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Quantized topological point defects in two-dimensional antiferromagnets

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We semiclassically quantize static topological point defects that exist within a continuum Heisenberg model of the two-dimensional antiferromagnet. The quantum corrections reduce the classical defect energy as defect size increases and induce an effective interaction between defects that can be attractive at short range.

The mechanism for superconductivity in the recently discovered class of ceramic high-temperature superconductors is still unknown. In order to understand the superconductivity in these systems it is important first to note the features which are special to these materials. Two properties that may be essential for the ceramic superconductors are (a) the two-dimensional nature of both the charge excitations and the magnetic excitations, and (b) the antiferromagnetic nature of the magnetic excitations. The crystal structure, for example, is highly planar[1] and band-structure calculations indicate the existence of two-dimensional electronic bands.[2] In addition, inelastic neutron-scattering measurements on insulating La_2CuO_4 show evidence for two-dimensional antiferromagnetic correlations parallel to the Cu-O planes at temperatures above the 3D Néel ordering temperature.[3] The above list of experimental facts indicates that the Cu-O planes in the ceramic superconductors may be essentially isolated two-dimensional antiferromagnets for insulating compositions.

The simplest theoretical description of a 2D antiferromagnet is a continuum Heisenberg model in terms of the Néel state. In the limit of zero temperature, it is represented by the following Lagrangian:

$$L=\tfrac{1}{2}J\int d^2x\,(c^{-2}|\partial_t \mathbf{n}|^2-|\nabla\mathbf{n}|^2)\,. \tag{1}$$

Above, $\mathbf{n}$ denotes the Néel unit vector characterizing the direction of the sublattice magnetization of the antiferromagnet, c is the velocity of the long-wavelength spin-waves, and J denotes the effective exchange coupling constant. Notice that Eq. (1) is just the Lagrangian for a nonlinear σ model in $2+1$ dimensions. This hydrodynamic model gives two acoustic spin-wave modes, which are expected of an antiferromagnet, and it should, therefore, describe the long-wavelength physics of an isolated antiferromagnetic plane. Recently, it has also been successfully used to explain the low-temperature behavior of the antiferromagnetic correlation length in La_2CuO_4.[4]

However, as was shown by Belavin and Polyakov,[5] this model also contains static, topologically nontrivial classical minima. In terms of the conformal representation[5,6]

$$w=(1+n_3)^{-1}(n_1+in_2)\,, \tag{2}$$

which is simply the stereographic projection of the Néel vector onto the complex plane, the Lagrangian (1) can be reexpressed as

$$L=8J\int d^2x\,(1+|w|^2)^{-2}\times(\tfrac{1}{4}c^{-2}|\partial_t w|^2-|\partial_z w|^2)-4\pi Jq\,, \tag{3}$$

where q is the topological charge of the configuration given by

$$q=\frac{1}{\pi}\int d^2x\,(1+|w|^2)^{-2}(\partial_{z^*}w\partial_z w^*-\partial_z w\partial_{z^*}w^*)\,. \tag{4}$$

Here, $\partial_z=\tfrac{1}{2}(\partial_{x_1}-i\partial_{x_2})$ and $\partial_{z^*}=\tfrac{1}{2}(\partial_{x_1}+i\partial_{x_2})$; likewise, $z=x_1+ix_2$ and $z^*=x_1-ix_2$. For configurations with a common value at infinity, $\mathbf{n}(\mathbf{x})$ is essentially a mapping of the sphere to itself and q measures the number of times $\mathbf{n}$ does this. Each topological equivalence class in the space of all possible configurations $\mathbf{n}(\mathbf{x})$ is uniquely labeled by its topological charge. From Eq. (3), it is evident that, within a given topological sector of the field theory, there exists static classical minima w_0 given by analytic functions of z^* satisfying $\partial_z w_0=0$ and having classical energies[5]

$$E_{\rm cl}=4\pi Jq\,. \tag{5}$$

The fundamental solitonic configuration with unit topological charge $q=1$, for example, is given by $w_0=\lambda_1/z^*$, where λ_1 is a complex parameter. Qualitatively, the configuration is radial, pointing down at the origin and up at infinity. The magnitude of λ_1 gives the extension of the defect, while the phase of λ_1 gives the rotational orientation of the defect configuration. In general, the q-soliton configuration is given by $w_0=\sum_{i=1}^{q}\lambda_i/(z^*-r_i^*)$, where λ_i and r_i^* are again complex parameters. It has q units of topological charge and describes q defects at positions r_i. Note, however, that antisoliton solutions, obtained by interchanging $z\leftrightarrow z^*$, are also local minima of Eq. (1) degenerate with respect to the above soliton solutions. Throughout this paper, all statements made about solitons apply equally to antisolitons. One must simply interchange $z\leftrightarrow z^*$ in all expressions.

From Eq. (5), we see that the classical energy of these static defect configurations depends only upon the total topological charge q. Thus, at the classical level there is no preferred size or orientation for a fundamental soliton. Nor do these solitons experience interactions classically. This results from the conformal invariance of Lagrangian (1). Quantization of these defects, however, will break the static conformal invariance. In this paper, we semiclassically calculate the quantum corrections to the classical energy of such static defect configurations arising from long-wavelength antiferromagnetic spin waves. This is done by calculating the zero-point energy due to the antiferromagnetic spin waves in the presence of the solitonic background. As in the case of $(1+1)$-dimensional solitons,[7] and of skyrmions,[8] we find that such contributions lower the classical energy of the unit-charge defect. In particular, the energy monotonically decreases as soliton size increases. It is suggested that electronic vacancies or interstitials in 2D antiferromagnets provide the nucleation site for such defects of the homogeneous Néel state. We also perform a similar calculation for the case of two solitons separated by a distance r to extract an effective interaction potential $V_{\rm eff}(r)$. We find that $V_{\rm eff}(r)$ has a repulsive r^{-2} tail at large separations and that it can have a short-range attractive well, depending upon the relative orientation between the two solitons. Assuming that the above vacancy-soliton states are mobile, we suggest that such an attractive interaction may result in Cooper pairing, and hence to superconductivity. Note that topological excitations in 2D antiferromagnets and their relation to high-temperature superconductivity have also recently been discussed.[9]

The object now is to calculate what effect such topological defects of the 2D homogeneous Néel state have on the associated long-wavelength antiferromagnetic spin waves. First, let us write the conformal representation for the Néel configuration (2) as $w=w_0+w_1$, where w_0 is the static classical minimum configuration. The deviation from the classical minimum, w_1, represents the antiferromagnetic spin wave. This can be seen by minimizing the action corresponding to Lagrangian (3) to second order in w_1. This yields the field equation

$$(\nabla^2-c^{-2}\partial_t^2)w_1=Vw_1\,, \tag{6}$$

where

$$V=8[\partial_{z^*}\ln(1+|w_0|^2)]\partial_z\,. \tag{7}$$

In the case of the homogeneous Néel state $w_0=0$ and $V=0$, and therefore, there exist two pure spin-wave solutions to Eq. (6), with frequencies $\omega_k=ck$. Thus, the lowest-order effect of an inhomogeneous solitonic background w_0 is to produce an elastic scattering center for the spin waves. Since the scattering potential (7) has a finite range on the order of the size of the soliton configuration, the asymptotic solutions to Eq. (6) are given by phase-shifted cylindrical spin waves of the form $w_1(\mathbf{x},t)=\psi_{km}(\mathbf{x})e^{ickt}$,[10] with

$$\psi_{km}(\mathbf{x})\underset{\rho\to\infty}{\sim}\tfrac{1}{2}\left[H^{(1)}_{|m|}(k\rho)e^{im\theta}+\sum_{m'}\exp[-2i\delta(k)]_{mm'}H^{(2)}_{|m'|}(k\rho)e^{im'\theta}\right]. \tag{8}$$

Above, $\delta_{mm'}(k)$ denotes the phase-shift matrix, coupling the different angular momentum channels m and m', and (ρ,θ) denote the cylindrical coordinates for $\mathbf{x}$. By a generalization of arguments used in the semiclassical quantization of solitons in $1+1$ dimensions,[7] it can be shown that the quantum correction to the classical soliton energy, given by the zero-point energy of the spin waves measured with respect to the vacuum, is

$$E=4\pi Jq-\hbar c\int_0^{k_D}\frac{dk}{\pi}\mathrm{tr}\delta(k)\,. \tag{9}$$

The second term above represents the zero-point energy contribution, where the trace is taken over the angular momentum indices. Here, we have assumed a Debye model for the spin-wave excitations, with k_D as the cutoff momentum. Notice that expression (9) is invariant to the choice of the origin. This results from the fact that a translation of the origin in Eq. (8) simply transforms the phase shift by a unitary transformation $\delta(k)\to U^\dagger\delta(k)U$, under which $\mathrm{tr}\delta(k)$ is invariant. Expression (9) for the energy depends only upon the sum of the diagonal elements of the phase shift. The first-order and second-order Born terms for the diagonal elements are given, in general, by

$$\delta_m^{(1)}(k)=-\frac{\pi}{2}\int_0^\infty\rho\,d\rho\langle J_{|m|}(k\rho)e^{-im\theta}Ve^{im\theta}J_{|m|}(k\rho)\rangle_\theta\,, \tag{10a}$$

$$\delta_m^{(2)}(k)=-\frac{\pi^2}{4}\sum_{m'}\int_0^\infty\rho\,d\rho\int_0^\infty\rho'd\rho'\langle J_{|m|}(k\rho)e^{-im\theta}Ve^{im'\theta}N_{|m'|}(k\rho_>)J_{|m'|}(k\rho_<)e^{-im'\theta'}V'e^{im\theta'}J_{|m|}(k\rho')\rangle_{\theta,\theta'}\,, \tag{10b}$$

where the symbol $\langle\cdots\rangle_\theta$ denotes an angular average, $\rho_<=\min(\rho,\rho')$, and $\rho_>=\max(\rho,\rho')$. Notice that $\mathrm{tr}\delta^{(1)}(k)$ vanishes identically for V given by Eq. (7). Hence, the lowest-order contribution to Eq. (9) comes from the second-order Born term (10b). Below, we calculate the phase shift and the associated zero-point energy contribution in the Born approximation for the case of a single soliton.

Case I: Fundamental soliton. Consider the case where the classical soliton configuration is given by $w_0=\lambda_1/z^*$.[11] This describes a fundamental soliton of unit topological charge and of size $|\lambda_1|$. The potential operator (7) associated with this configuration is cylindrically symmetric. Hence, angular momentum is a good quantum number and the phase-shift matrix $\delta_{mm'}(k)$ is diagonal. Each angular momentum channel of the phase shift can be calculated in the Born approximation via (10). The first-order phase shifts (10a) are given, in this case, by

$$\delta_m^{(1)}(k)=\begin{cases}2\pi k|\lambda_1|K_{m-1}(k|\lambda_1|)I_m(k|\lambda_1|), & \text{for } m\geq 1,\\ -\delta^{(1)}_{1-m}(k), & \text{for } m<1.\end{cases} \tag{11}$$

Notice that $\lim_{k\to 0}\delta_m^{(1)}(k)=0$. This indicates that the Born approximation is valid at long wavelengths for small defects. However, as mentioned above, the lowest-order contribution to the zero-point energy term in Eq. (9) comes from the second-order Born terms. In particular, the $m=0,1$ angular momentum channels give the lowest-order contribution to Eq. (9) in powers of $k\lambda_1$. Using the small argument expansion for the Bessel functions in Eq. (10b), we find that this contribution yields the following expression for the energy of a quantized fundamental soliton, measured with respect to the vacuum:

$$E_1 \underset{\lambda_1\to 0}{\sim} 4\pi J - \tfrac{2}{3}\zeta(2)\hbar c k_D^3 |\lambda_1|^2 . \tag{12}$$

The above Born approximation result is valid for *small* solitons, $k_D|\lambda_1|\ll 1$. To evaluate Eq. (9) in the limit of large skyrmions, $k_D|\lambda_1|\gg 1$, we must obtain the high-energy limit of the phase shifts. Using the conventional Wentzel-Kramer-Brillouin (WKB) expression for the phase shift after an appropriate similarity transform of Eq. (6) (see Ref. 10), it can be shown that[12] $\lim_{k\to\infty}\mathrm{tr}\delta(k)=\pi$. Thus, in the limit of large skyrmions $k_D|\lambda_1|\gg 1$, (9) gives

$$E_1 \underset{\lambda_1\to \infty}{\sim} 4\pi J - \hbar c k_D . \tag{13}$$

The complete function $E_1(\lambda_1)$ is likely to be a smooth interpolation between the limits (12) and (13), with the transition between these limits occurring at $k_D|\lambda_1|\sim 1$. In antiferromagnetic La_2CuO_4, the spin-wave velocity is on the order of $\hbar c \gtrsim 0.4$ eV Å and the lattice constant for the Cu-O plane is $a\simeq 5$ Å.[1,3] The exchange coupling constant is, therefore, on the order of $J\sim\hbar c/a\simeq 0.1$ eV. If we set $k_D\sim a^{-1}$, then both the first and the second terms in Eq. (13) are comparable. Thus, the energy cost of large topological defects in La_2CuO_4 may be substantially lower than the classical value.

We see, therefore, that semiclassical quantum corrections lower the classical soliton energy as soliton size increases. Anisotropy effects, such as a neighboring antiferromagnetic plane, will stabilize this quantum mechanically driven expansion to give a preferred soliton size $|\lambda_1|$. In addition, Eqs. (12) and (13) indicate that there may be a critical soliton size above which it is energetically favorable to make a soliton, i.e., $E_1<0$. Consider the square lattice nearest-neighbor Heisenberg antiferromagnet in the homogeneous Néel state ($q=0$) at zero temperature. If we remove a spin from the lattice, the nearest neighbors of that spin will have a coordination number of three, instead of the bulk-spin coordination number of four. Therefore, such boundary spins would have larger quantum fluctuations than the bulk spins and it is conceivable that the above considered soliton configurations, with reversed sublattice magnetization at the center, would preferentially nucleate about this vacancy. In the context of high-temperature superconductivity, such a conjecture motivates the following question; does the presence of antiferromagnetic spin-waves give rise to an attractive interaction between two defects of the Néel state, which would then be inherited by the electronic vacancy defect centers? Below we calculate the quantum corrections to the classical energy of two fundamental solitons separated by a distance r.

Case II: Two fundamental solitons. Consider now the case where the classical configuration is given by $w_0=\lambda_1/z^*+\lambda_2/(z^*-r^*)$, where λ_1, λ_2, and r^* are complex parameters. This field describes a unit soliton at the origin in the presence of another one at distance $|r|$ away. The effective potential experienced between the two defects is defined as

$$V_{\text{eff}}(r)=E_{1,2}(r)-E_1-E_2 , \tag{14}$$

where $E_{1,2}$ is the energy (9) of the bisolitonic configuration and E_1 and E_2 are the energies (9) of the isolated unit solitons. Thus, from the previous calculation of the energy of a fundamental soliton (12), we find that the value of the effective potential, in the limit that the separation vanishes, is given by

$$V_{\text{eff}}(r) \underset{r\to 0}{\sim} -\tfrac{2}{3}\zeta(2)\hbar c k_D^3(\lambda_1\lambda_2^*+\lambda_1^*\lambda_2)+O(k_D\lambda)^4 . \tag{15}$$

Let us now calculate the effective potential in the limit that the separation is large. Unlike the previous case, the operator V defined in Eq. (7) is no longer radially symmetric. The angular momentum is no longer a good quantum number, nor is the phase-shift matrix $\delta_{mm'}(k)$ any longer diagonal. The lowest-order term in powers of r^{-1} comes from the $m'=m\pm 1$ terms in Eq. (10b). Upon substituting in Eq. (7) and making suitable integrations by parts of Eq. (10b), we find that such terms result in an asymptotically *repulsive* interaction given by

$$V_{\text{eff}}(r) \underset{r\to \infty}{\sim} \tfrac{4}{3}\pi\beta\hbar c k_D^3 \frac{|\lambda_1|^2|\lambda_2|^2}{|r|^2}+O(k_D\lambda)^4 , \tag{16}$$

where

$$\beta=\int_0^\infty dx\,(J_1N_0+J_0N_1)(1-J_0^2) + 2\sum_{m=1}^{m_D}\int_0^\infty dx\,(J_mN_{m-1}-J_{m+1}N_m)J_m^2 . \tag{17}$$

The first term in Eq. (17) corresponds to transitions between the $m=0,1$ angular momentum channels and it vanishes. The remaining terms in Eq. (17) correspond to transitions between the m, $m+1$ and $-m$, $1-m$ angular momentum channels. Here, m_D denotes an angular momentum cutoff for the trace sum in Eq. (9). The first five terms of the series were calculated numerically and are well approximated by $(\pi m)^{-1}$. Hence, if we extrapolate this dependence to all angular momentum channel, then $\beta\simeq\pi^{-1}\ln m_D$ asymptotically. The cut-off angular momentum is given approximately by $m_D\sim k_D L$, where L is the length of the system, and thus $\beta\simeq\pi^{-1}\ln k_D L$.

Given Eqs. (15) and (16), we can make a reasonable qualitative picture now of the effective potential experienced between two small semiclassically quantized topological solitons. Asymptotically, the potential has an r^{-2} repulsive tail. For the case that both solitons are oriented within 90° of each other, Eq. (15) indicates a negative value for the potential at zero separation. Hence, in this case there is a short-range attractive well with a length scale on the order of $|\lambda_1+\lambda_2|$. On the other hand, if the solitons are oriented more than 90° with respect to each other, Eq. (15) indicates a positive value for the effective potential at zero separation, and it is then not clear whether or not a short-range potential well exists. Finally, Eq. (15) also indicates that it is energetically favorable for two small skyrmions to have the same orientation.

Above, we have shown that linearized spin-wave fluctuations about static solitonic configurations of the 2D Néel state (a) lower the classical energy of the fundamental soliton as soliton size increases and (b) induce an effective interaction potential between soliton pairs that can be attractive at short range. If we assume, as suggested earlier, that electronic vacancies in 2D antiferromagnets nucleate these topological defects, and that the resulting vacancy-soliton hybrids have metallic mobilities, then such an effective interaction could be a pairing mechanism for superconductivity in doped 2D antiferromagnets and have some relevance to high-temperature superconductivity. However, the calculation of the interaction energy (14) was performed in the Born approximation, which is valid for small solitons satisfying $k_D\lambda \ll 1$. Multiple scattering effects will be important outside of this regime and must be investigated in order to see if our present results extrapolate to the large-soliton regime.

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[10]The operator $-\nabla^2+V$ found in Eq. (6) is related by a similarity transform to the Hermitian operator $-4f^{-1}\partial_{z^*}f^2\partial_z f^{-1}$, where $f=(1+|w_0|^2)^{-1}$. Hence, the eigenvalues k^2 of Eq. (6) are real and positive. In addition, V is short ranged, which implies that the usual continuum states, with energies $\omega=ck$, exist.

[11]Actually, the most general $q=1$ solution is given by $w_0=u+\lambda_1/z^*$, where u is a complex parameter. Though it is classically degenerate with the rotationally symmetric solution $w_0=\lambda_1/z^*$, the semiclassical quantum corrections to the classical energy in Eq. (9) yield, to second-order in the Born approximation, an anisotropy term

$$E_{\rm ani}=\tfrac{4}{3}(\ln k_D L)\hbar c k_D^3|\lambda_1|^2|u|^2+O(u^4)\,.$$

To this order, the calculation is identical to that of the asymptotic effective potential experienced by two pure solitons (16). Hence, quantum effects favor rotationally symmetric solitons with $u=0$.

[12]J. P. Rodriguez (unpublished).