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Quantum dimer model for trimerized kagomé antiferromagnet

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Low-energy singlet states of a spin-1/2 trimerized kagomé antiferromagnet are mapped to an effective quantum dimer model on a triangular lattice. Mapping is done in the first-order of perturbation theory in a weaker coupling constant of the trimerized model. The derived quantum dimer model is dominated by kinetic energy terms (dimer resonances) on a few shortest loops of the triangular lattice.

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Resonating valence bond (RVB) state introduced by Anderson and co-workers long time ago [1] is nowdays a popular paradigm in the condensed matter physics. Short-range RVB states are considered to be probable candidates for an elusive spin-liquid phase of magnetic insulators. On a quantitative level the idea of short-range RVB states is formulated by so called quantum dimer models (QDM) [2 – 4]. In QDM each dimer represents a singlet state (valence bond) between a pair of neighboring spins. The QD Hamiltonian is defined on the Hilbert space of close-packed dimer coverings of a lattice. The dimer states are assumed to be properly orthogonalized. Local dynamics of an RVB state is typically described using only smallest plaquettes ($\square$), which are squares (square lattice) or rhombi (triangular lattice):

$$\hat{\mathcal{H}}_{\rm QD} = \tag{1}$$
$$= \sum_{\square}\Big[-t\big(|\,\overline{\underline{\;\;}}\,\rangle\langle\,|\,|\,| + |\,|\,|\,\rangle\langle\,\overline{\underline{\;\;}}\,|\big) + V\big(|\,\overline{\underline{\;\;}}\,\rangle\langle\,\overline{\underline{\;\;}}\,| + |\,|\,|\,\rangle\langle\,|\,|\,|\big)\Big].$$

The first term is a dimer kinetic energy, which flips a pair of parallel dimers around an arbitrary plaquette; the second term is a potential energy between such pairs. Rokhsar and Kivelson [3] have shown that a short-range RVB state given by a superposition of all dimer coverings of a square lattice is an exact eigen-state of the QD Hamiltonian for a special choice of the parameters $t = V$. On a bipartite square lattice the RVB state at the Rokhsar-Kivelson (RK) point has long-range power low correlations and describes, consequently, a gapless spin-liquid state [3, 5]. Small perturbations away from the RK point will drive the system into one of the ordered crystalline dimer states. The QDM on a triangular lattice exhibits quite a different behavior at the RK point [5 – 7]. The short-range RVB state has exponentially decaying correlators and, therefore, should be stable with respect to deviations from the RK point or on switching on extra perturbations to the QD Hamiltonian. Still, the question whether such states or Hamiltonians can describe realistic quantum spin systems remains to a large extent unsettled. In the present work we discuss a realization of QDM on a triangular lattice.

The most probable candidates for a singlet spin-liquid ground state are frustrated quantum antiferromagnets [8]. Numerical exact diagonalization studies of a spin-1/2 Heisenberg kagomé antiferromagnet have shown that this spin model has a nonmagnetic ground state with a large number of low-lying singlet excitations [9, 10]. Available cluster sizes do not allow to draw a definite conclusion on the possible nature of the singlet ground state.

One of a very few analytic approaches to such problems is a strong-coupling expansion from a small clusters. The main motif of a kagomé lattice is triangle. It is, therefore, natural to start from a trimerized kagomé lattice shown in Fig.1. Such a strong-coupling approach

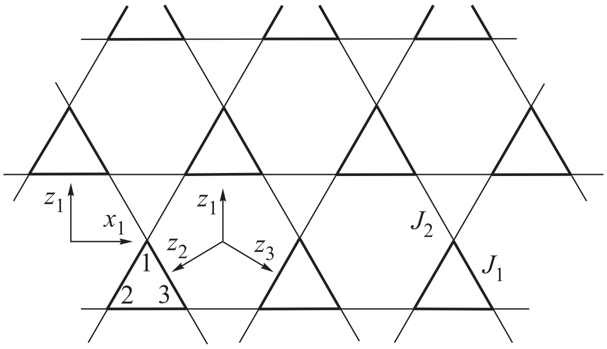

Fig.1. Trimerized kagomé lattice with two exchange constants. Indicated labeling of sites and axes is used in the text

has been pursued in relation to kagomé antiferromagnet in several theoretical works [11 – 14]. Recently, an experimental scheme to create a trimerized kagomé lattice

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has been suggested for ultracold atomic gases in optical traps [15]. This opens a possibility for experimental check of RVB physics in the corresponding spin model.

The Heisenberg model on a trimerized lattice

$$\hat{\mathcal{H}} = \sum_{\langle ij \rangle} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j \tag{2}$$

is described by two coupling constants: J_1 for a stronger interaction between spins in $\triangle$-triangles and J_2 for a weaker interaction inside ∇-triangles. An array of isolated $\triangle$-triangles is a zeroth order Hamiltonian, which has a highly degenerate ground state. Interactions between $\triangle$-triangles should lift such a degeneracy already in the first-order of the perturbation theory.

In the beginning, let us rederive the previous results on the effective first-order Hamiltonian [11−13] using somewhat different notations. One starts with an isolated triangle. Its Hamiltonian is

$$\begin{aligned}\hat{\mathcal{H}}_\triangle &= J_1\big(\mathbf{S}_1\cdot\mathbf{S}_2 + \mathbf{S}_2\cdot\mathbf{S}_3 + \mathbf{S}_3\cdot\mathbf{S}_1\big) = \\ &= \frac{J_1}{2}\big(\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3\big)^2 - \frac{3}{2}J_1 S(S+1).\end{aligned} \tag{3}$$

The energy levels are determined by the total spin. For $S = 1/2$, which is always assumed below, the levels are (i) two doublets with $S = 1/2$ and $E = -\frac{3}{4}J_1$ and (ii) one quartet with $S = 3/2$ and $E = \frac{3}{4}J_1$. In the lowest order of a perturbation expansion in J_2/J_1 one can neglect states with $S = 3/2$, which are separated from lowest doublets by a finite gap $\Delta E = \frac{3}{2}J_1$. The two degenerate states with $S = 1/2$ and $S^z = 1/2$ are

$$\begin{aligned}|d_\uparrow\rangle &= \frac{1}{\sqrt{2}}\big(\uparrow\uparrow\downarrow - \uparrow\downarrow\uparrow\big), \\ |p_\uparrow\rangle &= \frac{1}{\sqrt{6}}\big(2\downarrow\uparrow\uparrow - \uparrow\uparrow\downarrow - \uparrow\downarrow\uparrow\big),\end{aligned} \tag{4}$$

where $|d_\uparrow\rangle$ is a combination of the spin-up apex spin and a singlet bond between the two base spins (Fig.1). Spin-down states $|d_\downarrow\rangle$ and $|p_\downarrow\rangle$ are obtained from the spin-up states (4) by acting with S^- operator. The choice of the basis is, of course, not unique. The apex spin can be instead put into a singlet state either with its right or with left neighbor, which yields two other states $|d'_\uparrow\rangle = \frac{1}{\sqrt{2}}(\downarrow\uparrow\uparrow - \uparrow\uparrow\downarrow)$ and $|d''_\uparrow\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow)$ with appropriate orthogonal partners $|p'_\uparrow\rangle$ and $|p''_\uparrow\rangle$. The transformation from the old basis (4) to the new states is given by

$$\begin{aligned}|d'_\alpha\rangle &= -\frac{1}{2}|d_\alpha\rangle + \frac{\sqrt{3}}{2}|p_\alpha\rangle,\ |p'_\alpha\rangle = -\frac{\sqrt{3}}{2}|d_\alpha\rangle - \frac{1}{2}|p_\alpha\rangle, \\ |d''_\alpha\rangle &= -\frac{1}{2}|d_\alpha\rangle - \frac{\sqrt{3}}{2}|p_\alpha\rangle,\ |p''_\alpha\rangle = \frac{\sqrt{3}}{2}|d_\alpha\rangle - \frac{1}{2}|p_\alpha\rangle,\end{aligned} \tag{5}$$

where $\alpha = \uparrow,\downarrow$ is a spinor index. The main difference with the previous works [11, 12] is that we use real basis states (4) or (5) instead of defining complex chiral states. This yields a more transparent form of the first-order Hamiltonian and simplifies subsequent derivation of a QDM.

At this point we introduce two sets of the Pauli matrices: σ^i, which act between spin-up and spin-down states, and τ^i, which act in the orbital subspace (d,p) preserving the total spin. A convenient choice of orbital axes shown in Fig.1 corresponds to

$$\tau^{z_1}|d_\alpha\rangle = |d_\alpha\rangle, \quad \tau^{z_1}|p_\alpha\rangle = -|p_\alpha\rangle. \tag{6}$$

Then, the orbital operators projected onto the rotated axes $\tau^{z_2} = -\frac{1}{2}\tau^{z_1} - \frac{\sqrt{3}}{2}\tau^{x_1}$ and $\tau^{z_3} = -\frac{1}{2}\tau^{z_1} + \frac{\sqrt{3}}{2}\tau^{x_1}$ yield $\tau^{z_2}|d'_\alpha\rangle = |d'_\alpha\rangle$ and $\tau^{z_3}|d''_\alpha\rangle = |d''_\alpha\rangle$ and so on.

In order to find the effect of coupling J_2 between triangular blocks, we have to calculate matrix elements of the on-site spin operators between the basis states $|d_\alpha\rangle$ and $|p_\alpha\rangle$. This problem is greatly simplified once all symmetries are taken into account. The final result is

$$\begin{aligned}\mathbf{S}_1 &= \frac{1}{2}\,d^\dagger_\alpha\boldsymbol{\sigma}_{\alpha\beta}d_\beta - \frac{1}{6}\,p^\dagger_\alpha\boldsymbol{\sigma}_{\alpha\beta}p_\beta\ , \\ \mathbf{S}_{2,3} &= \frac{1}{3}\,p^\dagger_\alpha\boldsymbol{\sigma}_{\alpha\beta}p_\beta \pm \frac{1}{2\sqrt{3}}\left(p^\dagger_\alpha\boldsymbol{\sigma}_{\alpha\beta}d_\beta + \text{h. c.}\right).\end{aligned} \tag{7}$$

Spinor structure is a consequence of the spin-rotational symmetry, while the permutation symmetry P_{23} fixes the orbital part in (7). The above representation is further simplified once the total spin of a triangle $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$ is defined and the orbital operators operators τ^{z_k} are used. Then, the n^{th} spin $(n = 1,2,3)$ of the i^{th} triangular block is represented by

$$\mathbf{S}_{ni} = \frac{1}{3}\,\mathbf{S}_i\,(1 + 2\tau_i^{z_n})\,, \tag{8}$$

where $\hat{\mathbf{z}}_n$ goes from the center of a triangle in the direction of the corresponding spin, see Fig.1.

The effective Hamiltonian of the first order in a weaker coupling J_2 is found by substituting Eq. (8) into the Hamiltonian (2):

$$\hat{\mathcal{H}}_1 = \frac{J_2}{9}\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j(1+2\tau_i^{z_n})(1+2\tau_j^{z_m})\ , \tag{9}$$

where a trivial constant term $-\frac{3}{4}J_1 N_\triangle$ is omitted for convenience. The derived spin-orbital Hamiltonian $\hat{\mathcal{H}}_1$ is defined on a triangular lattice, such that every site corresponds to one $\triangle$-block of the trimerized kagomé model and is attributed with spin and orbital operators. The bond orientation uniquely determines the orbital axes for two participating sites. In the following we drop the common energy factor J_2, which is the same for all results obtained in the first-order perturbation theory.

Search for the low-energy states of the Hamiltonian (9) can be approached from a two-site problem (two adjacent $\triangle$-triangles of the original kagomé lattice) [12]. This problem is solved exactly and its ground state corresponds to a spin singlet with the orbital degrees fully polarized along the bond: $\langle\tau_i^{z_n}\rangle = \langle\tau_j^{z_m}\rangle = 1$. The ground-state energy is $-\frac{3}{4}$. A variational solution for the lattice problem (9) is constructed by splitting the whole lattice into a close-packed structure of dimers between nearest-neighbor sites, such that the dimer wave-function is given by the ground-state solution of the two-site problem. A remarkable feature of these variational states is that at the mean-field level with respect to orbital degrees of freedom the total energy is just a sum of energies of individual dimers and does not depend on a particular dimer covering of a triangular lattice [12]. Indeed, once $\langle\tau_i^{z_n}\rangle = 1$, then for the two other axes $\langle\tau_i^{z_m}\rangle = \langle\tau_i^{z_k}\rangle \equiv -\frac{1}{2}$. Therefore, the expectation value of any empty bond, *i.e.*, a bond without a dimer, identically vanishes over the variational wave-function: either one or both sites of the bond have $\langle\tau_i^{z_m}\rangle = -\frac{1}{2}$.

In the works [12, 16] the degenerate set of variational mean-field states has been identified with low energy states of spin-1/2 antiferromagnets on trimerized and isotropic kagomé lattices. The number of low-lying singlets of the kagomé model scales, then, as 1.15^N in good agreement with the full exact diagonalization study [10]. The previous works leave, however, without answer the following questions: (i) how good is the mean-field approximation? (ii) does the true singlet ground state break certain symmetries of the lattice? (iii) is there a finite gap between the ground state and the first excited singlet levels? We shall address these problems in the following.

In order to beyond the mean-field approximation, one has to consider off-diagonal matrix elements of the Hamiltonian (9) between various dimer configurations as well as the corresponding overlap matrix. The general rule to compute the overlap matrix for models, where every dimer represents a singlet pair, is to construct the transition or overlap graph by drawing two dimer configurations on the same lattice [2]. Every closed nonintersecting loop of dimers contributes $2/2^{l/2}$ to the overlap matrix, l being the length of the loop. The sign of the overlap matrix element depends on a sign convention for singlet wave-functions. We adopt the standard convention such that the singlet bond wave-function is $[ab] = \frac{1}{\sqrt{2}}(\uparrow_a\downarrow_b - \downarrow_a\uparrow_b)$, where b is an upper site in the pair or is directly to the right from a, see Fig.2.

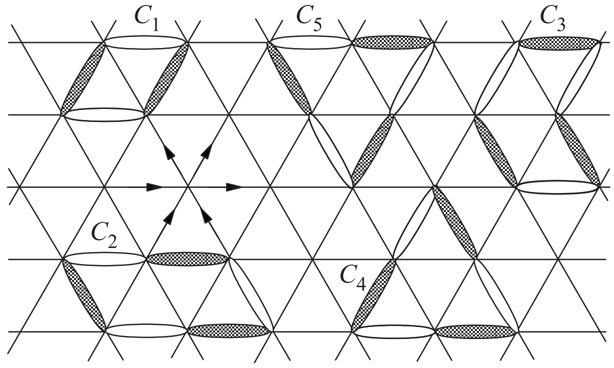

Fig.2. Effective triangular lattice with five shortest loops. The arrow direction indicates a sign convention for the singlet wave-function on each bond

To study local dynamics of valence bonds in trimerized kagomé model it is natural to select a few shortest loops on an effective triangular lattice shown in Fig.2. Taking into account the orbital part of the wave-functions the overlaps of two dimer configurations on each loop are calculated as $c_1 = -1/2^4$, $c_2 = c_3 = -1/2^7$, $c_4 = -1/2^8$, and $c_5 = 1/2^5$. These overlap matrix elements are significantly smaller than for singlet bond configurations on the original triangular lattice. In the latter case the corresponding loops have $c_1 = 1/2$, $c_2 = c_3 = 1/2^2$, $c_4 = c_5 = -1/2^2$. The difference reflects the fact that loops on an effective triangular lattice correspond to significantly longer loops on the original trimerized kagomé lattice. Note also, that loops C_4 and C_5 are different for the considered model because the trimerized kagomé lattice has only a three-fold rotation axis in the center of every triangle. Comparison of the overlap matrix elements explains why the QDM is a poor approximation for a spin-1/2 Heisenberg antiferromagnet on a triangular lattice, but might be a good one for the trimerized kagomé model.

In the work [3] the derivation of QDM from a particular spin Hamiltonian has been formulated in a general form via calculation of the inverse square root of the overlap matrix. The actual calculations can be done more straightforwardly by operating with the wave-functions. The final result are, of course, equivalent in both approaches. Specifically, let us consider two linearly independent, normalized states $|\psi_1\rangle$ and $|\psi_2\rangle$, which have a small (real) overlap $\langle\psi_1|\psi_2\rangle = c$. The matrix elements of the Hamiltonian between two states are assumed to be known $E_{11} = \langle\psi_1|\hat{H}|\psi_1\rangle$, $E_{12} = E_{21} = \langle\psi_1|\hat{H}|\psi_2\rangle$, and $E_{22} = \langle\psi_2|\hat{H}|\psi_2\rangle$. The aim is to compute the matrix elements in a new properly orthogonalized basis $|\varphi_n\rangle$. We write for this

$$|\varphi_{1,2}\rangle = \lambda\big(|\psi_{1,2}\rangle - \mu|\psi_{2,1}\rangle\big) \tag{10}$$

and demand that $\langle\varphi_1|\varphi_2\rangle = 0$, $\langle\varphi_1|\varphi_1\rangle = \langle\varphi_2|\varphi_2\rangle = 1$. This yields

$$\mu = \frac{c}{1+\sqrt{1-c^2}}, \quad \lambda^2 = \frac{1}{1+\mu^2-2\mu c}. \tag{11}$$

Calculating now the matrix elements between the new states and assuming $E_{11} = E_{22}$, for simplicity, we find

$$\begin{aligned} \tilde{E}_{11} &= E_{11} + \frac{c}{1-c^2}\big(cE_{11} - E_{12}\big), \\ \tilde{E}_{12} &= E_{12} + \frac{c}{1-c^2}\big(cE_{12} - E_{11}\big). \end{aligned} \tag{12}$$

Since $|c| \ll 1$, one can safely neglect c^2 in the denominators and also use $\mu \approx c/2$.

Returning back to the model (9) let us write explicitly the wave-functions of the two dimer configurations for the shortest loop C_1 numbering sites counterclockwise starting from the left lower vertex:

$$|\psi_1\rangle = [12][43]|d_1 d_2' d_3' d_4\rangle, \ |\psi_2\rangle = [32][41]|d_1' d_2' d_3'' d_4''\rangle. \tag{13}$$

Here, the first part of $|\psi_{1,2}\rangle$ is given by a product of two spin singlet states, while the second part is an orbital wave-function represented as a product of states (4) or (5), such that every site is in a fully polarized orbital states along one of the $\hat{\mathbf{z}}_n$-axes. An explicit calculation gives for the diagonal matrix element a sum of two dimer energies $E_{11} = \langle\psi_1|\hat{H}_1|\psi_1\rangle = \langle\psi_2|\hat{H}_1|\psi_2\rangle = -3/2$, while the off-diagonal matrix element is $E_{12} = \langle\psi_2|\hat{H}_1|\psi_1\rangle = 9/64$. Substituting the above values into Eq. (12) we obtain for the properly orthogonalized basis

$$\tilde{E}_{11} = -\frac{3}{2} + \frac{3}{2^{10}} \equiv E_{\rm MF} + V, \quad \tilde{E}_{12} = \frac{3}{2^6} \equiv -t. \tag{14}$$

The off-diagonal matrix element $\tilde{E}_{12}$ is identified with the kinetic energy term in the corresponding QDM Hamiltonian. It amounts to less than 5% of the coupling constant J_2. The diagonal matrix element $\tilde{E}_{11}$ is split into the mean-field energy $E_{\rm MF} = -\frac{3}{2}$ and an excess part determined by quantum fluctuations. This excess part is present only if two parallel dimers occupy an elementary plaquette and should be identified with the potential energy V of QDM. The ratio of the potential energy to the kinetic term constant is very small $V/|t| = 1/16$. Note, that $t < 0$ in the above calculation. As was noted in [3, 5] the sign of t is a matter of convention. A gauge transformation from real wave-functions used to calculate Eq. (14) to complex wave-functions with appropriately chosen phase factors leads to $t \to -t$ (see below).

Since the potential energy V is very small, then a next relevant interaction in the QDM Hamiltonian may be resonances along longer loops. Let us consider first loops C_4 and C_5, which can be investigated by a simple extension of the previous analysis. For two dimer configurations consisting of three dimers along the loop C_4 ($c_4 = -1/2^8$), the diagonal matrix elements coincide again with the mean-field result $E_{11} = E_{22} = -\frac{9}{4}$, while $E_{12} = -9/2^9$. Using Eq. (12) we find that for the properly orthogonalized basis $\tilde{E}_{12} = -27/2^{10} = -t$, while the potential energy term is vanishingly small $V/t = 1/2^8$. For the loop C_5 ($c_5 = 1/2^5$) explicit calculations yield $\tilde{E}_{12} \equiv 0$ or no tunneling. This can be understood by drawing the two dimer configurations on a corresponding cluster of a kagomé lattice and noticing that they are exact degenerate eigenstates for such a cluster.

Finally, let us consider the loops C_2 and C_3. One cannot use the previously derived Eq. (12) in this case since in addition to the two dimer configurations resonating along a perimeter of C_2 there is an extra state with three parallel dimers on the same parallelogram. The first two state are denoted by $|\psi_1\rangle$ and $|\psi_2\rangle$, $\langle\psi_2|\psi_1\rangle = c'$, and the third state by $|\psi_3\rangle$, $\langle\psi_3|\psi_{1,2}\rangle = c$. Three orthogonal states are constructed similar to Eq. (10):

$$\begin{aligned} |\varphi_{1,2}\rangle &\sim \big[|\psi_{1,2}\rangle - \mu'|\psi_{2,1}\rangle - \mu|\psi_3\rangle\big] , \\ |\varphi_3\rangle &\sim \big[|\psi_3\rangle - \mu(|\psi_1\rangle + |\psi_2\rangle)\big] . \end{aligned} \tag{15}$$

The orthogonality conditions yield $\mu \approx \frac{1}{2}c + O(c^2)$, which coincides in the leading order with Eq. (11). The second relation for the relevant case $|c'| \ll |c| \ll 1$ becomes $\mu' = \frac{1}{2}(c' - \frac{3}{4}c^2)$. Resonances around smaller loops lead to a renormalization of the large loop resonance. Calculating now the matrix elements of the Hamiltonian between states (15) we find that resonances on smaller loops, that is $\tilde{E}_{13}$ and $\tilde{E}_{23}$, do not change compared to Eq. (12), whereas the large loop resonance is

$$\tilde{E}_{12} \approx E_{12} + (c^2 - c')E_{11} - cE_{13} . \tag{16}$$

Using the above expression to calculate resonance of singlet bonds on C_2 and C_3 we find that in both cases $\tilde{E}_{12} = 15/2^{10} = -t$. The potential energy term is again extremely small.

Following [6] let us consider now more carefully the issue of the sign of the kinetic energy coefficients t. To change the sign of the resonance matrix element for the shortest loop, one multiplies the basis states by a factor $i^{n_r + n_{l,e} - n_{l,o}}$, where for a given dimer configuration n_r counts the number of dimers on links pointing upwards and right, $n_{l,e}$ ($n_{l,o}$) counts the number of dimers on links pointing upwards and left from sites with even (odd) vertical coordinates. Dimers on strictly horizontal bonds do not contribute to the phase factor. By this operation every resonance move along C_1 loops picks up an extra (-1) factor, changing $t_1 \to -t_1$. At the same time, resonance moves along C_2 and C_3 loops do not change sign, while the sign change takes place again for the C_4 loops: $t_{2,3} \to t_{2,3}$ and $t_4 \to -t_4$. An effective QD Hamiltonian for the trimerized kagomé antiferromagnet is, therefore, dominated by kinetic energy terms for resonance moves between orthogonal dimer configurations $|\varphi_{l_n}\rangle$ and $|\varphi'_{l_n}\rangle$ for every loop C_n of four different types $n = 1, \ldots, 4$ on an effective triangular lattice:

$$\hat{\mathcal{H}}_{\rm QD} = \sum_{l_n} -t_n |\varphi_{l_n}\rangle\langle\varphi'_{l_n}| \,. \tag{17}$$

The kinetic matrix elements are $t_1 = 3/2^6$, $t_2 = t_3 = -15/2^{10}$, and $t_4 = -27/2^{10}$. Tunneling matrix elements for the longer loops have no significant smallness compared to the strongest resonance move: $t_4/t_1 \approx -0.56$, $t_{2,3}/t_1 \approx -0.31$. They have also different signs, which leads to frustration and a sign problem for possible Quantum Monte Carlo investigations of this model [17].

The QDM (17) with only the shortest loop resonance has been investigated in [5, 6] via mapping to a frustrated Ising model in transverse field. The ground state of the dimer model is believed to be a crystalline $\sqrt{12} \times \sqrt{12}$ state, which consists of locally resonating dimer pairs and breaks translational symmetry of the lattice. Such a state should have a fully gapped excitation spectrum. The properties of the QDM (17) with several dimer resonances are not clear at the moment. Since the potential terms are vanishingly small, the QD Hamiltonian is far away from the RK pint and the ground state should break certain lattice symmetries. The excitation spectrum is also expected to be gapped unless a fine tuning of t_n drives the system towards a transition point between two crystalline states.

In conclusion, the presented derivation of QDM for a realistic spin model on trimerized kagomé lattice illustrates a generation of small energy scales in frustrated quantum magnets. The dimer resonance matrix elements in (17) are given by small fractions of a weaker exchange constant, e.g., $t_1 \approx 0.047 J_2$. In a wide temperature interval $t_1 \ll T \ll J_2$ the quantum spin systems is described by an RVB liquid of singlet pairs. At very low temperatures $T < t_1$ a valence bond crystal probably replaces an RVB state. The dimer crystallization is, however, driven by local resonances. Therefore, variational mean-field type approaches [12, 14] are not capable to describe the precise nature of the corresponding ground states.

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