

Short-range spin- and pair-correlations: a variational wave-function

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Abstract

A many-body wave-function is postulated, which is sufficiently general to describe superconducting pair-correlations, and/or spin-correlations, which can occur either as long-range order or as finite-range correlations. The proposed wave-function appears to summarize some of the more relevant aspects of the rich phase-diagram of the high- T_c cuprates. Some of the states represented by this wave-function are reviewed: for superconductivity in the background of robust anti-ferromagnetism, the Cooper-pairs are shown to be a superposition of spinquantum numbers $S = 0$ and 1. If the anti-ferromagnetism is weak, a continuous super-symmetric rotation is identified connecting s-wave superconductivity to anti-ferromagnetism.

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1. Introduction

The large variety of phenomena due to correlations between electrons in solids is one of the major challenges of contemporary physics. Over the past 80 years this subject has formed the arena of many new developments in theoretical physics. The most common approach to the many-body problem is, to define in the first step a model defined as a Hamiltonian, Lagrangian, or action, describing the most important interactions of the system one tries to understand. In the second step one tries to solve the corresponding equations of motion. Apart from a few special cases, no exact solution is known of the Schrödinger equation of a large number of interacting particles. To circumvent this problem two different approaches are most frequently used, often in combination with each other: one is to devise an analytical approximation scheme, which ultimately may provide an approximate solution. The other is to use computational techniques for a finite size cluster.

An alternative approach, which has sometimes been quite successful, is to start with designing a variational many-body ground-state wave-function with the desired characteristics of (for example) the pair-correlation function, spin-polarization, etc. One can then subsequently try to find a model Hamiltonian which will produce (i) the aforementioned many-body wave-function as it is ground-state

and (ii) the low energy excitations which are important for determining the thermal properties and the various spectral functions all of which can be measured experimentally.

The variational wave-function approach has been used with great success for superconductivity [1], the fractional quantum Hall effect [2], and the resonating valence bond [3–7]. Other striking examples of this ‘bottom-up’ approach are the Affleck-Marsten flux-phase [8–13], or d-density wave [14], the mixed anti-ferromagnetic/superconducting state [15], and the Gossamer superconducting wave-function [16,17].

Here we use the many-body wave-function approach to explore the possibility of (anti)-ferromagnetism, superconductivity, and local pairs within the same phase-diagram. Our ansatz for the many-body wave-function is

$$|\Psi\rangle = C \exp \left\{ \sum_G \sum_k f(k, G) c_{k\uparrow}^\dagger c_{-k+G\downarrow}^\dagger \right\} |0\rangle \quad (1)$$

where C is a normalization constant. The function $f(k, G)$ is a distribution function of the center-of-mass momentum (G) and the relative momentum ($2k$) of pairs of electrons. Below we will see, that $f(k, G)$ represents several types of different correlations within the interacting electronic system. Moreover, Eq. (1) is sufficiently general to capture, besides less familiar states of matter, several well known states of matter, such as superconductivity, anti-ferromagnetism, resonating valence bond states, and the non-interacting electron gas. It therefore may be a useful starting point for

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the rich phase-diagram of the high- T_c cuprates, and of the heavy-fermion superconductors. In the subsequent discussion we will frequently refer to the projection of Eq. (1) on the subspace with $2N$ electrons

$$|\Psi_{2N}\rangle = C \exp \left\{ \sum_G \sum_k f(k, G) c_{k\uparrow}^\dagger c_{-k+G\downarrow}^\dagger \right\}^N |0\rangle \quad (2)$$

This expression is a generalization of the many-body wave-function describing the simultaneous occurrence of superconductivity and anti-ferromagnetism [15] to arbitrary distributions $f(k, G)$, of the center of mass momentum G .

2. Superconductivity

Let us first consider the special case, that the distribution function $f(k, G)$ is a Dirac δ -function of the center-of-mass momentum: $f(k, G) = \delta(G, 0) \psi_k$.

$$|\Psi_{2N}\rangle = C \hat{P}_{2N} \exp\{A_0^\dagger\} |0\rangle \quad (3)$$

where \hat{P}_{2N} is the projection on states with $2N$ electrons, and

$$A_0^\dagger \equiv \sum_k \phi_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \quad (4)$$

creates a pair of electrons with zero center-of-mass momentum. The exponential function of A_0^\dagger appearing in Eq. (3), can be expanded in a Taylor's series. The term containing $2N$ electrons

$$|\Psi_{2N}\rangle = \{A_0^\dagger\}^N |0\rangle \quad (5)$$

is similar to a Bose–Einstein condensate of N composite bosons, each consisting of a pair of electrons. In a superconductor this state is realized if we cool an isolated lump of material with known number of electrons below the phase transition. Bardeen, Cooper, and Schrieffer considered a phase-coherent superposition of states containing different numbers of pairs:

$$|\Psi_\phi\rangle = C \sum_N e^{i\phi N} |\Psi_{2N}\rangle \quad (6)$$

which can be shown to be equivalent to the state

$$|\Psi_\phi\rangle = \prod_k (u_k + e^{i\phi} v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle \quad (7)$$

where $\psi_k = v_k/u_k$ and $|v_k|^2 + |u_k|^2 = 1$. In the limit case, where $|v_k|^2 \rightarrow 1$ for $|k| \leq k_F$ and $|v_k|^2 \rightarrow 0$ for $|k| > k_F$, this product is just the ground-state of the non-interacting electron gas

$$|\Psi_0\rangle = \prod_{k,\sigma} \theta_k^F c_{k\sigma}^\dagger |0\rangle \quad (8)$$

where the occupation number θ_k^F is 0 or 1 depending on whether the state is above or below the Fermi level, respectively.

3. Anti-ferromagnetism

Another well-documented limit of Eq. (2) is presented by the anti-ferromagnetic state. To be specific, we consider a square lattice in two space-dimensions, with site-alternating up- and down polarization. The anti-ferromagnetic Bragg vector is $Q = (\pi, \pi)$ in this case, and the operators which create an electron on the two sublattices are

$$a_{k\sigma}^\dagger = \frac{1}{\sqrt{2}}(c_{k\sigma}^\dagger - c_{k+Q\sigma}^\dagger), \quad b_{k\sigma}^\dagger = \frac{1}{\sqrt{2}}(c_{k\sigma}^\dagger + c_{k+Q\sigma}^\dagger), \quad (9)$$

respectively. The single particle operators of the anti-ferromagnetic state are

$$\begin{aligned} \varepsilon_k^- : \quad \alpha_{k\uparrow}^\dagger &= \mu_k c_{k\uparrow}^\dagger - v_k c_{k+Q\uparrow}^\dagger & \text{and} & \quad \beta_{k\downarrow}^\dagger = v_k c_{k\downarrow}^\dagger + \mu_k c_{k+Q\downarrow}^\dagger \\ \varepsilon_k^+ : \quad \beta_{k\uparrow}^\dagger &= v_k c_{k\uparrow}^\dagger + \mu_k c_{k+Q\uparrow}^\dagger & \text{and} & \quad \alpha_{k\downarrow}^\dagger = \mu_k c_{k\downarrow}^\dagger + v_k c_{k+Q\downarrow}^\dagger \end{aligned} \quad (10)$$

where the coefficients satisfy $\mu_k = \mu - k$, $v_k = v - k$, $\mu_k + Q = v_k$, $v_k + Q = \mu_k$, and $|\mu_k|^2 + |v_k|^2 = 1$. The energies ε_k^\pm are determined by the details of the energy–momentum dispersion of the $c_{k\sigma}^\dagger$ -operators and by the interactions giving rise to the anti-ferromagnetism. For simplicity we consider here the case where only one of the two sub-bands is occupied, which assumes that the anti-ferromagnetic splitting is very large. The ground-state wave-function is obtained by partially or fully occupying the lowest band

$$|\Psi_{AF}\rangle = \prod_k \theta_k^F \alpha_{k\uparrow}^\dagger \beta_{k\downarrow}^\dagger |0\rangle \quad (11)$$

The states with momentum k and $-k$ are degenerate, so we may replace $\alpha_{k\uparrow}^\dagger \beta_{k\downarrow}^\dagger$ with $\alpha_{k\uparrow}^\dagger \beta_{-k\downarrow}^\dagger$ in the above product. Because each electron-state can only be created once, this is equivalent to

$$|\Psi_{AF}\rangle = \left\{ 2^{-1/2} \sum_k \theta_k^F \alpha_{k\uparrow}^\dagger \beta_{-k\downarrow}^\dagger \right\}^N |0\rangle \quad (12)$$

The derivation of Eq. (12) employs the property that $\alpha_{k\uparrow}^\dagger$ and $\beta_{k\downarrow}^\dagger$ are orthogonal to each other, consequently all two-particle operators under the summation commute with each other. In the first (reduced) Brillouin-zone of the anti-ferromagnetic state the occupation function θ_k^F is either 1 or 0. In Eq. (12) and in later similar expressions the summation over k refers to the paramagnetic (extended) Brillouin-zone. The factor $2^{-1/2}$ compensates for the double counting. However, $\alpha_{k\sigma}^\dagger = -\alpha_{k+Q\sigma}^\dagger$ and $\beta_{k\sigma}^\dagger = \beta_{k+Q\sigma}^\dagger$. To avoid the complete cancellation of terms originating from the first and second reduced Brillouin-zone, it is therefore important to define $\theta_{k+Q}^F = -\theta_k^F$ for k in the second reduced Brillouin-zone.

To see the relation with Eq. (2) we substitute for $\alpha_{k\uparrow}^\dagger$ and $\beta_{-k\downarrow}^\dagger$ the original $c_{k\sigma}^\dagger$ -operators in the paramagnetic Brillouin-zone using Eq. (10). We then decompose the summation over k in separate terms corresponding to different

quantum numbers for the spin and the center-of-mass momentum

$$\begin{aligned} \sum_k \theta_k^F \alpha_{k\uparrow}^\dagger \beta_{-k\downarrow}^\dagger &= 2 \sum_k \theta_k^F (\mu_k v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \mu_k^2 c_{k\uparrow}^\dagger c_{-k+Q\downarrow}^\dagger) \\ &= \sum_k f_o^e(k) c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \sum_k (g^e(k) \\ &\quad + g^o(k)) c_{k+Q/2\uparrow}^\dagger c_{-k+Q/2\downarrow}^\dagger \end{aligned} \quad (13)$$

where

$$\begin{aligned} f_o^e(k) &= \theta_k^F (2\mu_k v_k) \\ g^e(k) &= \theta_{k+Q/2}^F (\mu_{k+Q/2}^2 - v_{k+Q/2}^2) \\ g^o(k) &= \theta_{k+Q/2}^F \end{aligned} \quad (14)$$

This concludes the proof, that Eq. (2) is sufficiently general to also contain the anti-ferromagnetic state as one of the possibilities. The distribution-function of the center-of-mass momentum, $f(k, G)$, is a superposition of two δ -functions: The first at $G = 0$ is an even function of k and therefore creates a pair with spin quantum number zero. The second δ -function at the anti-ferromagnetic Bragg-vector $G = (\pi, \pi)$ contains two contributions with different spin quantum-numbers. Since $\theta_{-k+Q/2} = \theta_{k-Q/2} = -\theta_{k+Q/2}$, and $\mu_{-k+Q/2}^2 = \mu_{k-Q/2}^2 = v_{k+Q/2}^2$, the functions $g^e(k)$ and $g^o(k)$ are even and odd functions of k respectively. Hence the first of the two terms with center-of-mass momentum Q corresponds to a $S = 0$ state. The other term is an odd function of k , and corresponds to the $m_S = 0$ member of the ($S = 1$) spin-triplet.

A well-known property of the anti-ferromagnetic state is the broken SU(2) symmetry. This symmetry breaking is illustrated by the fact, that Eq. (13) corresponds to a superposition of pair-states with different spin quantum numbers (i.e. $S = 0$ and 1). Eq. (13) is also a superposition of pair-states with different center-of-mass quantum numbers, and this illustrates the fact that the anti-ferromagnetic state also breaks the discrete translational invariance of the lattice.

The spin-polarization depends on the value of $\mu_k^2 = 1 - v_k^2$. For example $\mu_k = v_k = 1/\sqrt{2}$ corresponds to full spin-polarization, where the electrons move either completely in sublattice a with spin \uparrow , or in sublattice b with spin \downarrow . From Eq. (14) we see that the fully polarized anti-ferromagnetic state can be regarded as a simultaneous condensation in a singlet state with momentum $G = 0$ and a triplet with momentum $G = (\pi, \pi)$, both having the same amplitude.

4. Superconductivity and anti-ferromagnetism

The results of this section and the previous one can be summarized by a diagram displaying the center-of-mass distribution function $f(k, G)$ averaged over the relative coordinate $F(G) \equiv \sum_k |f(k, G)|^2$. In Fig. 1 this

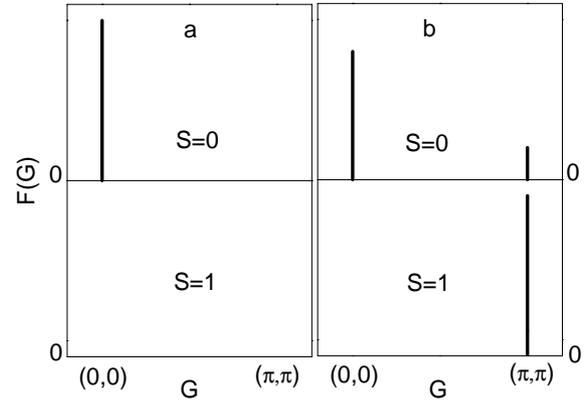


Fig. 1. Distribution of the center-of-mass momentum for (a) a BCS-superconductor (b) an anti-ferromagnet. The positive (negative) values correspond to the singlet (triplet) channels. The vertical bars indicate δ -functions, the area of which is represented by the length of the bar.

function is displayed for the superconducting state and the anti-ferromagnetic state. We point out two important aspects of the BCS-wave-function of the superconducting state:

- (1) The internal structure of the Cooper-pairs (i.e. the pairing symmetry and the degree of localization of the pairs) is completely determined by v_k and u_k in Eqs. (6) and (7): The function $\psi_k = v_k/u_k$ is the Fourier-transform of the wave-function describing the relative coordinate of the electrons forming a Cooper-pair [18].
- (2) All pairs are condensed in a state with zero center-of-mass momentum $G = 0$, regardless of the details of the internal structure of the pairs.

Although the long-range anti-ferromagnetic state is characterized by two δ -functions for the center-of-mass momentum G , Eq. (13) does not correspond to a true superconducting state, because the occupation function θ_k^F has a sharp cut-off at the Fermi-momentum.

4.1. Superconductivity in the background of anti-ferromagnetism

We first consider the situation, where the anti-ferromagnetism has been stabilized on a high energy scale, and superconductivity is a relatively weak phenomenon. Under those conditions it is a good approximation to assume that the onset of superconductivity does not affect the anti-ferromagnetic order parameter. The simultaneous occurrence of superconductivity and anti-ferromagnetism requires that θ_k^F is replaced with the smooth function $v_k = u_k$, as usual in a BCS-type superconductor. In principle this smooth function may be different for the three different terms with differing quantum numbers, and the corresponding many-body wave-function was described by Chen et al. [15], but in the fully polarized anti-ferromagnet we expect a single distribution function, so that the superconducting/anti-ferromagnetic wave-function can be

transformed to up- and down-spin sublattice-operators using Eq. (9)

$$|\Psi_{AF}\rangle = \prod_k \frac{v_k}{u_k} a_{k\uparrow}^\dagger b_{k\downarrow}^\dagger |0\rangle \quad (15)$$

Interestingly, in this example the Cooper-pairs are a superposition of an $S = 0$ and an $S = 1$ spin-state with equal amplitudes for the $S = 0$ and 1 contributions. In other words, the superconducting state of a fully polarized anti-ferromagnet is a condensate with a broken $SU(2)$ symmetry, with Cooper-pairs which have one spin-up electron on sublattice a , and one spin-down electron on sublattice b . In the partially polarized anti-ferromagnet the amplitude of the $S = 1$ contribution is different from the $S = 0$ weight a $Q = (\pi, \pi)$. The degree of polarization of the Cooper-pairs depends on the details of the pairing-mechanism and the degree of polarization of the underlying anti-ferromagnetic state. For vanishing spin-polarization $SU(2)$ -symmetry should be restored, and the Cooper-pairs are either in an $S = 1$ state or in an $S = 0$ state, depending on the parity of $v_k = u_k$.

5. Supersymmetric rotations and $SO(5)$

A different situation arises, when the anti-ferromagnetic correlations and the superconducting correlations are stabilized on comparable energy scales. In this case the anti-ferromagnetism can be partially or totally suppressed when superconducting order sets in and vice-versa. An elegant approach to this phenomenon is the group-theory, which uses the super-symmetric $SO(5)$ extension of the direct product of $U(1)$ corresponding to the superconducting phase, and of $SO(3)$ corresponding to the anti-ferromagnetic order parameter [19]. In this so-called $SO(5)$ theory, the anti-ferromagnetic state and the d-wave superconducting state are regarded as two different projections of a generalized higher dimensional order parameter. It is tempting to regard Eq. (13) as a manifestation of precisely this $SO(5)$ symmetry, namely, that the d-wave superconducting condensate can be transformed into anti-ferromagnetic state by adiabatically adding the additional triplet condensate at $G = (\pi, \pi)$. However, in Eq. (13) the singlet at $G = 0$ has s-wave symmetry. Hence, although our wave-function does support a super-symmetric rotation from anti-ferromagnetism to s-wave pairing by mixing in a triplet-condensate at $G = (\pi, \pi)$, a similar construction connecting d-wave pairing to anti-ferromagnetism appears to be absent [20]. In principle we could postulate an unconventional anti-ferromagnetic order parameter μ_k which has a d -wave symmetry with nodes along the diagonal directions. Such an order parameter transforms to a d -wave superconducting order parameter if we reduce the singlet and triplet condensates at $G = (\pi, \pi)$ to zero.

6. Local pairs

It has often been speculated that a remnant of the Cooper-pairs may exist even if the material is not superconducting. This would require that those pairs are not condensed in the same state. The variational wave-function proposed by Bardeen, Cooper, and Schrieffer does not include this possibility. On the other hand the situation sketched in Fig. 1a can be easily generalized to describe a paired state with no long range superconducting order, by replacing the Dirac δ -function of the center-of-mass coordinate with the Lorentzian $1/(1 + l^2|G|^2)$. The width of this distribution, $1/l$ then corresponds to the inverse of length over which the pairs maintain the phase-coherence. A transition to the superconducting state as a function of temperature, or another control parameter, is in this scenario characterized by the appearance of the Dirac δ -function at the origin. Note, that for the existence of superconductivity it is not necessary that the entire distribution collapses into the δ -function, not even at $T = 0$. This scenario, depicted in Fig. 2, is reminiscent of the experiments with Bose–Einstein condensation. Yet, the pairs in this wave-function are not real bosons. In principle it is not even required that they are strongly localized in space, although the conditions giving rise to this type of phase transition would typically cause the pairs to be rather small. States of the type displayed in Fig. 2a have a simple representation in real space. Starting from Eq. (2), we insert the real-space representation of the creation operators $c_{k\sigma}^\dagger = \sum_R e^{ikR} c_{j\sigma}^\dagger$, and obtain

$$|\Psi_{2N}\rangle = C \left\{ \sum_{m,n} \tilde{f}(r_m, r_n) c_{m\uparrow}^\dagger c_{n\downarrow}^\dagger \right\}^N |0\rangle \quad (16)$$

where $\tilde{f}(r_m, r_n) \equiv \sum_{k,G} e^{i(k(r_m-r_n)+G r_m)} f(k, G)$ is the double Fourier-transform of the momentum distribution function. A state with near-neighbor resonating bonds is

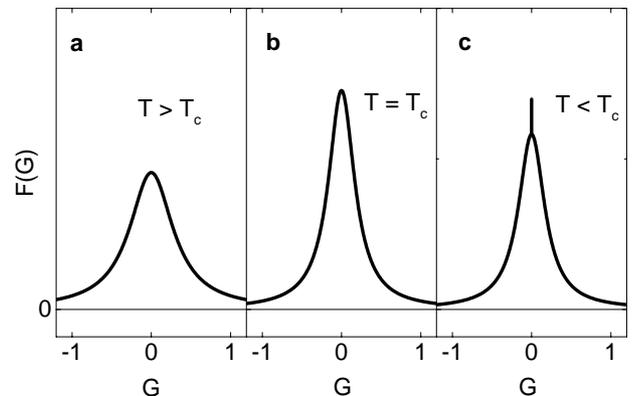


Fig. 2. Non-BCS scenario for the evolution from the normal to the superconducting state. Panels (a) and (b) correspond to a situation where pairs are already formed, but no condensation has yet occurred. The superconducting state is only reached when the δ -function gains a finite intensity, as indicated in panel (c).

constructed by defining

$$\tilde{f}(r_m, r_n) = e^{-|r_m + R_n|/(2l)} \delta_{\langle m, n \rangle} \{(x_m - x_n) + i(y_m - y_n)\}^L \quad (17)$$

where l measures the range of the RVB correlations, $\delta_{\langle m, n \rangle}$ selects out nearest-neighbor bonds, and the last factor selects the state with relative angular momentum L . A Gutzwiller projection is still required if we want to exclude the doubly occupied sites. The representation in k -space is

$$|\Psi_{2N}\rangle = C \hat{P} \left\{ \sum_{G,k} e^{i\phi(G)} \frac{\cos(k_x) \pm \cos(k_y)}{1 + l^2|G|^2} c_{k+G/2\uparrow}^\dagger c_{-k+G/2\downarrow}^\dagger \right\}^N |0\rangle \quad (18)$$

where the \pm sign refers to $L = 0$ or $L = 2$ angular momentum states respectively, $\phi(G)$ is a random phase, and \hat{P} is the Gutzwiller projection operator. The true RVB state [3–7] corresponds to taking the limit $l \rightarrow \infty$ in the above expression. In this limit this state becomes equivalent to a BCS-type superconducting wave-function with either extended s -wave symmetry or d -wave symmetry, with the two paired holes on a nearest-neighbor distance. In a superconductor with a small gap, the k -dependent factor inside the curly brackets has a strong k -dependence, corresponding to singlet-bonds on a range much longer than a nearest neighbor distance in $\tilde{f}(r_m, r_n)$.

7. Finite range magnetic correlations

Likewise a wave-function corresponding to a state of short-range magnetic correlations can be easily constructed by replacing the Dirac δ -functions in Fig. 2b with distribution functions with a finite width. The corresponding structure sketched in Fig. 3a corresponds to the magnetic structure-factor measured with neutron scattering, and the width of the distribution is inversely proportional to the anti-ferromagnetic correlation length. Like for the

superconducting state, long-range anti-ferromagnetic order is characterized by the condensation of part of the spectral weight into the δ -function at $G = (\pi, \pi)$. By shifting the peak in the distribution function from (π, π) to another value of the wavevector G , the formalism can be used to describe short- or long-range incommensurate spin-density waves.

8. Summary and conclusions

We have generalized earlier expressions of many-body wave-functions to a formula, Eq. (1), which envelopes many known or suspected types of spin- and pairing order of the high T_c cuprates and of some of the heavy fermion superconductors. We have used this approach to show that anti-ferromagnetism can be regarded as the simultaneous condensation of $S = 0$ singlets at $G = 0$ and Q , and of $S = 1$ triplets at $G = Q$ where Q is the anti-ferromagnetic Bragg-vector. The possibility of superconductivity and anti-ferromagnetism occurring simultaneously can be easily described this way. In principle the calculation of matrix-elements of the Hamiltonian, as well as most operators corresponding to experimentally measurable quantities, is unproblematic at least in the examples where the center-of-mass momentum, G , has a single discrete value. The general case presented by the proposed wave-function allows G to be distributed over a finite range of k -space. In the latter case it appears to be more problematic to obtain analytical expressions of the aforementioned matrix-elements. The latter forms, as yet, the main obstacle for using Eq. (1) in a variational calculation of the ground state and the excitation spectrum. If this obstacle can be taken, this could offer a straightforward analytical approach to the rich phase diagram of the high- T_c cuprates.

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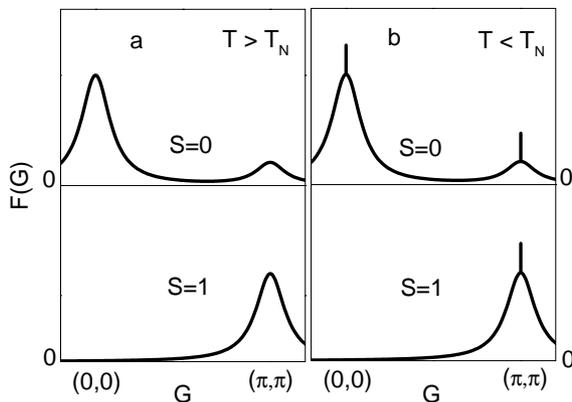


Fig. 3. Scenario for the evolution from a state with short range anti-ferromagnetic order (panel a) to the Néel state with long range order (panel b).

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