Isolated ferromagnetic bonds in the two-dimensional anisotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnet

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An isolated ferromagnetic bond of coupling constants K_z and K_{xy} replacing an antiferromagnetic link in the spin-$\frac{1}{2}$ anisotropic Heisenberg antiferromagnet of coupling constants $J_z \geq J_{xy}$ on a square lattice is investigated within the linearized spin-wave approximation. Two competing interactions affect the local ordered magnetic moment $\langle S_i^z \rangle$ and the correlation $\langle S_i^x S_j^x \rangle$: The longitudinal terms J_z tend to enhance the sublattice magnetization, while the transverse terms J_{xy} represent the quantum fluctuations that suppress the long-range order. We analyze the interplay between these two effects as a function of K_z and K_{xy} at the impurity link. The linearized spin-wave approximation breaks down for sufficiently large K_z and K_{xy} as a consequence of the frustration of the two plaquettes adjacent to the ferromagnetic bond.

I. INTRODUCTION

The discovery of numerous high-temperature superconductors has revived the interest in the two-dimensional Heisenberg antiferromagnet. Several mechanisms for high-T_c superconductivity invoke the strong antiferromagnetic correlations within the CuO planes. Properties of the high-T_c compounds are believed to be related to defects in the planes, e.g., static vacancies,[1,2] mobile holes,[3,4] and ferromagnetic bonds.[5-7]

The addition of holes in La_2CuO_4, e.g., by doping with Sr, introduces a local effective ferromagnetic exchange coupling between the Cu spins.[8] The resulting frustration affects the antiferromagnetic correlations in the neighborhood of the ferromagnetic link. In Ref. 8 it is argued that these ferromagnetic defects are the origin of the spin-glass[9] and superconducting phases of $La_{2-x}Sr_xCuO_4$.

In a previous paper[5] we studied the effects of an isolated isotropic ($K_z = K_{xy} = K$) ferromagnetic link on an otherwise antiferromagnetic square lattice with isotropic Heisenberg nearest-neighbor coupling ($J_z = J_{xy}$). We assumed that the simple linearized spin-wave theory provides a reasonable description of the antiferromagnet at $T = 0$. The ground state has a broken symmetry (Néel state) and quantum fluctuations reduce the sublattice magnetization to an ordered moment of about 0.3. This is in reasonable agreement with the available numerical results for the square lattice.[10] Since the scattering potential arising from the impurity link is factorizable, the problem of one isolated ferromagnetic bond embedded in an antiferromagnetic lattice can be solved exactly within the linearized spin-wave approximation (LSWA).

The main results of Ref. 5 are the following. There are two competing interactions affecting the sublattice magnetization: The longitudinal terms, involving S_z, tend to enhance the ordered staggered magnetic moment, while the transverse terms, involving S_x and S_y, represent the quantum fluctuations that suppress the sublattice magnetization. For small K, the quantum fluctuations are reduced in the neighborhood of the impurity link and the local magnetic moment is enhanced. This process is reversed with increasing K, i.e., the staggered magnetization is gradually suppressed close to the impurity link and the two spins joined by the ferromagnetic bond tend to form a triplet state. This ultimately leads to the breakdown of the LSWA.

In this paper we extend our investigation of the interplay of the longitudinal and transversal terms in the Hamiltonian by studying an anisotropic ferromagnetic link ($K_z \neq K_{xy}$) embedded in an antiferromagnetic Ising-Heisenberg square lattice ($J_z \geq J_{xy}$). We discuss the ordered magnetic moment at the impurity bond, as well as the $\langle S_i^x S_j^x \rangle$ correlation across the link, which again can be obtained exactly within the LSWA. Although the excitation spectrum of the lattice now has a gap for $J_z > J_{xy}$, the LSWA still breaks down for sufficiently large K_z and K_{xy}.

The rest of the paper is organized as follows. In Sec. II, we introduce the model and obtain its exact solution within the LSWA. Our results and concluding remarks are presented in Sec. III.

II. MODEL AND CALCULATION

We consider the two-dimensional spin-$\frac{1}{2}$ antiferromagnet on a square lattice with nearest-neighbor coupling only. The link joining the sites 0 and 1 is replaced by a ferromagnetic one of strength K_z and K_{xy}. The Hamiltonian then has the following form:

$$H = \frac{1}{2} \sum_{\langle ij \rangle} [J_z S_i^z S_j^z + J_{xy}(S_i^x S_j^x + S_i^y S_j^y)] - \frac{1}{2}(J_z + K_z) S_0^z S_1^z - \frac{1}{2}(J_{xy} + K_{xy})(S_0^x S_1^x + S_0^y S_1^y) , \quad (1)$$

with $J_z \geq J_{xy} > 0$. Here $\langle ij \rangle$ denotes a single term for each nearest-neighbor pair.

Within the spin-wave theory, the lattice is divided into two interpenetrating sublattices denoted by a and b, respectively, and the spin operators are replaced by two sets of boson operators ($a_i, a_i^\dagger$ and $b_j, b_j^\dagger$) by means of the Holstein-Primakoff transformation.[11,12] Suppressing all terms higher than bilinear in boson operators (LSWA), we have

$$H=-\tfrac{1}{2}NJ_z+\sum_{\mathbf{k}}[J_{xy}\gamma_{\mathbf{k}}(a_{\mathbf{k}}b_{\mathbf{k}}+a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger)+J_z(a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+b_{\mathbf{k}}^\dagger b_{\mathbf{k}})]$$
$$+\tfrac{1}{8}(J_z+K_z)-\frac{1}{4N}(J_{xy}+K_{xy})\sum_{\mathbf{k},\mathbf{k}'}(e^{ik_x'd}a_{\mathbf{k}}b_{\mathbf{k}'}+e^{-ik_x'd}a_{\mathbf{k}}^\dagger b_{\mathbf{k}'}^\dagger)-\frac{1}{4N}(J_z+K_z)\sum_{\mathbf{k},\mathbf{k}'}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}+e^{-i(k_x-k_x')d}b_{\mathbf{k}}^\dagger b_{\mathbf{k}'})\ , \quad (2)$$

where d is the lattice constant, the impurity link is oriented along the x direction, and

$$\gamma_{\mathbf{k}}=\tfrac{1}{2}[\cos(k_xd)+\cos(k_yd)]\ . \quad (3)$$

We now follow the same procedure as in Ref. 5 (see also Refs. 1 and 2) and introduce the standard one-particle Green's function in matrix form

$$\hat{G}_{\mathbf{k},\mathbf{k}'}(z)=\begin{bmatrix}\langle\langle a_{\mathbf{k}}^\dagger;a_{\mathbf{k}'}\rangle\rangle_z & \langle\langle a_{\mathbf{k}}^\dagger;b_{\mathbf{k}'}^\dagger\rangle\rangle_z\\ \langle\langle b_{\mathbf{k}};a_{\mathbf{k}'}\rangle\rangle_z & \langle\langle b_{\mathbf{k}};b_{\mathbf{k}'}^\dagger\rangle\rangle_z\end{bmatrix}\ . \quad (4)$$

Since the Hamiltonian is bilinear in boson operators and the scattering potential is factorizable, the exact Green's function is obtained by applying the standard equation of motion method

$$\hat{G}_{\mathbf{k},\mathbf{k}'}(z)=\hat{G}_{\mathbf{k}}^0(z)\delta_{\mathbf{k},\mathbf{k}'}-\frac{J_z+K_z}{4N}\hat{G}_{\mathbf{k}}^0(z)\begin{bmatrix}1&0\\0&e^{-ik_xd}\end{bmatrix}\hat{X}\begin{bmatrix}1&0\\0&e^{ik_x'd}\end{bmatrix}\hat{G}_{\mathbf{k}'}^0(z)-\frac{J_{xy}+K_{xy}}{4N}\hat{G}_{\mathbf{k}}^0(z)\begin{bmatrix}0&1\\e^{-ik_xd}&0\end{bmatrix}\hat{X}\begin{bmatrix}1&0\\0&e^{ik_x'd}\end{bmatrix}\hat{G}_{\mathbf{k}'}^0(z)\ , \quad (5)$$

where $\hat{G}_{\mathbf{k}}^0(z)$ is the Green's function for the lattice in the absence of impurity links

$$\hat{G}_{\mathbf{k}}^0(z)=\frac{J_z\hat{I}-J_{xy}\gamma_{\mathbf{k}}\hat{\sigma}_x-z\hat{\sigma}_z}{z^2-J_z^2+J_{xy}^2\gamma_{\mathbf{k}}^2}\ , \quad (6)$$

and

$$\hat{X}=\frac{A\hat{I}-B\hat{\sigma}_x-C\hat{\sigma}_y-D\hat{\sigma}_z}{A^2-B^2-C^2-D^2}\ . \quad (7)$$

Here $\hat{I}$ and $\hat{\sigma}_i$ denote the identity and Pauli matrices, and

$$A=1+\frac{1}{4N}\sum_{\mathbf{k}}\frac{J_z(J_z+K_z)-J_{xy}(J_{xy}+K_{xy})\gamma_{\mathbf{k}}^2}{z^2-J_z^2+J_{xy}^2\gamma_{\mathbf{k}}^2}\ ,$$
$$B=\frac{1}{4N}\sum_{\mathbf{k}}\frac{J_z(J_{xy}+K_{xy})-J_{xy}(J_z+K_z)\gamma_{\mathbf{k}}^2}{z^2-J_z^2+J_{xy}^2\gamma_{\mathbf{k}}^2}\ , \quad (8)$$
$$C=\frac{1}{4N}\sum_{\mathbf{k}}\frac{-iz(J_{xy}+K_{xy})}{z^2-J_z^2+J_{xy}^2\gamma_{\mathbf{k}}^2}=i\frac{J_{xy}+K_{xy}}{J_z+K_z}D\ .$$

In the absence of impurity link, the sublattice magnetization and the transversal correlation are given by

$$\langle S_{ai}^z\rangle=\tfrac{1}{2}-\langle a_i^\dagger a_i\rangle=\frac{1}{2}-\frac{2}{\pi^2}\int_{\sqrt{\eta^2-1}}^{\eta}dx\left[\frac{\eta-x}{\eta+x}\right]^{1/2}K(x^2+1-\eta^2)\ ,$$
$$\langle S_{ai}^xS_{bj}^x\rangle=\tfrac{1}{2}\langle a_i^\dagger b_j^\dagger\rangle=-\frac{1}{\pi^2}\int_{\sqrt{\eta^2-1}}^{\eta}dx\sqrt{\eta^2-x^2}K(x^2+1-\eta^2)\ . \quad (9)$$

Here $\eta=J_z/J_{xy}$ and $K(x)$ is the complete elliptical integral of the first kind. Expressions (9) follow from the unperturbed Green's function $\hat{G}_{\mathbf{k}}^0(z)$. The changes of the local ordered magnetic moment and the transverse correlation as a consequence of the impurity link, $\delta\langle S_{ai}^z\rangle$ and $\delta\langle S_{ai}^xS_{bj}^x\rangle$, are obtained from the second and third terms of the Green's function, Eq. (5). The momentum integrations can be expressed in terms of modified Bessel functions of integer order I_n, which appear in pairs (two-dimensional integral) in integrals of the form

$$\tilde{I}_n^m(y)=\int_0^\infty dt\, I_n\left[\frac{t}{2\eta}\right]I_m\left[\frac{t}{2\eta}\right]\exp[-t\sqrt{1+y^2}]\ , \quad (10)$$

where $y=-iz/J_z$ is an imaginary frequency. For the sites joined by the ferromagnetic link, we obtain

$$\delta\langle S_{a0}^z\rangle=\frac{1}{64\pi J_z^3}\int_0^\infty dy\frac{-(J_z+K_z)X_1+(J_{xy}+K_{xy})X_2}{(1+y^2)(A^2-B^2-C^2-D^2)}\ , \quad (11a)$$

$$\delta\langle S_{a0}^xS_{b1}^x\rangle=\frac{1}{128\pi J_z^3}\times\int_0^\infty dy\frac{-(J_z+K_z)X_3+(J_{xy}+K_{xy})X_4}{(1+y^2)(A^2-B^2-C^2-D^2)}\ , \quad (11b)$$

where

$$X_1=16J_z^2[A(1-y^2)+2iyD][\tilde{I}_0^0(y)]^2+J_{xy}^2A[\tilde{I}^*(y)]^2+8BJ_zJ_{xy}\tilde{I}_0^0(y)\tilde{I}^*(y)\ ,$$
$$X_2=16J_z^2[B(1-y^2)+2yC][\tilde{I}_0^0(y)]^2+J_{xy}^2B[\tilde{I}^*(y)]^2+8AJ_zJ_{xy}\tilde{I}_0^0(y)\tilde{I}^*(y)\ ,$$
$$X_3=16J_z^2B(1+y^2)[\tilde{I}_0^0(y)]^2+J_{xy}^2B[\tilde{I}^*(y)]^2+8J_zJ_{xy}(A+iD)\tilde{I}_0^0(y)\tilde{I}^*(y)\ ,$$
$$X_4=16J_z^2A(1+y^2)[\tilde{I}_0^0(y)]^2+J_{xy}^2A[\tilde{I}^*(y)]^2+8J_zJ_{xy}(B+C)\tilde{I}_0^0(y)\tilde{I}^*(y)\ . \quad (12)$$

Here $\tilde{I}^*(y)=\tilde{I}_0^0(y)+\tilde{I}_2^0(y)+2\tilde{I}_1^1(y)$ and the functions A, B, C, and D, Eqs. (8), take the form

$$A=1-\frac{J_z+K_z}{4J_z}(1+y^2)^{-1/2}\tilde{I}_0^0(y)-\frac{J_{xy}+K_{xy}}{4J_{xy}}[1-(1+y^2)^{1/2}\tilde{I}_0^0(y)]\ ,$$

$$B=-\frac{J_{xy}+K_{xy}}{4J_z}(1+y^2)^{-1/2}\tilde{I}_0^0(y)$$
$$-\frac{J_z+K_z}{4J_{xy}}[1-(1+y^2)^{1/2}\tilde{I}_0^0(y)]\ , \qquad (13)$$
$$C=-\frac{J_{xy}+K_{xy}}{4J_z}(1+y^2)^{-1/2}y\tilde{I}_0^0(y)=i\frac{J_{xy}+K_{xy}}{J_z+K_z}D\ .$$

The t and y integrations are now performed numerically. The results for $\delta\langle S_{a0}^z\rangle$ and $\delta\langle S_{a0}^x S_{b1}^x\rangle$ are presented in Sec. III.

III. RESULTS AND DISCUSSION

From symmetry considerations the magnetic moments at the two sites joined by the ferromagnetic link have equal magnitude and opposite sign. It is then sufficient to discuss only one of these sites. If $K_z+J_z=0$ and $K_{xy}+J_{xy}=0$, the impurity link has the same antiferromagnetic coupling strength as all other bonds, so that it is actually not an impurity. The sublattice magnetization in this case decreases monotonically as a function of J_{xy}/J_z from 0.5 (Ising limit $J_{xy}=0$) to 0.3034 for the isotropic antiferromagnet ($J_{xy}=J_z$). The transversal correlation between nearest neighbors is zero in the Ising limit (no quantum fluctuations) and its antiferromagnetic character grows monotonically with J_{xy} and reaches -0.1378 for the isotropic antiferromagnet. The J_z and J_{xy} terms of the lattice Hamiltonian give rise to competing effects: the longitudinal terms yield the ordered magnetic moment, i.e., the Néel state, while the transversal terms represent the quantum-mechanical fluctuations which tend to suppress the long-range order.

The situation $K_z=K_{xy}=0$ corresponds to a missing link. Our numerical results show that the absence of the bond slightly increases the local magnetic moment at the sites labeled 0 and 1 for all values of the anisotropy $\eta>0$. As expected, the transverse correlation across the missing link is antiferromagnetic but strongly reduced with respect to an unperturbed antiferromagnetic bond. The value of $\langle S_{a0}^x S_{b1}^x\rangle$ is zero in the Ising limit and its magnitude slowly increases with J_{xy} to -0.05 for the isotropic case.

With increasing K_z and K_{xy}, the basis of the LSWA, namely, the Néel state, breaks down locally. In Ref. 5 we found this breakdown of the approximation scheme for the isotropic case at $K_{xy}=K_z=J_{xy}=J_z$. Similarly, for the Ising limit the breakdown can be visualized as the frustration of the two plaquettes adjacent to the impurity link, so that the Néel state is locally not the state with lowest energy. The spins at sites 0 and 1 tend to form a triplet with zero spin projection in the z direction, and the antiferromagnetic bonds of the plaquettes can no longer all be satisfied. Mathematically the breakdown is caused by zeros in the denominator of the integrals (11a) and (11b). The function $\phi(y)=A^2-B^2-C^2-D^2$ is monotonically increasing with y for all values of the coupling parameters, so that the integrals are finite as long as $\phi(y=0)>0$. The boundary for the instability is then given by $\phi(y=0)=0$ and is shown in Fig. 1 as a function of the anisotropy of the lattice $J_{xy}/J_z=\eta^{-1}$. The curves

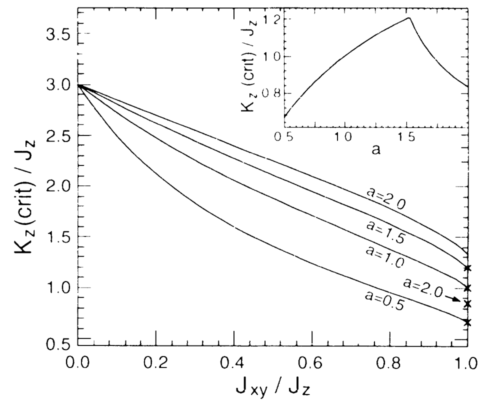

FIG. 1. Boundaries for the breakdown of the LSWA as given by the condition $\phi(y=0)=0$ as a function of η^{-1} and various ratios a. At these boundaries both $\langle S_{a0}^z\rangle$ and $\langle S_{a0}^x S_{b1}^x\rangle$ diverge, so that the approximation actually becomes inaccurate before reaching the curves from below. The inset corresponds to the boundary if $\eta=1$. The behavior for $a>1.54$ is anomalous as a consequence of the vanishing gap in the excitation spectrum for $\eta=1$.

represent anisotropy ratios of the impurity link proportional to those of the lattice

$$K_z/K_{xy}=a\eta=aJ_z/J_{xy}\ . \qquad (14)$$

In the Ising limit the boundary is at $K_z=3J_z$, while for finite values of η (>1) the boundary is an increasing function of a. For all $\eta>1$, the excitation spectrum for the pure lattice has a gap. This gap vanishes for $\eta=1$ and, as a consequence, the value of K_z at the instability for $\eta=1$ does not necessarily agree with its limit as $\eta\to1$. These two values are different for $a>1.54$ as shown in the inset of Fig. 1. At $a=1.54$ there is a crossing of two curves satisfying $\phi(y=0)=0$, which only happens if $\eta=1$. For $a=\eta=1$ we recover the instability discussed in Ref. 5.

Our results for the local magnetization and the transversal spin-spin correlation function[13] are summarized in Figs. 2 and 3 as a function of K_z/J_z for fixed η and a. Both $\langle S_{a0}^z\rangle$ and $\langle S_{a0}^x S_{b1}^x\rangle$ diverge at the instability line, but the approximation is, of course, already invalid somewhat before. This is indicated by the dashed lines in the figures. Although for small K_{xy} and K_z the local ordered moment is slightly enhanced over the corresponding sublattice magnetization for the pure lattice, this trend is reversed by increasing the ferromagnetic couplings. This is the consequence of increased quantum fluctuations and the trend of the spins at sites 0 and 1 to form an $S_z=0$ triplet state. The quantum fluctuations decrease with increasing a and, hence, $\langle S_{a0}^z\rangle$ increases while $\langle S_{a0}^x S_{b1}^x\rangle$ decreases (the spins are less ferromagnetically aligned in the xy plane). Note the deviations from this trend for $\eta=1$ and $a>1.54$ [Figs. 2(d) and 3(d)], since the limit $\eta\to1$ is not equal to the corresponding values at $\eta=1$, as a consequence of the vanishing gap in the excitation spectrum.

In summary, we studied the behavior of a ferromagnetic link embedded in a two-dimensional antiferromagnet on a square lattice within the LSWA. Two competing interactions affect the ordered magnetic moment and the transversal correlations locally, namely, the z component

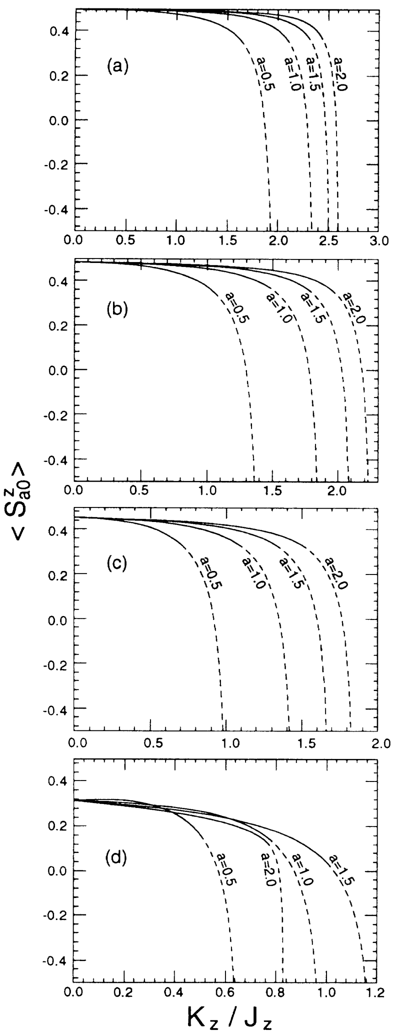

FIG. 2. Magnetic moment for a site at the impurity link $\langle S_{a0}^z \rangle$ as a function of K_z/J_z for various a ratios [see Eq. (14)] and (a) $\eta=4$, (b) $\eta=2$, (c) $\eta=\frac{4}{3}$, and (d) $\eta=1$. The corresponding sublattice magnetizations for the pure lattice are (a) $\langle S_{ai}^z \rangle=0.4960$, (b) 0.4824, (c) 0.4520, and (d) 0.3034. The dashed lines indicate the region where the approximation is not believed to be accurate.

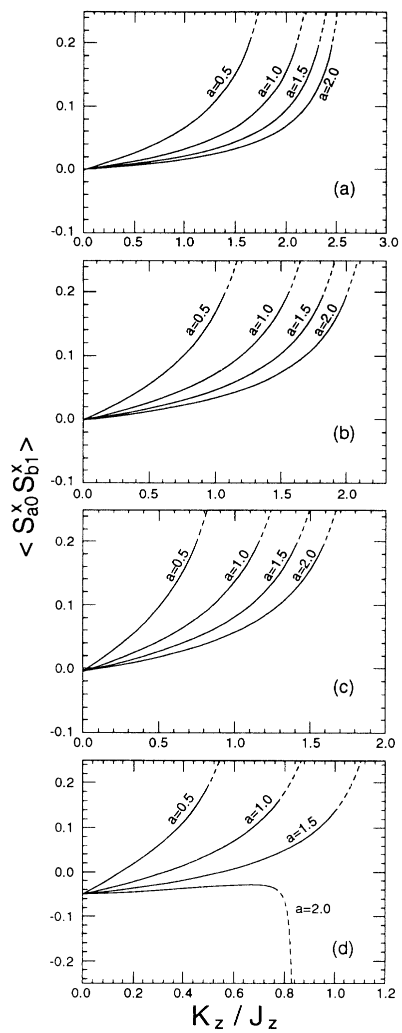

FIG. 3. Transversal correlation across the impurity link $\langle S_{a0}^x S_{b1}^x \rangle$ as a function of K_z/J_z for various a ratios [see Eq. (14)] and (a) $\eta=4$, (b) $\eta=2$, (c) $\eta=\frac{4}{3}$, and (d) $\eta=1$. The corresponding correlations for the pure lattice are (a) $\langle S_{ai}^x S_{bj}^x \rangle=-0.0159$, (b) -0.0338, (c) -0.0578, and (d) -0.1378. The dashed lines indicate the region where the approximation is not believed to be accurate.

of the interaction (Ising terms) and the transversal terms (fluctuations). For sufficiently large ferromagnetic couplings the LSWA breaks down as a consequence of the frustration of the two plaquettes adjacent to the impurity link. With increasing a, the transversal interaction is reduced giving rise to an increased ordered moment and a reduced transversal correlation across the link. Only if the coupling constants of the impurity link are very weak is there an enhancement of the local order with respect to the pure lattice and a strongly reduced transversal correlation.

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