Exactly soluble spin-$\frac{1}{2}$ models on three-dimensional lattices and non-abelian statistics of closed string excitations

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Exactly soluble spin-$\frac{1}{2}$ models on three-dimensional lattices are proposed by generalizing Kitaev model on honeycomb lattice to three dimensions with proper periodic boundary conditions. The simplest example is spins on a diamond lattice which is exactly soluble. The ground state sector of the model may be mapped into a $p$-wave paired state on cubic lattice. We observe for the first time a topological phase transition from a gapless phase to a gapped phase in an exactly soluble spin model. Furthermore, the gapless phase can not be gapped by a perturbation breaking the time reversal symmetry. Unknotted and unlinked Wilson loops arise as eigen excitations, which may evolve into linked and knotted loop excitations. We show that these closed string excitations obey abelian statistics in the gapped phase and non-abelian statistics in the gapless phase.

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**Introductions:** Non-abelian anyons in two dimensions provide a promising candidate for quantum computation, which is topologically protected from decoherence [1]. Recently, this topic has attracted great interests [2]. The most possible system in which the quasiparticles obey non-abelian statistics is two-dimensional electron gas which is closely related to the monodromy matrix in conformal field theory [11]. The statistics of non-abelian anyons is two-dimensional electron gas in the gapped phase and non-abelian statistics in the gapless phase.

In search for non-abelian statistics in exact soluble models, Kitaev proposed an exactly soluble spin model on honeycomb lattice and showed that in a wider parameter region, the vortex excitations obey non-abelian statistics [3]. Since the exotic statistics of the vortices, Kitaev model has attracted many research interests [6, 7]. It has been shown that Kitaev model in the same universality class with $p_x + ip_y$-wave paired state [8].

The point-like anyons are strictly restricted in two dimensions. In three dimensions (3-d), the point-like particles can only be either bosons or fermions. However, the exotic statistics may arise in the closed string excitations. In a seminal paper [9], Witten has shown that the Wilson loops in 3-d Chern-Simons field theory obey non-abelian statistics, which is closely related to the monodromy matrix in conformal field theory [11]. The statistics of unknotted, unlinked closed strings is described by loop braid groups [12]. The quantum loop gas applied to topological quantum computation is a rapidly developing field [13]. Topological quantum order in brane systems was also an interesting subject [14].

In this paper, we will generalize Kitaev model to that on a diamond lattice as well as multi-layer honeycomb lattices in which the closed string excitations obey non-abelian statistics. This 3-d generalization of Kitaev model is also exactly soluble and the ground state sector is equivalent to 3-d $p$-wave paired state. The phase diagram consists of two topological phases, a gapped one and gapless one. The gapped phase is a strong pairing phase whose topological nature is characterized by Hopf invariant and then the ground state is topologically trivial. The singularity of the Hopf mapping in the gapless phase implies that the ground state is topologically non-trivial. Removing the singular points, a non-zero winding number may appear. Thus, in the gapped phase, the closed strings obey abelian anyonic statistics while in the gapless phase, the strings obey non-abelian statistics, which is tantamount to Wilson loops in SU(2)$_3$ Chern-Simons field theory [9]. The Majorana fermion excitations in the gapless phase is always gapless even there is a perturbation with time-reversal symmetry breaking. A topological phase transition between gapped and gapless phases [10] is found for the first time in an exactly soluble model.

**Model and Solution:** We begin with a Kitaev-type coupled spin-$\frac{1}{2}$ model on a diamond lattice (Fig. 1a), whose Hamiltonian reads

$$H_d = \sum_i (J_x \sigma^x_i \sigma^x_{i+e_1} + J_y \sigma^y_i \sigma^y_{i+e_2} + J_z \sigma^z_i \sigma^z_{i+e_3} + J_0 \sigma^z_i \sigma^z_{i+e_3}),$$

where the translational invariant vector is $i = me_1 + ne_2 + le_3 - (m + n + l)e_2$. This Hamiltonian has a set of integrals of motion $\{S_p, p = 1, 2, ...\}$ in which anyone commutes with the Hamiltonian as well as another member in the set. $S_p$ is a loop operator, i.e., an unknotted and unlinked closed string operator along $e_{1,3} = e_2 - e_1$ if we take periodic boundary condition along $e_{1,3}$. The explicit form of $S_p$ is $S_p = \prod_{i=me_{1,3}}^{n-e_{1,3}} \sigma^x_i + \sigma^y_i \sigma^y_{i+e_2}$, which reduces to $S_p = \prod_{i=0}^{m-1} \sigma^x_i \sigma^y_{i+e_3}$ under the periodic constraint $\sigma^z_{i+me_{1,3}} = \sigma^z_i$. Each $S_p$ projects a sector of the to-
consistent with all fermions living in the same loop. Defining the link fermions living in a loop excitation and in fact is a nontrivial Wilson loop. The loop excitation-free Hamiltonian may be written as

$$H_d = i J_z \sum s u_{s,bw} c_{sb} c_{sw} + i J_z \sum s u_{s,bw} (c_{sb} c_{s-e_1,w} - c_{s,w} c_{s-e_1,b}) + J_y y + J_n n$$

(2)

where $s$ is the position of the $z$-links. Note that $[H_d, u_{ij}] = 0$, $u^2 = 1$ and $S_p$ is the product of a set of $u_{ij}$. Therefore, one may take $u_{ij} = \pm 1$ and the eigen value of $S_p$ may be determined by product of $u_{ij}$. According to Lieb’s theorem, the ground state is included in the sector with all $u_{sw} = 1$, which is consistent with all $S_p = 1$. If there are odd numbers of $u_{sw} = -1$ along a loop, this gives $S_p = -1$. This is a loop excitation and in fact is a nontrivial Wilson loop. Defining the link fermions living in $z$-links, $d_s = (c_{s,b} + ic_{s,w})/2$, $d^*_s = (c_{s,b} - ic_{s,w})/2$ and deforming the lattice to a cubic lattice (Fig. 1) in a similar way deforming the honeycomb to a square lattice in two dimensions. The loop excitation-free Hamiltonian may be written as

$$H_0 = \sum_p \xi_p d^*_p d_p + \frac{\Delta_p}{2} (d^*_p d^*_p - d^*_p d_p) + i \frac{\Delta_p}{2} (d^*_p d^*_p - d^*_p d_p)$$

(3)

where $d_p$ is the Fourier component of $d_s$; the dispersion and the pairing functions are

$$\xi_p = J_z - J_x cos p_x - J_y cos p_y - J_v cos p_v$$

$$\Delta_{a,p} = \Delta_{ax} sin p_x + \Delta_{ay} sin p_y + \Delta_{az} sin p_z$$

(4)

This is a p-wave paired state. At present, $\Delta_{1b} = 0$ and $\Delta_{2b} = J_0$ with $b = x, y, v$. Furthermore, one can follow a previous work by Wang and one of the authors (Y.Y) and introduce three-spin couplings and four-spin couplings etc. This leads to the parameters $J_{x,y}$ and $\Delta_{ax,y}$ become tunable. To let $J_z$ and $\Delta_{a}$ be tunable, one needs to add terms like $\sigma^x_{s,b} \sigma^x_{s+e_1,b} + \sigma^x_{s,w} \sigma^x_{s+e_1,w}$ and $\sigma^z_{s,b} \sigma^z_{s+e_1,b}$ etc. These are not nearest neighbor couplings. One can rewritten them as $\sigma^x_{s,b} (b^z_{s+e_1,b} b^z_{s+e_1,w}) \sigma^x_{s+e_1,b} + \sigma^x_{s,w} (b^z_{s,b} b^z_{s,w}) \sigma^x_{s+e_1,w}$ and $\sigma^z_{s,b} (b^z_{s,b} b^z_{s,w}) (b^z_{s+e_1,b} b^z_{s+e_1,w}) \sigma^z_{s+e_1,b}$ because $b_1 b_2 = 1$. Thus, these terms can also be bilinear since $u_{ij}$ are correctly inserted. Thus, the model with these terms added is still exactly soluble but these pairing parameters $\Delta_{ab}$ become tunable. Hereafter, we discuss this general p-wave paired state. The quasiparticle excitations are governed by the BdG equations

$$E_p u_p = \xi_p u_p - \Delta_p^* v_p$$

$$E_p v_p = -\xi_p u_p - \Delta_p^* u_p$$

(5)

where $E_p = \sqrt{\xi_p^2 + (\Delta_p^*)^2 + (\Delta_p)^2}$ is the quasiparticle dispersion, $\Delta_p = \Delta_{1p} + i \Delta_{2p}$, and $(u_p, v_p)$ are the coherence factors with $|u_p|^2 = \frac{1}{2} (1 + \frac{\xi_p}{\Delta_p})$ and $|v_p|^2 = \frac{1}{2} (1 - \frac{\xi_p}{\Delta_p})$ and $v_p/u_p = -(E_p - \xi_p)/\Delta_p$.

The phase diagram can be drawn in a similar way to that for the two-dimensional copy. The phase boundary is determined by $\xi_p = 0$ for any $\Delta_{ab}$. That is, the band insulator/free Fermi gas transition determines the phase boundary, which is given by $|cos p^*| = 1$ with $p^* = (0, 0, 0), (0, 0, \pm \pi), (0, \pm \pi, 0), (\pm \pi, 0, 0), (0, \pm \pi, \pm \pi), (\pm \pi, \pm \pi, 0)$ and $(\pm \pi, \pm \pi, \pm \pi)$ where $J_z \neq J_x \neq J_y \neq 0$. The phase where $\xi_p > 0$ is always gapped. In the $p$-wave sense, this is the strong pairing phase as that in two dimensions. However, out of the gapped phase, there are a pair of $p^*$ so that $E_p = 0$ for general $\Delta_{ab}$. This means that there is a phase transition from the gapped phase to a gapless phase even the time reversal symmetry (or the generalized inversion symmetry) is broken.

**Topology of Phases:** Now, the question is whether the phase transition from the gapped to gapless phases is a topological phase transition. First, we do not observe the spontaneous breaking of any continuous symmetry. This implies the phase transition may be topological. However, in general, a topological phase transition requires an energy gap between the degenerate ground state and any excitation state. To check if the phase with a gapless Majorana fermion excitation is topologically non-trivial, we calculate the topological invariants of both phases in the continuum limit. The momentum space is $D^2 \times S^1$ due to the periodic boundary condition. Note that the coherent function $\psi^1 = (u^*, v^*)$ defines a mapping from $p \in D^2 \times S^1$ to $(u, v) \in S^2$. The unit vector $m = \psi d\psi/|\psi^1|/E_p$ parameterizes this mapping. If we compact $D^2 \times S^1$ to $S^3$ by defining $m = m_0$ on the boundary torus $T^2$, the mapping is called the Hopf mapping. Associated with Hopf mapping, there is a topological invariant, the Hopf invariant, which is defined by

$$Hf = \frac{1}{8\pi^2} \int_{S^3} d^3 p \epsilon_{ijk} A_i F^{jk}$$

(6)

with $A_i(p) = \frac{i}{2} (\psi^1 \partial_p \psi - \psi \partial_p \psi^1)$ and $F_{ij}(p) = \partial_p A_j(p) - \partial_j A_i(p) - \partial_i \times \partial_j M$. This is an abelian Chern-Simons in the momentum space. On the other hand, we know that the Hopf invariant describes the linking numbers of closed strings. Due to the duality between the cubic lattice and dual momentum lattice, the linking number in momentum space is equal to that in the co-ordinate space. For the strong pairing ground state, this linking number is zero because there is
no closed string excitation. One may also directly prove that \((u(\infty), v(\infty)) = (u(0), v(0)) = (0,1)\) in the ground state and thus, \(H_f=0\).

Note that the unit vector \(\mathbf{m}(p^*)\) is singular in the gapless phase because at Dirac points \(p^*, E_{p^*} = 0\). For a set of given parameters in the gapless phase, there are two such Dirac points except at the phase boundary where \(p_1^* = p_2^* = 0\). The unit vector \(\mathbf{m}\) can not be defined in these singular points. To see the topological property, one may pick off these two Dirac points for given parameters. Then, \(S^2\) is reduced to \(S^2 - \{p_1^*, p_2^*\}\), which can contract to an \(S^2\) while at the phase boundary it is \(D^3\) which can contract to origin. The later fact means there is a discontinuity of the mapping at the phase boundary. Inside of the gapless phase, the Hopf mapping now is reduced to a mapping \((u, v)\) from \(S^2\) to \(S^2\). Taking \((px, py)\) as the coordinate in the source \(S^2\), then the winding number of this mapping [18] is the same as that defined in two-dimensional Kitaev-type model

\[
\nu = \frac{1}{4\pi} \int_{S^2} dp_x dp_y (\partial_{px} \mathbf{m}(p)) \times (\partial_{py} \mathbf{m}(p)) \cdot \mathbf{m}(p)
\]

Since \((u(\infty), v(\infty)) = (1, 0)\) is the north pole of the target \(S^2\) and \((u(0), v(0)) = (0, 1)\) is the south pole, we know that \(\nu = 1\). Therefore, the ground state of the gapless phase is topologically non-trivial [19]. (As explained in [19], although there is a phase transition from gapless to gapped phase transition in Kitaev’s original model, both phases are topologically trivial.)

**Loops, Knots and Links:** We now define the loops, knots and links. Loops are excited if \(S_P = -1\). Two loops may merge into a single loop by operation of plaquette operator. Knot and link excitations are created by this operations. To see these operators more clearly, we show it by using a model on a multi-layer honeycomb lattice which is in the same university class with the diamond lattice model in the long wave length limit, i.e., they both are described by a 3-d \(p\)-wave paired state. The links arrangement of the new model is shown in Fig. 2a and the Hamiltonian reads

\[
H_z = \sum_i J_z (\sigma_i^x \sigma_{i+e_1}^x + \sigma_i^y \sigma_{i+e_2}^y + \sigma_i^z \sigma_{i+e_3}^z) + J_y (\sigma_i^y \sigma_{i+e_2}^y + \sigma_i^y \sigma_{i+e_3}^y) + J_z (\sigma_i^z \sigma_{i+e_3}^z + \sigma_i^z \sigma_{i+e_1}^z) + J_c (\sigma_i^z \sigma_i^z + \sigma_i^z \sigma_i^z)
\]

where the fundamental translational invariant vector is \(i = m(e_1 - e_3) + n(e_2 - e_3) + 2le_z\), with basis \(e_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)\), \(e_2 = (\frac{1}{2}, -\frac{\sqrt{3}}{2}, 0)\), \(e_3 = (-1, 0, 0)\), \(e_z = (0, 0, 1)\). Again, there exist a series of string operators \(S_p \equiv \prod_{m=0}^{n-1} \iota^x \sigma^x_{m+e_3}\) which commute with the Hamiltonian under periodic boundary condition. Using Majorana fermions, we obtain bilinear fermionic Hamiltonian and the closed string excitation-free Hamiltonian has a dispersion \(E = |E_1 E_2|^{1/2}\). The gapless phase falls in the area given by the inequalities \(|J_{e3}||J_{e1}| + |J_{e2}| + |J_{e3}| \leq \sum_j \{ |J_{e1}e_1j| + |J_{e2}e_2j| + |J_{e3}e_3j|^2 \}^2 \). One may prove that \(H_z\) is also equivalent to a \(p\)-wave paired model.

The lattice for \(H_z\) is topologically equivalent to a solid torus \(D^2 \times S^1\) with \(e_{1,3}\) as its tangent vector (Fig. 3a). All the loop operators following the geodesic circles commute with the Hamiltonian and they are good quantum numbers. Two neighboring loops following zigzag geodesic circle are the product of plaquette operators \(P\) sandwiched between them, \(P_1 P_2 \cdots P_{n-1} = S_{1}^{0} S_{1}^{0+e_3}\), where \(P_i = \sigma^x \sigma^y \sigma^z\) is the plaquette operator defined on the hexagon. In this way, we merge two loops into a single loop. These loops form a loop gas. Links and knots can be obtained by twisted boundary conditions (See Figs. 3b and 3c). These knots and links may also be thought \(Z_2\) Wilson loops but they are not exact eigen excitations of \(H_z\). However, the non-commutativity between \(H_z\) and the knots and links may only happen in the bonds connecting two geodesic circles. Therefore, one can ignore this non-commutativity in the thermodynamic and long wave length limits and takes these Wilson loops to be quasi-exact eigen excitations. The above analysis may also be done on diamond lattice. However, since there is a shift between two adjacent layers, the illustrations are not so direct.

**Statistics:** One can calculate the linking number of a closed string configuration. In the gapped phase, the Hopf invariant [19] counts the linking number of the dual links in momentum space, which is equal to the linking number on the original co-ordinate space. The fact that the Hopf invariant is the abelian Chern-Simons implies these closed string excitations obey abelian statistics.

To see the closed string excitations obey non-abelian statistics in the gapless phase, we follow Witten’s discussion in dealing with knots and links in SU(N) Chern-
By using the monodromy B punctured complicated stuff but the right piece, we consider two Wilson loops in $S^3$. Using an $S^2$ cuts $S^3$ into two pieces as shown in Fig. 4a, the left piece $M_L$ may contain very complicated stuff but the right piece $M_R$ is simple. Then, two Wilson loops puncture four points which are corresponding to creating two spin fields $\sigma$ and destroying two $\sigma$ on $S^2$. The low energy limit of BdG equations \[ \psi \rightarrow e^{-i\sigma/2} \] is the 3+1-dimensional Dirac equations. Hence, the Hilbert space of the massless Majorana fermions restricted on $S^2$ is determined by $c = 1/2$ conformal field theory. The fusion rule $\sigma \cdot \sigma = 1 + \psi$ implies the Hilbert space on this punctured $S^2$ is two-dimensional. Therefore, three states $L_+, L_0$ and $L_-$ showed in Fig. 4b are linear-dependent. By using the monodromy B matrix \[ [11] \] these states may relate to each other through

\[ L_0 = BL_+, \quad L_- = BL_0 = B^2L_+ \] \[ (9) \]

where the $B$ matrix is not proportional to identity. Obviously, the operation through the $B$ matrix is an exchange of these vortices $\sigma$ and then they obey non-abelian statistics. Any spin-$\frac{1}{2}$ has an SU(2) gauge symmetry if the spin is represented by fermion or boson operators because the Hilbert space is enlarged \[ 20, 21 \]. So is the present model. Fixing $u_{ij} = \pm 1$ is corresponding to a gauge fixing, i.e., reducing the gauge symmetry from SU(2) to Z_2. After gauge transformation, $\sigma$ carries a unit SU(2) charge. By using the non-abelian bosonization \[ 22 \], the massless Majorana fermion theory on $S^2$ is bosonized to an SU(2)/U(1) coset Wess-Zumino-Witten model. The $k = 2$ turns out that the Wilson loops indeed obey non-abelian statistics in the sense Witten defined. Due to the gauge group is in its defining representation, the $B$ matrix has two eigenvalues $\lambda_1 = e^{-i\pi/8}$, $\lambda_2 = -e^{i\pi/8}$. Thus, the three states in Fig. 4b satisfy the skein relation

\[ qL_0 + (q^{1/2} - q^{-1/2})L_0 + q^{-1}L_- = 0 \] \[ (10) \]

with $q = e^{i\pi/2}$. Witten took this relation as the definition of knot polynomials on $S^3$ \[ 9 \]. As Witten pointed out, the physical meaning of the skein relation is clear: all links and knots can be resolved by the skein relation. Therefore, if we know the physical behavior of unknotted and unlinked quantum loop gas, the system with knots and links may be understood. This means that the study of the quantum loop gas is fundamental \[ 13 \].

In conclusions, we constructed a 3-d exactly soluble spin model with closed string excitations obeying non-abelian statistics. This is closely related to Witten’s original proposal to the statistics of the Wilson loops in the Chern-Simons field theory. A topological phase transition between gapless and gapped phases was first time predicted.

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\[ e^{\frac{1}{2}(q_x + (2 + \sqrt{3})q_y)}(J_x J_z - J_y J_z) + J_z^2, \quad E_2 = e^{i(q_x + 4q_y)}J_x^2 - e^{i(5 - \frac{2}{\sqrt{3}})q_y + i2q_z}(-e^{i\frac{1}{2}((\sqrt{3} - 2)q_y)}(J_x^2 + J_y^2) - e^{i\frac{1}{2}(2q_x + (\sqrt{3} - 2)q_y)}J_x^2 - e^{i\frac{1}{2}((\sqrt{3} - 2)q_y + e^{i\frac{1}{2}(5\sqrt{3} - 6)q_y)}J_x J_y - e^{i\frac{1}{2}(q_x + 2(\sqrt{3} - 2)q_y)}(e^{i\sqrt{3}q_y} - 1)(J_x - J_y) J_z). \]

One may construct another exactly solvable model which is on the lattice as shown in Fig. 2b. However, the dispersion is more complicated.