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The quantum Heisenberg antiferromagnet on the square lattice is known to model the magnetic interactions in the copper ion planes of many high-T_c superconductors and their parent compounds. The thermodynamics of the model is approached by the *Pure-Quantum Self-Consistent Harmonic Approximation*, that reduces the quantum problem to the study of an effective classical antiferromagnetic system. The effective exchange, weakened by quantum fluctuations, enters as a temperature scale the classical-like expressions for the thermal averages, and the quantum spin correlation length is then obtained from its classical counterpart in a simple way. The theory compares very well, for any value of the spin and without need for adjustable parameters, with high-temperature expansions, quantum Monte Carlo simulations and recent neutron and NQR experiments.

The two-dimensional quantum Heisenberg Antiferromagnet (2d-QHAF) is described by the isotropic Hamiltonian

$$\hat{\mathcal{H}} = \frac{J}{2}\sum_{\mathbf{i},\mathbf{d}} \hat{\boldsymbol{S}}_{\mathbf{i}} \cdot \hat{\boldsymbol{S}}_{\mathbf{i}+\mathbf{d}} \ , \tag{1}$$

where the index $\mathbf{i} \equiv (i_1, i_2)$ runs over the sites of the square lattice, and $\mathbf{d} \equiv (\pm 1, \pm 1)$ represents the displacements of the 4 nearest-neighbors of each site. The quantum spin operators $\hat{\boldsymbol{S}}_{\mathbf{i}}$ satisfy $|\hat{\boldsymbol{S}}_{\mathbf{i}}|^2 = S(S+1)$.

Being a two-dimensional model with a continuous symmetry, this model is disordered at any finite temperature; the study of the spin correlations is then a matter of characterizing the disorder itself and its evolution as temperature and spin magnitude S vary. At T=0 and S=∞, i.e. when neither thermal nor quantum fluctuations are active, the system's ground state is the perfectly ordered Néel state. Increasing the quantum effects, by lowering the spin value, makes the ground state evolve towards different configurations which can be rigorously demonstrated [1] to be ordered as far as $S \geq 1$. No definite answer about the S=1/2 ground state is available yet, though many works, including this one, strongly suggest an ordered ground state even in the extreme quantum case. This conclusion is actually drawn out of results obtained at finite temperature through the extensive comparison with the experimental data.

What in fact makes the quantum HAF so much interesting is the existence of several real compounds whose magnetic behaviour is described by Eq. (1) which are either parent compounds of high-T_c superconductors or superconductors themselves. Also from the experimental point of view the interest mainly focuses on the spin correlations and the signature of unusual responses of the system to an external perturbation; as a consequence, amongst the most interesting physical observables that have been measured are the spin correlation length ξ, the magnetic susceptibility χ and both the dynamical and statical structure factors $S(q,\omega)$ and $S(q)$.

In this work we tackle this problem by the Pure-Quantum Self-Consistent Harmonic Approximation (PQSCHA) which has never been used in this framework, though successfully applied to the study of other magnetic systems. Beside the very good agreement we find between our results and experimental and simulation data, the importance of this work resides also in the novelty of such results being obtained in a completely new way and hence free from typical problems of previous approaches.

The 2d-QHAF can be related with the quantum field theory of the nonlinear σ model (QNLσM) in different ways. The procedure used by Haldane and Affleck [2] starts with the parametrization of the quantum spin operators by two canonically conjugated vector fields, and leads to an effective action for the QHAF which is indeed that of the QNLσM. Being based on a precise mapping, the coefficients of the model (typically the spin stiffness ρ_s and the spin wave velocity c) are univocally defined in terms of the parameters of the original Hamiltonian, i.e. S, J, the lattice constant a and the dimensionality d. This approach is justified only in the semiclassical limit $S \to \infty$ so that the comparison with experimental data from real compounds, mainly with $S \leq 5/2$, cannot be safely carried out. Haldane suggested an *ad hoc* replacement of S with $\sqrt{S(S+1)}$ to make the results more appropriate for the quantum case, but, as we have already pointed out elsewhere, the combination in which the spin length enters the results of any theory, should indeed be defined unambiguously by the theory itself.

The subsequent work by Chakravarty, Halperin and Nelson (CHN) [3] connects QHAF and QNLσM in a rather different way, i.e. showing that, because of symmetry reasons, the short-wavelength, low-energy physics of the former must be the same of that of the latter. The results obtained are valid for any value of the spin, as far as there is LRO at T=0, and can then be easily compared with experimental data. The price to pay for this gain in generality is that the theory, though depending on both ρ_s and c, does not fix their values. They have to be considered as phenomenological input parameters and determined from either experiments or simulations.

Among the many interesting results contained in the works cited above, we mainly concentrate on those for the correlation length. For models with $S \geq 1/2$, i.e. in the so-called renormalized classical regime, CHN find ξ to behave as in the classical model but with renormalized coefficients ρ_s and c; their curves fit nicely, being in fact ρ_s and c the fit parameters, with experimental data for $S=1/2$. Quite surprisingly, things get worse for higher values of S; not only further adjustment of the fit parameters are necessary to reproduce the experimental data, but the very dependence of ξ upon S cannot be physically neither understood, nor justified.

A recent work by Elstner et al. [4] highlighted the weak points of the CHN approach and showed results from high-temperature expansions which, though not actually extended to those low temperatures where most of the experimental data are available, are in good agreement with simulation data ($S=1/2$) and with some of the experimental data for $S=1$. They also find, for $S>1$ and $T \geq JS$ that the quantum correlation length is $\xi(S,T)=\xi_{\rm cl}(T_{\rm cl})$ with $T_{\rm cl} \equiv TS(S+1)$ where the appearance of $S(S+1)$ is due to a purely phenomenological substitution of S^2 with $S(S+1)$, such as that suggested by Haldane.

Let us now describe our new approach to this problem, based on the effective Hamiltonian method, which allows to express quantum thermodynamic properties and static correlation functions as renormalized classical-like averages. The procedure leading to the effective Hamiltonian, i.e. the PQSCHA, is described in Ref. [5] and has already been applied to anisotropic spin systems [6].

One of the distinctive features of the PQSCHA is that of separating the classical from the pure-quantum contribution, so that the one-loop approximation we introduce to deal with the former, does not affect the latter. If we then consider that the longer is the wavelength of an excitation, the more classical is its character, we conclude that the PQSCHA not only exactly takes into account linear excitations, but also very accurately describes the long-wavelength non-linear ones. Besides all the advantages deriving from this property, in the 2d-QHAF case we must add that of making the first step of the PQSCHA, i.e. the introduction of a spin-boson transformation, easily acceptable. Because of the symmetry of Eq. (1) we cannot use the Villain transformation, mainly designed for easy-plane systems, but at the same time neither the Holstein-Primakoff (HP) nor the Dyson-Maleev (DM) transformations do apparently give a suitable alternative, as they both break the symmetry of the problem. However, we know that the broken symmetry of the 2d-QHAF's ground state is restored at finite temperature by those non linear excitations that are very well described, for their being essentially classical, by the PQSCHA: This indeed permits us the use of the HP and DM transformations in a wide range of temperatures. The possibility of a completely disordered ground state is not considered in this paper, as we think that for any physical value of the spin (i.e. for $S \geq 1/2$) the ground state of the 2d-QHAF has long range order. The good agreement we find between our results and experimental and simulation data indirectly confirms this statement.

Moving towards the final expression of the effective Hamiltonian we subdivide the lattice in the usual AFM *positive* and *negative* sublattices, being $(-)^{\mathbf{i}}=+$ or $-$ depending on whether the site labelled by $\mathbf{i}$ belongs to the former or the latter. The DM transformation for spins on the positive sublattice is

$$\begin{aligned} \hat{S}^+_{\mathbf{i}} &= (2S)^{\frac{1}{2}}\, \hat{a}_{\mathbf{i}} \;, \\ \hat{S}^-_{\mathbf{i}} &= (2S)^{-\frac{1}{2}}\, \hat{a}^\dagger_{\mathbf{i}}\, (2S - \hat{a}^\dagger_{\mathbf{i}} \hat{a}_{\mathbf{i}}) \;, \\ \hat{S}^z_{\mathbf{i}} &= S - \hat{a}^\dagger_{\mathbf{i}} \hat{a}_{\mathbf{i}} \;, \end{aligned} \tag{2}$$

while that for those sitting on the negative sublattice is obtained by Eqs. (2) by replacing $\hat{S}^\mu_{\mathbf{i}} \to -(\hat{S}^\mu)^\dagger$ ($\mu=z,+,-$). Both transformations are canonical, being the spin commutation relations consequence of $[\hat{a}_{\mathbf{i}}, \hat{a}^\dagger_{\mathbf{i}}] = 1$, and satisfy $|\hat{\boldsymbol{S}}|^2 = S(S+1)$; they are normally ordered in the boson operators $(\hat{a}^\dagger, \hat{a})$ and transform Eq. (1) in a normal ordered boson Hamiltonian with quartic interaction $\hat{\mathcal{H}}(\hat{a}^\dagger, \hat{a})$; its normal symbol $\mathcal{H}_{\rm N}(a^*, a)$ is simply obtained replacing the Fock operators with commuting holomorphic variables, $(\hat{a}^\dagger, \hat{a}) \to (a^*, a)$, and its Weyl symbol [5,7] $\mathcal{H}(a^*, a)$ obtained by the relation [7] $\mathcal{H}(a^*, a) = \exp\big(-\frac{1}{2}\partial_a \cdot \partial_a\big)\, \mathcal{H}_{\rm N}(a^*, a)$. The Weyl symbols for the DM spin operators in the positive sublattice are

$$\begin{aligned} S^+_{\mathbf{i}} &= (2S)^{\frac{1}{2}}\, a_{\mathbf{i}} \;, \\ S^-_{\mathbf{i}} &= (2S)^{-\frac{1}{2}}\, (2\widetilde{S} - a^*_{\mathbf{i}} a_{\mathbf{i}})\, a^*_{\mathbf{i}} \;, \\ S^z_{\mathbf{i}} &= \widetilde{S} - a^*_{\mathbf{i}} a_{\mathbf{i}} \;, \end{aligned} \tag{3}$$

in which the substitution $\hat{S}^\mu_{\mathbf{i}} \to -(\hat{S}^\mu)^*$ gives those for $(-)^{\mathbf{i}}=-$. As a consequence of having properly considered the ordering problem, we see that $|\boldsymbol{S}_{\mathbf{i}}|^2 = S^z_{\mathbf{i}} S^z_{\mathbf{i}} + S^+_{\mathbf{i}} S^-_{\mathbf{i}} = \widetilde{S}^2$ and the effective spin length $\widetilde{S} \equiv S + \frac{1}{2}$ naturally appears: No need then for any *ad hoc* or *purely empirical* definition of it! In what follows, the reduced temperature is consequently defined as $t \equiv T/(J\widetilde{S}^2)$.

Following the procedure described in [5] and [8] we obtain the effective Hamiltonian

$$\mathcal{H}_{\rm eff} = -\frac{J\widetilde{S}^2\theta^4}{2} \sum_{\mathbf{i},\mathbf{d}} \boldsymbol{s}_{\mathbf{i}} \cdot \boldsymbol{s}_{\mathbf{i}+\mathbf{d}} + NJ\widetilde{S}^2\, \mathcal{G}(t) \;, \tag{4}$$

where $\boldsymbol{s}_{\mathbf{i}}$ are classical unit vectors. The term $\mathcal{G}(t) = tN^{-1}\sum_{\mathbf{k}} \ln[\sinh f_k/(\theta^2 f_k)] - 2\theta^2\mathcal{D}$ is uniform and does not play any role in calculating thermal averages.

The renormalization parameter $\theta^2 \equiv 1 - \mathcal{D}/2$ represents the effect of pure-quantum fluctuations,

$$\mathcal{D} = \frac{1}{\widetilde{S}\,N} \sum_{\mathbf{k}} (1-\gamma^2_{\mathbf{k}})^{\frac{1}{2}} \Big(\coth f_{\mathbf{k}} - \frac{1}{f_{\mathbf{k}}} \Big) \;, \tag{5}$$

where $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$ and $f_{\mathbf{k}} = \omega_{\mathbf{k}}/(2\widetilde{S}T)$. A further low-coupling approximation leads to the coupled equations

$$\omega_{\mathbf{k}} = 4\kappa^2\sqrt{1-\gamma_{\mathbf{k}}} \quad ;$$
$$\kappa^2 = 1 - \frac{1}{N\widetilde{S}}\sum_{\mathbf{k}}\sqrt{1-\gamma_{\mathbf{k}}^2}\coth\left(\frac{\omega_{\mathbf{k}}}{2\widetilde{S}t}\right)$$

whose self-consistent solution finally closes the whole scheme. At variance with previous applications of the PQSCHA, the frequency spectrum does not depend upon the pure-quantum coefficient θ^2, but rather upon the SCHA renormalization coefficient κ^2; this is due to the use of a slightly different and more refined LCA made necessary by the pronounced instability of the ground state. The well known unphysical break-down of the SCHA frequencies renormalization $\kappa^2(t)$ occurring at $t=\theta^4$ can be avoided by inserting a proper cut-off for the contributions of wavelengths larger than 2ξ, as described in Refs. [8].

The PQSCHA expressions for the spin-spin correlation functions are similarly found to be

$$(-)^{\mathbf{r}}\langle\hat{\boldsymbol{S}}_{\mathbf{i}}\cdot\hat{\boldsymbol{S}}_{\mathbf{i}+\mathbf{r}}\rangle = (-)^{\mathbf{r}}\widetilde{S}^2\theta_{\mathbf{r}}^4\langle\boldsymbol{s}_{\mathbf{i}}\cdot\boldsymbol{s}_{\mathbf{i}+\mathbf{r}}\rangle_{\rm eff}\ , \qquad (6)$$

where $\langle\boldsymbol{s}_{\mathbf{i}}\cdot\boldsymbol{s}_{\mathbf{i}+\mathbf{r}}\rangle_{\rm eff}$ is the classical like average with the effective Hamiltonian and the parameter $\theta_{\mathbf{r}}^4$ tends to a constant value as $|\mathbf{r}|$ increases. Because of the symmetry of Eq. (1), the renormalization coefficient $\theta^4(S,t)$ enters the effective Hamiltonian Eq. (4) just as a multiplying factor, so that any $\langle\,\cdot\,\rangle_{\rm eff}$ at a given temperature t is just equal to the classical average at a higher temperature $t/\theta^4(S,t)$. As for the correlation length this means that the quantum correlation length $\xi(S,t)$ is related to its classical counterpart by

$$\xi(t,S) = \xi_{\rm cl}(t_{\rm cl}) \quad \text{where} \quad t_{\rm cl}{=}\frac{t}{\theta^4(S,t)}\ . \qquad (7)$$

Given the value of J and the classical $\xi_{\rm cl}(t)$, we do not need any external parameter or input of any kind to obtain, from Eqs. (7), the curves to compare with experimental and simulation data, or with results from other approaches. Values for $\xi_{\rm cl}$ in the range $1 \lesssim \xi \lesssim 8$ have been obtained by Monte Carlo simulation [9] and by high-temperature expansion [4] (HTE); we ourselves have performed some more Monte Carlo simulations to extend this data range [8]. All the available classical data sets agree with each other, so we have used the data of Ref. [4] and ours, and fitted them by a (polynomial × exponential) curve in the range $1 \lesssim \xi \lesssim 50$. In Fig. 1 we report our result for $\xi(t)$ at spin $S=\frac{1}{2}$ together with experimental data for $Sr_2CuO_2Cl_2$ [10,11], for La_2CuO_4 [12,13] and with quantum Monte Carlo results [14]. In Fig. 2 we compare our curve at spin $S=1$ with experimental data for La_2NiO_4 [15] and for K_2NiF_4 [11].

Our results appear to explain all the experimental data [10–13,15,11] for different values of S without any fitting parameters and they also agree with the HTE results of Ref. [4]. This gives evidence of our approach being an important step forward in the direction of the full understanding of the real quantum Heisenberg antiferromagnet, and perhaps in the possible overtaking of the QNLσM approach.

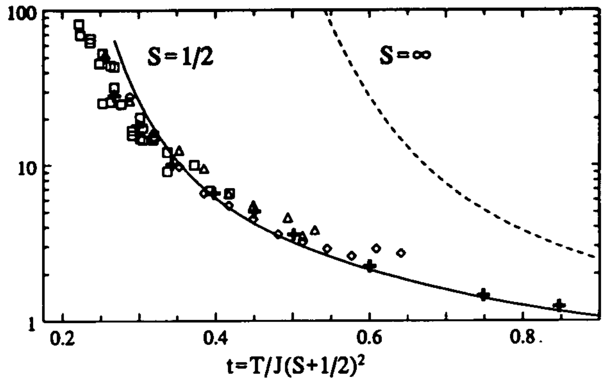

FIG. 1. Correlation length $\xi(t)$ for spin $S=\frac{1}{2}$. Continuous line: this work; dashed line: classical results from [9] and [8]. Squares: experimental data [10,11] for $Sr_2CuO_2Cl_2$; triangles and diamonds: data for La_2CuO_4 from neutron scattering [13] and from ^{63}Cu NQR relaxation [12] experiments, respectively; crosses: quantum Monte Carlo results [14].

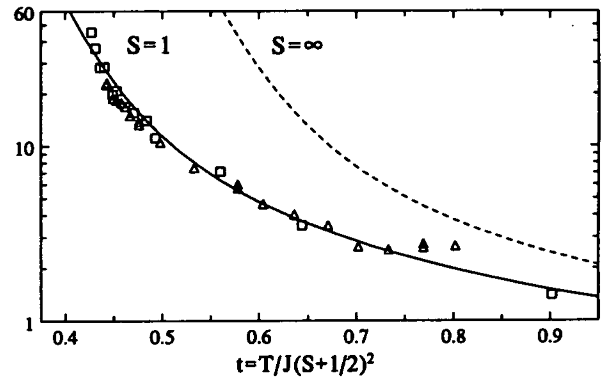

FIG. 2. Correlation length for spin $S=1$. Triangles: experimental data [15] for La_2NiO_4; squares: experimental data [11] for K_2NiF_4. Lines as in Fig. 1.

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