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Spin-liquid state for two-dimensional Heisenberg antiferromagnets on a kagomé lattice

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Abstract. The magnetic properties of the spin liquid state of the antiferromagnetic Heisenberg model on the kagomé lattice are investigated within the self-consistent mean-field theory. The results show that the spin liquid ground-state energy per site is $E_g/N_sJ = -0.859$, which is in very good agreement with the best numerical estimates. The spin structure factor and spin susceptibility are also discussed.

PACS. 75.10.Jm Quantized spin models – 67.40.Db Quantum statistical theory; ground state, elementary excitations – 75.50.Ee Antiferromagnetics

The magnetic properties of the two-dimensional (2D) frustrated quantum Heisenberg antiferromagnet have received considerable attention in the last decade, which perhaps is motivated partly by the search for the quantum disordered spin liquid ground-state and possible relationship to the high temperature superconductivity in copper oxide materials [1]. The numerical simulation and analytical approaches strongly support the existence of the antiferromagnetic (AF) long-range-order (AFLRO) for the Heisenberg antiferromagnet on the square lattice with the reduced moment of about 60% of its classical value [2]. Anderson [3] argued that strong spin frustration on the triangular lattice may generate a novel resonating-valence-bond spin liquid ground-state without AFLRO, in particular, Kalmeyer and Laughlin [4] argued that the resonating-valence-bond state for the triangular lattice is similar to the fractional quantum Hall state for bosons. Several numerical simulations were interpreted as not in favour of their arguments [5]. However, the situation seems less clear on the kagomé lattice due to the geometric frustration, as in the triangular lattice, but the lower coordination number, as in the square lattice. Although the classical ground-state of the kagomé lattice is highly degenerate as shown by many authors [6], it is believed that such degeneracies may be lifted by thermal or quantum fluctuations [7]. The interest in the AF Heisenberg model on the kagomé lattice is that it is an attractive candidate in 2D involving only nearest-neighbor coupling with a low coordination number to display a quantum disordered spin liquid ground-state for the spin one-half. On the other hand, a series of experiments on the multilayer ^{3}He films have shown that some anomalous physical properties of ^{3}He absorbed on graphite can be described by the AF Heisenberg model on the kagomé lattice [8]. Various numerical and analytical techniques have been used to study the kagomé lattice [9–16], and several different types of the quantum ground-state have been proposed, in particular, Singh and Huse [10] have calculated the three-sublattice magnetism based on the high-order perturbation theoretical treatment, which is believed to be accurate, and predicted that the ground-state is strongly disordered due to the large degeneracy of the classical ground-state configurations.

In this paper, we study the magnetism of the AF Heisenberg antiferromagnet on the kagomé lattice within the self-consistent Tyablikov's spin Green's function theory [17] under the Kondo-Yamaj decoupling scheme [18]. The advantage of this approach is that the unwanted hard-core condition of the quantum spin operators, *i.e.*, the spin one-half raising and lowering operators behave as fermions on the same site and as bosons on different sites, is satisfied by the Pauli algebra. Within this theoretical framework, we obtain the spin liquid ground-state energy per site $E_g/N_sJ = -0.859$, which is in very good agreement with the best numerical results [9].

The simple way to visualize the kagomé lattice is to regard the triangular lattice as consisting of four sublattices and remove the spin on one of the sublattices, therefore there are three inequivalent sublattices A, B, and C even without AFLRO, where the spins in A, B, and C sublattices pointing to the vertices of an equilateral triangle are placed with no two nearest-neighbors pointing in the same direction (Fig. 1), then the kagomé lattice structure

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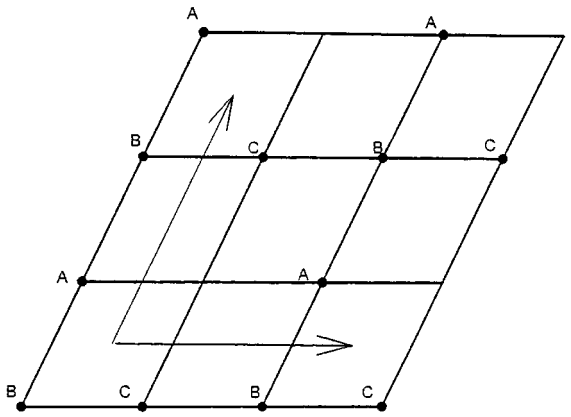

Fig. 1. The spin configuration of the sublattice A, B, and C on the kagomé lattice.

is much more complicated than the square and triangular lattices. For convenience, the equilateral triangle A, B, C is chosen as the cell as shown in Figure 1, in this case the kagomé lattice is reduced as the triangular structure, then the position of the spins in a cell i is specified by the vector $X_{i_s} = R_i + d_s$, with $s = A$, B, C, *i.e.*, each cell contains three spins, while the lattice vector R_i and the reciprocal lattice vector K_j satisfy the relationship as $R_i \cdot K_j = 2\pi\delta_{ij}$. With the above definition, the AF Heisenberg model on the kagomé lattice is described by the Hamiltonian as,

$$H = J\sum_{i_s,\eta_s} S_{i_s}\cdot S_{i_s+\eta_s} = J\sum_{i_s,\eta_s}[\frac{1}{2}(S^+_{i_s}S^-_{i_s+\eta_s} + S^-_{i_s}S^+_{i_s+\eta_s}) + S^z_{i_s}S^z_{i_s+\eta_s}], \quad (1)$$

where $J > 0$, the sum is over all sites X_{i_s} and for each X_{i_s}, it is over nearest-neighbors η_s of the kagomé net, and $S^+_{i_s}$ and $S^-_{i_s}$ are the raising and the lowering operators of $S^z_{i_s}$ respectively.

The quantum spin operators obey the Pauli spin algebra, which can be discussed in terms of the two-time spin Green's function within the Tyablikov's scheme [17]. In our present case, because there are three inequivalent spins A, B, and C, then the spin two-time Green's function is a matrix which can be defined as,

$$D(k,t-t') = \begin{pmatrix} D^{AA}(k,t-t') & D^{AB}(k,t-t') & D^{AC}(k,t-t') \\ D^{BA}(k,t-t') & D^{BB}(k,t-t') & D^{BC}(k,t-t') \\ D^{CA}(k,t-t') & D^{CB}(k,t-t') & D^{CC}(k,t-t') \end{pmatrix}, \quad (2)$$

where $D^{ss'}(i_s - j_{s'}, t-t') = \langle\langle S^+_{i_s}(t); S^-_{j_{s'}}(t')\rangle\rangle$. Since the time-Fourier transform of the two-time Green's function satisfies the equation,

$$\omega\langle\langle \hat{A};\hat{B}\rangle\rangle_\omega = \langle[\hat{A},\hat{B}]\rangle + \langle\langle[\hat{A},H];\hat{B}\rangle\rangle_\omega, \quad (3)$$

then the equation of motion of the spin two-time Green's function $G^{ss'}(i_s - j_{s'}, t-t')$ in equation (2) can be evaluated as,

$$\omega G^{ss'}(i_s - j_{s'},\omega) = \delta_{i_s j_{s'}}\langle S^z_{i_s}\rangle + \sum_{\eta_s}\langle\langle S^+_{i_s+\eta_s}S^z_{i_s} - S^+_{i_s}S^z_{i_s+\eta_s}; S^-_{j_{s'}}\rangle\rangle_\omega. \quad (4)$$

The second order spin Green's functions appear in the right hand side of equation (4), therefore in common practice the second-order spin Green's function is decoupled based on the Tyablikov's scheme [17]. However, the absence of the simple three sublattice magnetic order on the kagomé lattice has been convincingly demonstrated by Singh and Huse [10], then in the following discussions, we only study the system in the case $\langle S^z_{i_s}\rangle = 0$, *i.e.*, the quantum disordered spin liquid state without AFLRO. In this case, the first term in the right hand of equation (4) for the Green's function $G^{AA}(i-j,\omega)$ is equal to zero, and therefore the standard Tyablikov's approximation is not valid, and we should decouple the spin Green's function (4) at a stage one-step further than the Tyablikov's decoupling and make the equation of motion of the higher order of fluctuations, *e.g.*, that for the term in equation (4) is,

$$\begin{aligned}\omega\langle\langle S^+_{i_s}S^z_{i_s+\eta_s}; S^-_{j_{s'}}\rangle\rangle_\omega &= 2\delta_{i_s j_{s'}}\langle S^z_{i_s}S^z_{i_s+\eta_s}\rangle \\ &- \delta_{i_s+\eta_s j_{s'}}\langle S^+_{i_s}S^-_{i_s+\eta_s}\rangle + 2J\sum_{\eta'_{s''}}\langle\langle\frac{1}{2}S^+_{i_s}S^+_{i_s+\eta_s}S^-_{i_s+\eta_s-\eta'_{s''}} \\ &- \frac{1}{2}S^+_{i_s}S^+_{i_s+\eta_s-\eta'_{s''}}S^-_{i_s+\eta_s} + S^+_{i_s+\eta'_{s''}}S^z_{i_s}S^z_{i_s+\eta_s} \\ &- S^+_{i_s}S^z_{i_s+\eta'_{s''}}S^z_{i_s+\eta_s}; S^-_{j_{s'}}\rangle\rangle_\omega. \quad (5)\end{aligned}$$

Kondo and Yamaji [18] have generalized this Green's function theory to discuss the one-dimensional AF Heisenberg model, they obtained the ground-state energy of the one-dimensional AF Heisenberg model to be $E_g = -0.4156(2J)$, which is only 6% higher than the exact Bethe-ansatz value [19] of $E_g = -0.4431(2J)$, and is close to the result of $E_g = -0.4196(2J)$ obtained [20] based on the Jordan-Wigner transformation [21]. The theory has been used to discuss the 2D square lattice in the case of $\langle S^z_i\rangle = 0$ by many authors [22,23], and the result [22,23] of the ground-state energy per bond of the 2D AF Heisenberg model is $E_g/NZJ = -0.310$, which is in very good agreement with the result of $E_g/NZJ = -0.319$ obtained [24] based on the resonating-valence-bond state. This theory has been applied to study the 2D doped antiferromagnet within the t-J model [25]. In this paper, we apply this theory to the kagomé lattice. Following previous discussions [18,22,23], we decouple the four operator terms in the right-hand side of equation (5) as,

$$\begin{aligned}\langle\langle S^+_{i_s}S^+_{i_s+\eta_s}S^-_{i_s+\eta_s-\eta'_{s''}}; S^-_{j_{s'}}\rangle\rangle_\omega \rightarrow & \\ \alpha\langle S^+_{i_s+\eta_s}S^-_{i_s+\eta_s-\eta'_{s''}}\rangle\langle\langle S^+_{i_s}; S^-_{j_{s'}}\rangle\rangle_\omega & \\ + [\delta_{\eta_s\eta'_{s''}} + (1-\delta_{\eta_s\eta'_{s''}})]\langle S^+_{i_s}S^-_{i_s+\eta_s-\eta'_{s''}}\rangle\langle\langle S^+_{i_s+\eta_s}; S^-_{j_{s'}}\rangle\rangle_\omega, & \quad (6a)\end{aligned}$$

$$\langle\langle S^+_{i_s}S^+_{i_s+\eta_s-\eta'_{s''}}S^-_{i_s+\eta_s};S^-_{j_{s'}}\rangle\rangle_\omega \rightarrow \alpha\langle S^+_{i_s}S^-_{i_s+\eta_s}\rangle\langle\langle S^+_{i_s+\eta_s-\eta'_{s''}};S^-_{j_{s'}}\rangle\rangle_\omega + \alpha\langle S^+_{i_s+\eta_s-\eta'_{s''}}S^-_{i_s+\eta_s}\rangle\langle\langle S^+_{i_s};S^-_{j_{s'}}\rangle\rangle_\omega, \quad \eta_s\neq\eta'_{s''}, \tag{6b}$$

$$\langle\langle S^+_{i_s+\eta'_{s''}}S^z_{i_s}S^z_{i_s+\eta_s};S^-_{j_{s'}}\rangle\rangle_\omega \rightarrow \alpha\langle S^z_{i_s}S^z_{i_s+\eta_s}\rangle\langle\langle S^+_{i_s+\eta'_{s''}};S^-_{j_{s'}}\rangle\rangle_\omega = \frac{1}{2}\alpha\langle S^+_{i_s}S^-_{i_s+\eta_s}\rangle\langle\langle S^+_{i_s+\eta'_{s''}};S^-_{j_{s'}}\rangle\rangle_\omega, \quad \eta_s\neq\eta'_{s''}, \tag{6c}$$

$$\langle\langle S^+_{i_s}S^z_{i_s+\eta'_{s''}}S^z_{i_s+\eta_s};S^-_{j_{s'}}\rangle\rangle_\omega \rightarrow [\delta_{\eta_s\eta'_{s''}}+(1-\delta_{\eta_s\eta'_{s''}})]\langle S^z_{i_s+\eta'_{s''}}S^z_{i_s+\eta_s}\rangle\langle\langle S^+_{i_s};S^-_{j_{s'}}\rangle\rangle_\omega = \frac{1}{2}[\delta_{\eta_s\eta'_{s''}}+(1-\delta_{\eta_s\eta'_{s''}})]\langle S^+_{i_s+\eta'_{s''}}S^-_{i_s+\eta_s}\rangle\langle\langle S^+_{i_s};S^-_{j_{s'}}\rangle\rangle_\omega, \tag{6d}$$

where $2\langle S^z_{i_s}S^z_{i_s+\eta_s}\rangle=\langle S^+_{i_s}S^-_{i_s+\eta_s}\rangle$ and $2\langle S^z_{i_s+\eta'_{s''}}S^z_{i_s+\eta_s}\rangle=\langle S^+_{i_s+\eta'_{s''}}S^-_{i_s+\eta_s}\rangle$ have been used since there is the rotational symmetry in the quantum spin systems without AFLRO. In order not to violate the sum rule of the correlation function $\langle S^+_{i_s}S^-_{i_s}\rangle=1/2$ in the case $\langle S^z_{i_s}\rangle=0$, the important decoupling parameter α has been introduced as discussed by Kondo and Yamaji [18] and many others [22,23], which can be regarded as the vertex corrections. With the help of the above decoupling scheme, we obtain the two-time spin Green's functions of the kagomé lattice as,

$$D(k,\omega)=\sum_{j=1}^{3}\begin{pmatrix}\Gamma_{1j}(k,\omega)a_{j1}(k) & \Gamma_{1j}(k,\omega)a_{j2}(k) & \Gamma_{1j}(k,\omega)a_{j3}(k)\\ \Gamma_{2j}(k,\omega)a_{j1}(k) & \Gamma_{2j}(k,\omega)a_{j2}(k) & \Gamma_{2j}(k,\omega)a_{j3}(k)\\ \Gamma_{3j}(k,\omega)a_{j1}(k) & \Gamma_{3j}(k,\omega)a_{j2}(k) & \Gamma_{3j}(k,\omega)a_{j3}(k)\end{pmatrix}\times\frac{1}{[\omega^2-\omega^2_1(k)][\omega^2-\omega^2_2(k)][\omega^2-\omega^2_3(k)]}, \tag{7}$$

where $\Gamma(k,\omega)$ is the adjugate matrix of

$$\Delta(k,\omega)=\begin{pmatrix}\omega^2-(Z_{11}+Z_{12}\gamma_{k1}) & Z_{13}\gamma_{k4}-Z_{12}\gamma_{k5} & Z_{13}\gamma_{k6}-Z_{12}\gamma_{k7}\\ Z_{13}\gamma^*_{k4}-Z_{12}\gamma^*_{k5} & \omega^2-(Z_{11}+Z_{12}\gamma_{k2}) & Z_{13}\gamma_{k8}-Z_{12}\gamma_{k9}\\ Z_{13}\gamma^*_{k6}-Z_{12}\gamma^*_{k7} & Z_{13}\gamma^*_{k8}-Z_{12}\gamma^*_{k9} & \omega^2-(Z_{11}+Z_{12}\gamma_{k3})\end{pmatrix}, \tag{8}$$

and

$$a(k)=8J\chi\begin{pmatrix}-2 & \gamma_{k4} & \gamma_{k6}\\ \gamma^*_{k4} & -2 & \gamma_{k8}\\ \gamma^*_{k6} & \gamma^*_{k8} & -2\end{pmatrix}, \tag{9}$$

with $Z_{11}=8J^2(2\alpha C+1)$, $Z_{12}=8J^2\alpha\chi$, $Z_{13}=Z_{11}/2+2Z_{12}$, $\gamma_{k1}=\cos k_y+\cos(k_y-k_x)$, $\gamma_{k2}=\cos k_x+\cos k_y$, $\gamma_{k3}=\cos k_x+\cos(k_y-k_x)$, $\gamma_{k4}=(1+e^{ik_y})/2$, $\gamma_{k5}=(e^{ik_x}+e^{i(k_y-k_x)})/2$, $\gamma_{k6}=(1+e^{i(k_y-k_x)})/2$, $\gamma_{k7}=(e^{-ik_x}+e^{ik_y})/2$, $\gamma_{k8}=(1+e^{-ik_x})/2$, $\gamma_{k9}=(e^{-ik_y}+e^{i(k_y-k_x)})/2$, and the order parameters $\chi=\langle S^+_{i_s}S^-_{i_s+\eta_s}\rangle$ and $C=\sum_{\eta_s\neq\eta_{s'}}\langle S^+_{i_s+\eta_s}S^-_{i_s+\eta_{s'}}\rangle$, while three branch spectra $\omega_1(k)$, $\omega_2(k)$, and $\omega_3(k)$ are the solution of the determinant $|\Delta(k,\omega_j)|=0$. According to the spectral representation of the correlation function,

$$\langle\hat{B}\hat{A}\rangle=i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\langle\langle\hat{A};\hat{B}\rangle\rangle_{\omega+i0^+}-\langle\langle\hat{A};\hat{B}\rangle\rangle_{\omega-i0^+}}{e^{\beta\omega}-1}e^{-i\omega(t-t')}, \tag{10}$$

the self-consistent equations based on the spin Green's function (7) can be obtained to determine the order parameters χ, C and decoupling parameter α, while the ground-state energy per site obtained from equation (1) is $E_g/N_sJ=\sum_{\eta_s}\frac{3}{2}\langle S^+_{i_s}S^-_{i_s+\eta_s}\rangle=6\chi$.

We are now ready to discuss the magnetic property of the AF Heisenberg model on the kagomé lattice. We have performed the numerical calculation, and the result of the spin liquid ground-state energy per site is $E_g/N_sJ=-0.859$. For the comparison, some results of the ground-state energy obtained from the numerical simulations and our present theoretical result are listed in Table 1. As shown in Table 1, the present spin liquid energy seems to be closer to the extrapolated finite lattice result of Leung and Elser [12], and only is 3% higher than the best numerical estimates by Zeng and Elser [9]. Our result is almost identical with that of the variational calculation by Sindzingre, Lecheminant and Lhuillier [14]. For further understanding the ground-state property, the spin-spin correlations have been calculated, and the results are given in Table 2, where the spin pairs are identified in terms of their separation, *i.e.*, the distance r as well as the minimum path length of bonds n connecting the two spins. These results are in very good agreement with the numerical simulations [9,12], and show that the correlations decay rapidly with separation, which is the characteristic property of the spin liquid ground-state. As a by-product, we have also studied the spin liquid state of the 2D AF Heisenberg model on the triangular lattice, the result shows that the spin liquid energy per site is $E_g/NJ=-0.966$, which is essentially identical to the results obtained by Kalmeyer and Laughlin [4] and Lee and Feng [5] based on the resonating-valence-bond state without AFLRO, but higher than the results of Huse and Elser [5] for an AFLRO state, the correlations decay slowly with separation. This result, in the comparison with the kagomé lattice case, suggests the possibility of an ordered ground-state on the triangular lattice.

An important experimental characterization of the ground-state is the spin structure factor $S(k)=\frac{1}{N}\sum_{ij}\langle S^+_iS^-_j\rangle\exp[ik(R_i-R_j)]$, which has been computed within the present framework at the zero temperature, and the result is plotted in Figure 2, where for convenience the original coordinate system has been transformed to an orthogonal one. The maxima of $S(k)$ in

Table 1. A comparison of the ground-state energy per site for the antiferromagnetic Heisenberg model on the two-dimensional kagomé lattice.

Authors	E_g/N_sJ	Method
Zeng and Elser [9]	-0.882	Finite lattice
Yang, Warman and Girvin [13]	-0.788	Variational Monte-Carlo
Leung and Elser [12]	-0.877	Finite lattice
Sindzingre, Lecheminant and Lhuillier [14]	-0.84	Variational Monte-Carlo
The present work	-0.859	Green's function method

Table 2. A comparison of the spin-spin correlation for the antiferromagnetic Heisenberg model on the kagomé lattice, where space of the nearest neighbor spins is unity.

n path length	r distance	Zeng and Elser [9] $\langle S^z_{i_s} S^z_{i_s+\eta_s}\rangle$	Leung and Elser [12] $\langle S^z_{i_s} S^z_{i_s+\eta_s}\rangle$	The present work
1	1	-0.0728	-0.0731	-0.0716
2	$\sqrt{3}$	0.0097	0.0039	0.0138
2	2	0.0137	0.0176	0.0121
3	2	$-0.0004 \sim 0.0005$	-0.0030	-0.0085

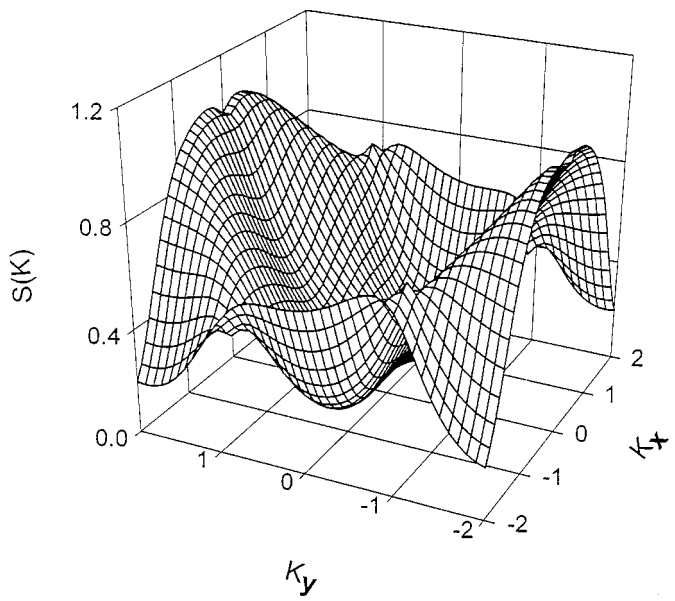

Fig. 2. Zero temperature spin structure factor $S(k)$ of the antiferromagnetic Heisenberg model on the kagomé lattice. The global maxima are at four wave vectors.

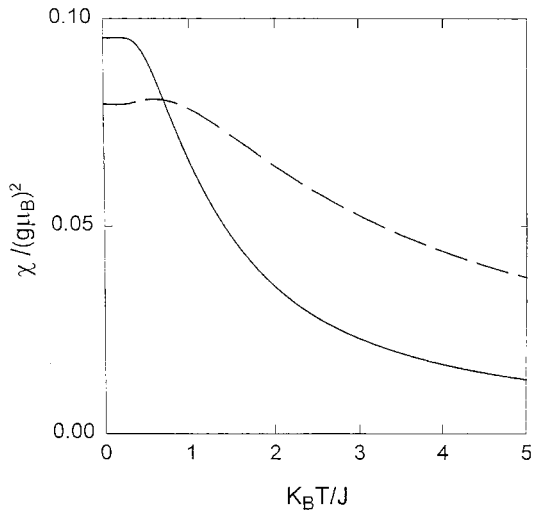

Fig. 3. The spin susceptibility of the antiferromagnetic Heisenberg model on the kagomé lattice (solid line) and the triangular lattice (dashed line) as a function of temperature.

Figure 2 occur at four wave vectors, which is consistent with the results obtained within the large-N expansion [15]. The interesting magnetic quantity associated with the spin structure factor in the present spin liquid state is the temperature dependence of the spin susceptibility $\chi = (g^2\mu_B^2/NK_BT)\sum_{ij}\langle S_i^z S_j^z\rangle$, where g is the Landa factor and μ_B is the Bohr magneton, and the result of the spin susceptibility is shown in Figure 3 (solid line). For comparison, the result of the spin susceptibility of the 2D AF Heisenberg antiferromagnet on the triangular lattice is also plotted in Figure 3 (dashed line). These results indicate that values of the spin susceptibility on the kagomé lattice are decreased rapidly with increasing temperatures for temperature $T > J$, which is in contrast to the triangular lattice case, where the values of the spin susceptibility are decreased slowly with increasing temperatures for temperature $T > J$. However, we should mention that at very low temperatures the spin susceptibility in the kagomé lattice decay slowly with decreasing temperatures, which is not consistent with the common spin liquid behavior. Kondo and Yamaj's treatment [18] for the one-dimensional AF Heisenberg model suffers from the same weakness. Probably, it can be cured by including fluctuations beyond the mean-field theory. Finally we also note that the spin excitation spectrum of the kagomé lattice has been discussed by Waldtmann and Everts [27].

A natural question is why is this self-consistent mean-field Green's function theory so useful to treat the quantum spin systems without AFLRO? To our present understanding, there are at least three reasons: (1) the unwanted hard-core condition of the quantum spin operators is exactly satisfied in the actual calculations. (2) The sum rule of the spin Green's function is always satisfied, and (3) the rotational symmetry in the quantum spin systems without AFLRO is not unphysically broken in this self-consistent mean-field Green's function theory. For the spin systems without AFLRO, the low lying excitations described are essentially spin waves propagating in a short-range-order with a correlation length. Many authors [18,22,23] have employed this self-consistent mean-field Green's function theory to study the one-dimensional Heisenberg spin system and 2D AF Heisenberg spin system on the square lattice, they obtained results which have a satisfactory temperature dependence over the whole temperature region from a qualitative view point.

In summary, we have discussed the magnetic property of the spin liquid state of the AF Heisenberg model on the kagomé lattice within the self-consistent mean-field Green's function theory under the Kondo and Yamaji's decoupling scheme [18,22]. It is shown that the spin liquid ground-state energy per site of the kagomé lattice is $E_{\rm g}/N_s J = -0.859$, which only is 3% higher than the best numerical estimate [9]. The theory also gives reasonable gross features of the spin structure factor and spin susceptibility for the kagomé lattice.

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