature $T_c$ of this model (we use $T_{KT}$ for the pure model) is a function of the impurity concentration $\rho_v$ decreasing monotonically with increasing $\rho_v$ [18, 19]. It vanishes at the site percolation threshold $\rho_v \approx 0.41$ for a square lattice[18, 19].

Numerically we simulated the thermal equilibrium spin dynamics of Hamiltonian (1) at several different dilutions $\rho_v$ on $L \times L$ square lattices ($16 \leq L \leq 96$, in units of lattice spacing $a$) with periodic boundary conditions. The number of spins in the system is $N = (1 - \rho_v)L^2$. The numerical method is a combined MC-SD technique, which include effects due to all thermodynamically allowed excitations available to the microscopic spin dynamics. The techniques used here have been described in Ref. 20 and are based on the simulation methods developed in Refs. 5, 21, and the MC part has been applied recently in the diluted easy-plane Heisenberg model[19, 22]. Averages for the diluted model were made over different realizations of the vacancy positions (averaging over the disorder). Now we summarize the main results. Figure 1 shows $S_{xx}(\vec{q}, \omega)$ at temperature $T = 0.350J$, $\vec{q} = (\pi/4a, 0)$, $L = 64a$ for various impurity concentrations, $\rho_v = 0.0, 0.16, 0.20$. The critical temperatures related to these impurity concentrations are, respectively, $0.700J, 0.453J$ and $0.384J$ [19]. Note that an almost infinitesimally narrow spike around $\omega = 0$ takes place. This is completely different from the pure case. In general, for $T \leq T_c$, the central peak becomes narrower as $\rho_v$ increases. At the same time the spin wave peak (SWP) moves towards lower frequencies and becomes wider as $\rho_v$ increases. Besides the SWP, another interesting inelastic peak at a finite frequency independent of $q$ arises. In order to better see this new structure, we use intermediate values of $q$. For small values of momentum, the spin wave peak is centralized at positions of low frequencies, dominating the region where the new peak arises, and hence, small $|\vec{q}|$ is not appropriate to observe it. This inelastic peak moves slightly towards lower $\omega$ and becomes narrower and higher as $\rho_v$ increases. We also notice that this peak moves continuously towards lower $\omega$ as the lattice size increases (see Fig.(2)). In fact, it is observed that $\omega_v = C(\rho_v, T)/L$ (in units of $J$), where the factor $C(\rho_v, T)$ depends on impurity concentration and temperature. As $\rho_v$ and $T$ increase, the factor $C(\rho_v, T)$ tends to decrease. The effect of $\rho_v$ on $C(\rho_v, T)$ is much stronger than that of $T$. Indeed, Paula *et al.*[16] have shown that the presence of other vacancies decreases considerably the vortex-on-vacancy pinning energy. In figure 3 we plot $C(\rho_v, T)$ versus $\rho_v$ for $T = 0.200J$. Essentially, for a given temperature $T$, $C(\rho_v, T)$ decreases linearly with $\rho_v$. It should be interesting to study the behavior of $C(\rho_v, T)$ in the limit of very low impurity concentration ($\rho_v \to 0$). Extrapolating the results of Fig.(3) to the limit $\rho_v \to 0$, we get $C(\rho_v, 0.200) \to 12.09Ja$. We also studied the behavior of $C(\rho_v \to 0, T)$ for other values of $T$ (not shown here). As the temperature is decreased, $C(\rho_v \to 0, T)$ increases and extrapolating the results to the limit $T \to 0$, we get $C(\rho_v \to 0, T \to 0) \approx 13.10Ja$ leading to $\omega_v \approx (13.10/L)J$. This result is very suggestive. Indeed, Pereira *et al.*[17] have shown that a single vortex can oscillate around a nonmagnetic impurity and such motion could be characterized by some normal modes with well defined frequencies, which have the same behavior with the system size as the peak obtained here. Their calculations were done for a system at zero temperature containing only one vortex and only one vacancy and therefore, valid in the limit $\rho_v \to 0$. The main mode of the oscillatory vortex motion was found to have a frequency given by $\omega_0 \approx (13.57/L)J$, which is very close to $\omega_v$ in the limit $\rho_v \to 0, T \to 0$. The relation $\omega_v(\rho_v \to 0, T \to 0) \approx \omega_0$ strongly suggests that the cause of the new peak observed here is vortex-vacancy interactions.

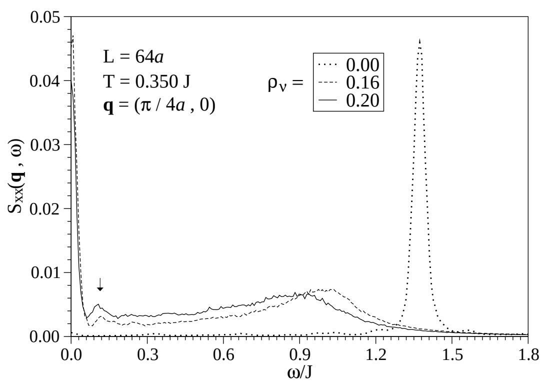


FIG. 1: The correlation function $S_{xx}(\vec{q}, \omega)$ versus $\omega$ for some impurity concentrations $\rho_v = 0$ (dotted line), $\rho_v = 0.16$ (dashed line) and $\rho_v = 0.20$ (solid line). It was used $\vec{q} = (\pi/4a, 0)$, $L = 64a$ and temperature $T = 0.350J$.

As we have already seen, for a given temperature $T$, the position of the spin wave peak moves towards lower $\omega$ as $\rho_v$ increases, and the peak widens slightly. It is somewhat similar to what happens for pure systems as the temperature increases, indicating that the non-magnetic disorder is, to some extent, similar to thermal disorder. Theoretical calculations using the spin wave approximation show that the static spin-spin correlation function exponent of the diluted system $\eta_v$ has the same form of the exponent $\eta$ of the pure system, differing only by a constant which renormalizes the temperature [18]. The approximate relation between $\eta_v$ and $\eta$ is then given by $\eta_v \simeq \eta/(1-2\rho_v)$ [18]. Writing this expression as $\eta_v = 1/2\pi J\beta_v$, we have $\beta_v = \beta(1-2\rho_v)$ and then, the effect of vacancies is to increase the effective temperature of the system. The substitution of $\eta$ by $\eta_v$ in the Villain [23] or Nelson and Fisher [24] dynamical correlation functions, implies that the spin wave peak must widen as $\rho_v$ increases, which is in qualitative agreement with our simulations.

While the behavior of the spin wave peak is relatively qualitatively well understood for the diluted problem, the additional small inelastic structure at a frequency $\omega_v$, not observed in pure systems, is a new and interesting peak that needs explanation. Theoretical expectations based on the vortex-vacancy interactions[17] may justify this structure. A simple phenomenological model based on oscillating vortices is developed now. Vortices are created in pairs of vortex-antivortex and, in impurity systems, it must be energetically favorable for a pair to nucleate near a vacancy, preferentially with one of the two vortex centers located exactly at the vacancy center [25]. Then the system may contain some impurity-pinned vortices (antivortices) and their respective antivortices (vortices) in the neighborhood (and in general, not pinned at impurities, at least for low impurity concentrations). Considering a specific pinned vortex, we will define its partner as the antivortex the shortest distance away. The energy of this configuration can be estimated as $E_i \cong E_{2v} + U_{vi}$, where $E_{2v}$ is the pair creation energy (for a discrete lattice, Landau and Binder[27] found $E_{2v} \approx 6.39J$) and $U_{vi} \approx -3.178J$ is the vortex-on-vacancy pinning energy[15].

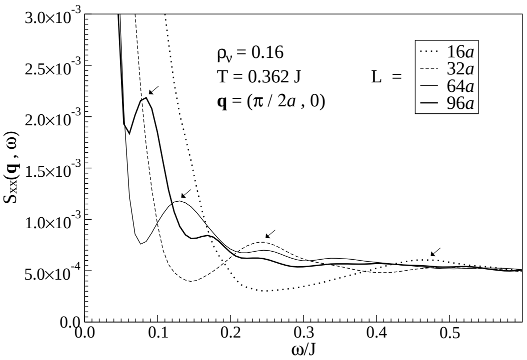


FIG. 2: $S_{xx}(\vec{q},\omega)$ versus frequency $\omega$ for some values of $L$.

The time-dependent spin correlation function is obtained after the following assumptions. First we assume that the magnetization at any point $\vec{r}_i$ in the lattice is from vortices located at vacant sites $\vec{r}_\gamma$ with $S^x(\vec{r}_i,t) = \sum_\gamma S^x(\vec{r}_i - \vec{r}_\gamma, t)$. In reality, the respective partners (not pinned) of each impurity-pinned vortex (i.e., its nearest antivortex) also contribute to the magnetization and they must also be considered. Such a partner is localized by vectors $\vec{r}_\gamma + \vec{R}_\gamma$, where $\vec{R}_\gamma$ determines the partner position in relation to $\vec{r}_\gamma$ (note that $\mid \vec{R}_\gamma \mid = R_\gamma$ gives the $\gamma$-pair size). In this notation the planar vortex-antivortex solution is written, in polar coordinates $(\Phi,\Theta)$, as $\Phi_p = \arctan[(y-y_\gamma)/(x-x_\gamma)] - \arctan[(y-y_\gamma-\vec{R}_\gamma\cdot\hat{y})/(x-x_\gamma-\vec{R}_\gamma\cdot\hat{x})]$, $\Theta_p = \pi/2$. In the simplest analysis, when not centered on an impurity, a partner contributes only to the static structure factor since it may not move considerably on the lattice. It is not completely true because these structures must affect the central peak in the sense proposed by Mertens and Bishop [12](of course with less intensity than the pure case). The time dependence is assumed from the vortex oscillations around the vacancy. It has been shown[17] that such oscillations are not so simple and that the amplitude of oscillation is of the order of one lattice spacing $a$. However, as a further simplification we will assume a harmonic approximation writing $S^x(\vec{r}_i,t) = \sum_\gamma S^x(\vec{r}_i - \vec{r}_\gamma - \vec{a}_\gamma \sin(\omega_v t))$, where vectors $\vec{a}_\gamma$ ($\mid \vec{a}_\gamma \mid = a$) indicate the direction of the oscillatory motion (in relation to the x-axis) and $\omega_v$ is the vortex oscillation frequency. Using the above considerations, the correlation function $S_{xx}(\vec{r},t) =< S^x(\vec{r},t)S^x(\vec{0},0) >$ is calculated as

$$S_{xx}(\vec{r},t) \approx n_v \int \mu(R) d^2r_\gamma dR < S^x(\vec{r}_\gamma, R, \alpha) \times S^x(\vec{r}-\vec{r}_\gamma-\vec{a}_\gamma\sin(\omega_v t), R, \alpha) >_{\alpha,\vartheta}, \quad (2)$$

where $n_v$ is the impurity-pair density, $\mu(R)$ is the pair size distribution function[26] and $\alpha, \vartheta$ are the angles that vectors $\vec{R}_\gamma$ and $\vec{a}_\gamma$ make with the x-axis respectively. The symbol $< ... >_{\alpha,\vartheta}$ represents an average over these two angles. In the low impurity concentration and low temperature regimes, we estimate the impurity-pair density $n_v$ substituting $\beta$ by $\beta_v$ in the Boltzmann factor, obtaining $n_v(\rho_v) \approx B(\rho_v)\exp(-\beta E_i)$, where the coefficient $B$ is given by $B(\rho_v) \approx \exp(2\rho_v \beta E_i)$. As expected, the geometric (or nonmagnetic) disorder contributes to the pair formation.

The spatial and temporal Fourier transformations of Eq.(2) yield

$$S_{xx}(\vec{q},\omega) \approx n_v F_{xx}(\vec{q}) \int < \exp[-i\vec{q}\cdot\vec{a}_\gamma \sin(\omega_v t)] >_\vartheta \times \exp(i\omega t) dt, \quad (3)$$

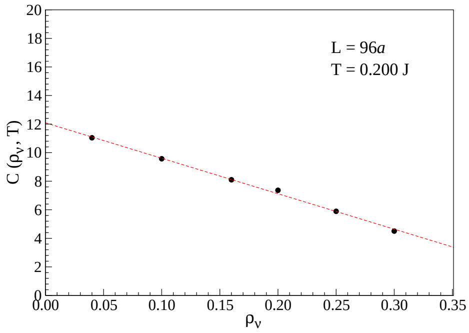


FIG. 3: The factor $C(\rho_v, T)$ versus impurity concentration $\rho_v$ for $L = 96$ and $T = 0.200J$. The dotted line is a good fit to the data. Note that $C(\rho_v \to 0, T = 0.200J) \to 12.09Ja$.

where $F_{xx}(\vec{q}) = \int \mu(R) <\mid f_{xx}(\vec{q}, R, \alpha) \mid^2>_\alpha dR$, with

$$\mid f_{xx}(\vec{q}, R, \alpha) \mid^2 = \frac{1}{2}[\mid f_x(\vec{q}, R, \alpha) \mid^2 + \mid f_y(\vec{q}, R, \alpha) \mid^2]. \quad (4)$$

The static structure factors in Eq.(4), $f_x(\vec{q}, R, \alpha) = \int \cos[\Phi_p(\vec{q}, R, \alpha)] \exp(i\vec{q} \cdot \vec{r}) d^2r$ and $f_y(\vec{q}, R, \alpha) = \int \sin[\Phi_p(\vec{q}, R, \alpha)] \exp(i\vec{q} \cdot \vec{r}) d^2r$ are calculated as in Ref. 9 ($f_x \sim O(R^2)$). After averaging over $\vartheta$, the integral in Eq.(3) is written as

$$\int [J_0(qa \sin(\omega_v t)) \cos(\omega t) + H_0^s(qa \sin(\omega_v t)) \sin(\omega t)] dt, \quad (5)$$

where $J_0$ and $H_0^s$ are the Bessel and Struve functions respectively. Integration of Eq.(5) leads to two sharp peaks at well defined frequencies $\omega = 0$ and $\omega = \omega_v$. The central peak is much more intense and then we approximate

$$S_{xx}(\vec{q}, \omega) \cong n_v(\rho_v) F_{xx}(\vec{q}) [b_1 \delta(\omega) + b_2 \delta(\omega - \omega_v)], \quad (6)$$

where $b_1$ and $b_2$ are constants that give the strength of the peaks. These simple analytical results suggest that the pinned-vortex contributions to the correlation function imply two infinitely high and infinitesimally narrow peaks, which in some respects resemble results of simulations. Of course, like the divergent spin wave-peaks obtained theoretically[23, 24], this double delta-function correlation is only an approximation. This sharp spectrum may be modified by the occurrence of other interactions, which cause a broadening of the lineshape. The simple analytical model introduced here reproduces the qualitative behavior of $S_{xx}(\vec{q}, \omega)$ observed in simulations.

In summary, vortices interacting with vacancies in diluted classical easy-plane 2D magnets result in an inelastic peak in the dynamical correlation function. Since there are several contributions to the central peak, the mechanism proposed here may be more effective to experimentally detect vortices in layered magnetic materials. Using typical values for ferromagnetic samples, $J \cong 0.1eV$, $a \cong 1\AA$ and considering $L$ as large as $1mm$, one gets the the frequency associate to the new peak as $\omega_v \cong 10^9 s^{-1}$.

This work was supported by CNPq, CAPES and FAPEMIG (Brazil). GMW is very grateful for support from FAPEMIG as a visiting researcher and for the hospitality of the Universidade Federal de Viçosa, Brazil.

[1] T. Pokhil, D. Song, and J. Nowak, J. Appl. Phys. **87**, 6319 (2000).
[2] M. Schneider, H. Hoffmann, and J. Zweck, Appl. Phys. Lett. **77**, 2909 (2000).
[3] M. Rahm, R. Höllinger, V. Umansky, and D. Weiss, J. Appl. Phys. **95**, 6708 (2004).
[4] A.R. Pereira, J. Appl. Phys. **97**, 094303 (2005).
[5] F.G. Mertens, A.R. Bishop, G.M. Wysin, and C. Kawabata, Phys. Rev. Lett. **59**, 117 (1987); Phys. Rev. B **39**, 591 (1989).
[6] M.E. Gouvêa, G.M. Wysin, A.R. Bishop, and F.G. Mertens, Phys. Rev. B **39**, 11840 (1989).
[7] C.E. Zaspel, T.E. Grigereit, and J.E. Drumheller, Phys. Rev. Lett. **74**,4539 (1995).
[8] K. Subbaraman, C.E. Zaspel, and J.E. Drumheller, Phys. Rev. Lett. **80**, 2201 (1998).
[9] A.R. Pereira and A.S.T. Pires, Phys. Rev. B **60**, 1 (1999).
[10] D.A. Dimitrov and G.M. Wysin, Phys. Rev. B **53**, 8539 (1996).
[11] B.V. Costa, J.E.R. Costa, and D.P. Landau, J. Appl. Phys. **81**, 5746 (1997).
[12] F.G. Mertens and A.R. Bishop, cond-mat/9903037 (1999).
[13] C.E. Zaspel and J.E. Drumheller, Int. J. Mod. Phys. B **10**, 3649 (1996).
[14] A.R. Pereira, L.A.S. Mól, S.A. Leonel, P.Z. Coura, and B.V. Costa, Phys. Rev. B **68**, 132409 (2003).
[15] G.M. Wysin, Phys. Rev. B **68**, 184411 (2003).
[16] F.M. Paula, A.R. Pereira, L.A.S.Mól, Phys. Lett.A **329**, 155 (2004).
[17] A.R. Pereira, S.A. Leonel, P.Z. Coura, and B.V. Costa, Phys. Rev.B **71**, 014403 (2005).
[18] B. Berche, A.I. Farinas-Sanches, Y. Holovatch, and R. Paredes, Eur. Phys. J. B **36**, 91 (2003).
[19] G.M. Wysin, A.R. Pereira, I.A. Marques, S.A. Leonel, and P.Z. Coura, cond-mat/0504145 (2005).
[20] G.M. Wysin and A.R. Bishop, Phys. Rev. B **42**, 810 (1990).
[21] C. Kawabata, M. Takeuchi and A.R. Bishop, J. Magn. Mater. **54-57**, 871 (1986);*ibid.*, J.Stat. Phys. **43**, 869 (1986).
[22] G.M. Wysin, Phys. Rev. B **71**, 094423 (2005).
[23] J. Villain, J. Phys.**35**,27 (1974).
[24] D.R. Nelson and D.S. Fisher, Phys. Rev. B **16**,4945 (1977).
[25] A.R. Pereira, J.Magn. Magn. Mater.**279**, 396 (2004).
[26] H.J. Jensen and H. Weber, Phys. Rev. B **45**, 10468 (1992).
[27] D.P. Landau and K. Binder, Phys. Rev.B **24**, 1391 (1981).