Calculated magnetic exchange interactions in Dirac magnon material Cu$_3$TeO$_6$

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Recently topological aspects of magnon band structure have attracted much interest, and especially, the Dirac magnons in Cu$_3$TeO$_6$ have been observed experimentally. In this work, we calculate the magnetic exchange interactions $J$'s using the first-principles linear-response approach and find that these $J$'s are short-range and negligible for the Cu-Cu atomic pair apart by longer than 7 Å. Moreover there are only 5 sizable magnetic exchange interactions, and according to their signs and strengths, modest magnetic frustration is expected. Based on the obtained magnetic exchange couplings, we successfully reproduce the experimental spin-wave dispersions. The calculated neutron scattering cross section also agrees very well with the experiments. We also calculate Dzyaloshinskii-Moriya interactions (DMIs) and estimate the canting angle ($\sim 1.3^\circ$) of the magnetic non-collinearity based on the competition between DMIs and $J$'s, which is consistent with the experiment. The small canting angle agrees with that the current experiments cannot distinguish the DMI induced nodal line from a Dirac point in the spin-wave spectrum. Finally we analytically prove that the “sum rule” conjectured in [Nat. Phys. 14, 1011 (2018)] holds but only up to the 11th nearest neighbour.

I. INTRODUCTION

The non-trivial topological nature of electronic bands has been studied extensively during the past decade [1, 2]. Plenty of topological materials have been discovered, such as topological insulator [1, 2], Dirac semimetal [3–8], Weyl semimetal [9–11] and node-line semimetal [12–16], etc [17]. In addition to the above topological phases, the rich variety of spatial symmetries in condensed matter systems results in various novel topological crystalline insulators/seminmetals [18–24]. By exploiting the mismatch between the real and momentum-space descriptions of the band structure, a complete classification scheme of band topology has been proposed [25–28]. A comprehensive database search for ideal non-magnetic topological materials has been finished [29] by combining first-principles calculation and the symmetry-indicator theory [30]. Meanwhile, thousands of electronic topological materials have also been proposed based on the graph theory [31] and the complete mapping between the symmetry representation of occupied bands and the topological invariants [32].

It is worth mentioning that the topological feature is not only restricted to electronic systems. The band crossings in systems of photons [33–36] and phonons [37, 38] have also been intensively investigated. Moreover, recent research in the magnon systems has led to the discovery of topological magnon insulators [39, 40], magnonic Dirac semimetals [41–43] and Weyl semimetals [44–46].

In 2017, Li et al. [47] proposed Dirac magnons may occur in the three-dimensional antiferromagnetic material Cu$_3$TeO$_6$. As shown in Fig. 1, Cu$_3$TeO$_6$ crystallizes in the centrosymmetric cubic crystal structure (space group $Ia-3$) [48, 49]. Temperature ($T$) dependent magnetic susceptibility ($\chi(T)$) reveals that this compound displays a long-range antiferromagnetic (AFM) ordering below $T_N \sim 60$ K [50]. Within the range of $T = 180 - 330$ K, $\chi(T)$ can be fitted very well by the Curie-Weiss (CW) law with the CW temperature $\theta_{CW} = -130$ K [50]. The $\chi(T)$ deviates from CW behavior below 180 K, which is three times larger than $T_N$. This may indicate the frustrated magnetic feature [50]. A clear bulk magnetic transition at around 62 K has also been observed by muon-spin relaxation/rotation measurement [51]. Neutron powder diffraction experiment [50] suggests two possible magnetic configurations: (i) collinear AFM order (ii) non-collinear configuration. In the collinear case, the two spins connected by inversion ($P$) have opposite spin orientations [50], thus Cu$_3$TeO$_6$ is invariant under $PT$ symmetry ($P$ is the time-reversal transformation), protecting robust magnon Dirac points [47]. For the non-collinear magnetic case [50], Li et al. [47] propose that non-collinearity breaks the U(1) symmetry. As a result, the Dirac point in the collinearly magnetically ordered state expands into a nodal line [47].

Motivated by this theoretical prediction, Yao et al. [52] and Bao et al. [53] have measured spin excitations of Cu$_3$TeO$_6$ with inelastic neutron scattering (INS), respectively. Both of them have observed the existence of band crossing points in the magnon spectra [52, 53]. In addition to Dirac points, at $\Gamma$ and $H$ points of the Brillouin zone (BZ) Bao et al. [53] also observed the triply degenerate nodes which can also occur in electronic bands [54, 55]. Bao et al. [53] found that the experimental magnon band dispersion can be well reproduced by a spin Hamiltonian dominated by only the 1st nearest-neighbour (NN) exchange interaction $J_1$. While Yao et al. [52] suggested that the magnetic moments in this compound couple over a variety of distances, and even the ninth-nearest-neighbour $J_9$ plays an important role. Strikingly they found an interesting relation between magnon eigenvalues at different high symmetry points of BZ which was dubbed as “sum rule” [52].

Generally, spin-orbit coupling (SOC) always exists...
and leads to the Dzyaloshinskii-Moriya interactions (DMIs) [56, 57] even in the centrosymmetric compound \( \text{Cu}_3\text{TeO}_6 \), as discussed in the following sections. The DMIs could result in a non-collinearity in the ground magnetic state, leading to nodal lines in magnetic excitations [47]. As mentioned above, the two experiments [52, 53] have observed the existence of Dirac points but cannot identify the nodal lines from the band crossing points. Note that the size of nodal lines strongly depends on the canting angle of the non-collinearity, which is determined by the competition between exchange interaction \( J \) and DMI [47]. Therefore it is an interesting issue to obtain accurate spin exchange parameters \( J \)'s and DMIs, which we address in the current work.

In this paper, based on first-principles calculations, we systematically study the electronic and magnetic properties of \( \text{Cu}_3\text{TeO}_6 \). The calculations show that \( \text{Cu}_3\text{TeO}_6 \) is an insulator with a band gap about 2.07 eV. The calculated magnetic moment of Cu ions is about 0.81 \( \mu_B \), which is larger than the experimental value (0.64 \( \mu_B \)) measured by the neutron powder diffraction [50]. Using a first-principles linear-response (FPLR) approach [58], we calculate the spin exchange parameters \( J \)'s. Based on these spin exchange parameters, we calculate the magnetic excitation spectra using linear spin wave theory (LSWT) and the calculated spin wave spectra agree with the experiments very well, as well as the positions of the Dirac and triply degenerate magnons in the BZ [52, 53]. We also calculate the neutron scattering cross section, which is consistent with the experiment [52, 53]. The calculated exchange interactions are short-range and negligibly weak for the distance more than 7 Å. There are only five sizable magnetic exchange terms and all them favor antiferromagnetic ordering. These spin exchange parameters are compatible with the modest frustration in \( \text{Cu}_3\text{TeO}_6 \) according to their signs and magnitudes. We also analytically prove that the magnon energies at high symmetry points of BZ cannot own a general “sum rule” conjectured in Ref. [52] which is found to be only satisfied up to the 11th NN. Moreover, we also calculate the DMIs and estimate the canting angle of non-collinearity which is about 1.3°, consistent with the experimental value \( \sim 6° \) [50]. This may be the reason why the recent experimental works only observed the existence of Dirac points instead of the nodal lines [52, 53].

II. METHOD

The electronic band structure and density of states calculations are carried out by using the full potential linearized augmented plane wave method as implemented in WIEN2K package [59]. Local spin density approximation (LSDA) for the exchange-correlation potential is used here. A \( 10 \times 10 \times 10 \) k-point mesh is used for the Brillouin zone integral. Using the second-order variational procedure, we include the SOC interaction [60]. The self-consistent calculations are considered to be converged when the difference of the total energy of the crystal does not exceed 0.01 mRy. We utilize the LSDA + \( U \) scheme [61] to take into account the effect of Coulomb repulsion in Cu-3d orbital. The value of \( U = 10 \) eV and \( J = 1 \) eV for Cu-oxides works well in the previous theoretical work [62, 63]. We vary the parameter \( U \) between 8.0 and 10.0 eV and find that our results are not sensitive to the values of \( U \) in this range. Thus in this paper we show our results for \( U = 10 \) eV.

The spin exchange parameters \( J \)'s are the basis to understand magnetic properties. By fitting \( J \) to reproduce experimental results, such as \( \chi(T) \) and magnon dispersion, one can extract the exchange interaction parameters \( J \)'s. However, an unambiguous fitting is basically impossible. For example, as mentioned above, though the INS experimental results of Yao et al. and Bao et al. are consistent with each other, their fitting results of the spin exchange interactions are completely different [52, 53]. In addition to this phenomenological approach, theoretical calculations can also be used to estimate the exchange interaction parameters. A popular numerical method to calculate \( J \) is to calculate the total energies of the \( N + 1 \) magnetic configurations, and map it by a spin Hamiltonian to extract \( N \) exchange constants. Unfortunately this theoretical method has several drawbacks: (i) the calculated magnetic moments may depend on the magnetic ordering, which significantly affect the accuracy of the obtained \( J \); (ii) it is not clear that how many exchange interactions \( J \) one need to use when mapping the total energies from the first-principles calculation on the spin Hamiltonian. An alternative but much more efficient method to calculate spin exchange interactions by first-principles is based on combining magnetic force theorem and linear-response approach [64]. The exchange interaction parameters are determined via calculation of second variation of total energy for small deviation of magnetic moments [64]. This method allows one to calculate \( J(q) \), the lattice Fourier transform of the exchange interactions \( J(R_d) \). Thus one can easily calculate long-range exchange interactions accurately even in complicated systems like \( \text{Cu}_3\text{TeO}_6 \) here owing a highly-interconnected three-dimensional spin network. Recently this technique has been used successfully for evaluating magnetic interactions including DMIs in a series of materials [58, 63–71], and is employed in this work to estimate the spin exchange parameters \( J \)'s and DMIs [58].

III. RESULTS

As shown in Fig. 1, \( \text{Cu}_3\text{TeO}_6 \) crystallizes in the centrosymmetric spin-web compound. The highly-interconnected three-dimensional spin network consists of 12 Cu ions per primitive cell, where six Cu ions form an almost coplanar hexagon and each Cu ion is shared by two hexagons. Based on the collinear antiferromagnetic configuration suggested by neutron powder diffraction experiment [50] as shown in Fig. 1, we perform the
first-principles calculations. Here we adopt the LSDA + $U$ (= 10 eV) scheme, which is adequate for the magnetically ordered insulating states [72]. The band structures and the density of states are shown in Fig. 2 and Fig. 3, respectively. Our calculations indicate that Cu$_3$TeO$_6$ is an insulator with a band gap about 2.07 eV from LSDA + $U$ (= 10 eV) calculations. The O-2p states are mainly located between $-8.0$ and 0.0 eV, while Te 5s and 5p bands appear mainly above 3.0 eV. Hence the nominal valence for Te is +6 while that for O is −2. As a result, Cu ions have the nominal valence of +2, indicating the 3$d^9$ electronic configuration. The nine 3$d$ occupied states of Cu ions are mainly located from $-8.0$ to $-3.0$ eV, implying strong hybridization between Cu and O states. Meanwhile the only one unoccupied state of Cu$^{2+}$ ions appears mainly between 3.0 to 5.0 eV. Despite of strong hybridization between Cu and O states, the calculated magnetic moment at the O site is negligible ($\sim 0.01 \mu_B$), and the major magnetic moment is located at the Cu site. The calculated magnetic moment of the Cu ions is 0.81 $\mu_B$, which is smaller than the ideal 3$d^9$ ($S=1/2$) configuration and larger than the experimental value 0.64 $\mu_B$ [50].

Based on the calculated electronic structures, we estimate the spin exchange parameters $J_i$'s (we refer to the exchange interaction of the $i$th NN as $J_i$) [58]. The FPLR approach allows us to calculate long-range exchange interactions accurately, and the results show that these exchange parameters decrease rapidly with increasing distance. We summarize the results up to 20th NN interaction $J_{20}$ in Table I. The fitted spin exchange parameters in the previous experimental work are also shown for comparison [52, 53]. As the FPLR approach automatically incorporates all the symmetry restrictions on exchange interactions, we can distinguish the inequiv-
TABLE I. Calculated spin exchange parameters (in meV) evaluated from LSDA + U (= 10 eV) scheme. The Cu-Cu distances and the corresponding number of neighbors are presented in the 2nd and 3rd columns. The fitting spin exchange parameters in the experimental work are also presented for comparison.

| Distance(A) | NN | Ref. [53] | Ref. [52] | Our results |
|------------|----|-----------|-----------|-------------|
| $J_1$      | 3.18 | 4 | 9.07 | 4.49 | 7.05 |
| $J_2$      | 3.60 | 4 | 0.89 | -0.22 | 0.51 |
| $J_3$      | 4.77 | 2 | -1.81 | -1.49 | 0.04 |
| $J_4$      | 4.81 | 2 | 1.91 | 1.33 | 2.18 |
| $J_5$      | 4.81 | 2 | 1.91 | 1.79 | 0.09 |
| $J_6$      | 5.48 | 4 | 0.09 | -0.21 | 0.01 |
| $J_7$      | 5.73 | 4 | 1.83 | -0.14 | -0.01 |
| $J_8$      | 5.97 | 4 | - | 0.11 | 0.04 |
| $J_9$      | 6.21 | 4 | - | 4.51 | 3.77 |
| $J_{10}$   | 6.34 | 2 | - | - | -0.01 |
| $J_{11}$   | 6.34 | 2 | - | - | -0.02 |
| $J_{12}$   | 6.74 | 4 | - | - | -0.06 |
| $J_{13}$   | 7.17 | 2 | - | - | -0.04 |
| $J_{14}$   | 7.17 | 2 | - | - | 0.00 |
| $J_{15}$   | 7.27 | 4 | - | - | 0.00 |
| $J_{16}$   | 7.46 | 4 | - | - | 0.02 |
| $J_{17}$   | 7.64 | 4 | - | - | 0.10 |
| $J_{18}$   | 7.83 | 4 | - | - | 0.00 |
| $J_{19}$   | 8.26 | 4 | - | - | -0.02 |
| $J_{20}$   | 8.26 | 4 | - | - | 0.00 |

The magnetic excitation spectra of the two experimental works [52, 53] are consistent with each other, but there is only one picture containing discrete points which can be used for comparison in Ref. [52].
intensities in Figs. 5(a) and (b) are distributed in both acoustic and optical branches, while the INS intensity in Fig. 5(c) is mainly located at the optical branches between 15 and 20 meV. At $\Gamma_1(1,1,2)$ point, the INS intensity is mainly located at the acoustic branch and the triply degenerate point, while the intensity at $\Gamma_2(2,0,2)$ point appears mainly at the Dirac point of 16.6 meV. Both at $H_1(2,1,2)$ and $H_2(1,0,2)$ point, the intensity is mainly located at the branch of the highest energy. As $Q$ moves from $P_2(\frac{1}{2}, \frac{1}{2}, \frac{3}{2})$ to $H_1(2,1,2)$, the main intensity is located at the lowest energy branch, as well as in the path $P_2(\frac{3}{2}, \frac{1}{2}, \frac{3}{2}) - N_2(\frac{1}{2}, 1, \frac{3}{2})$. These results are consistent with the experimental works [52, 53].

In Ref. [52], through checking the magnon eigenvalue $\omega_m(q)$ at four high symmetry points, $\Gamma = (0,0,0), P = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), H = (0,1,0), N = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, Yao et al. obtained an interesting relation expressed by the following eigenvalue-version of compatibility relation:

$$\sum_m (\omega_{P,m}^2 + 4\omega_{N,m}^2 + \omega_{H,m}^2) = \sum_m 6\omega_{N,m}^2, \quad \text{(1)}$$

which they called “sum rule” and proved that it holds at least up to the 9th NN [52]. Such kind of sum rule is surprised to us for conventional compatibility relation is usually only about the symmetry representations. Hence in the following we analytically investigate whether there exists a general sum rule on earth. We adopt the Heisenberg magnetic model as written by $\hat{H} = \frac{1}{2} \sum_{l,n,l',n'} J(R_l + R_n - R_{l'} - R_{n'}) S_{l,n} S_{l',n'}$ where $l, l'$ label the unit cell and $n, n'$ label the Cu ions: $n, n' = 1, 2, \ldots, 6$ represent Cu with up spin while $n, n' = 7, 8, \ldots, 12$ represent Cu with down spin. The positions for these Cu ions in the primitive unit cell are key for the following analysis, we thus shown them in Tables I of the Appendix.

Based on the antiferromagnetic ground state and using the LSWT, the magnon spectra are obtained by diagonalizing the following matrix and then extracting the non-negative eigenvalues for genuine magnon excitations [74]:

$$\mathcal{H}_{SW}(q) = \begin{bmatrix} \mathcal{J}(q) & \mathcal{J}'(q) \\ -\mathcal{J}'(q) & -\mathcal{J}(q)^\top \end{bmatrix}, \quad \text{(2)}$$

where $\mathcal{J}(q)$ and $\mathcal{J}'(q)$ (both are $12 \times 12$ matrices) are expressed by:

$$\mathcal{J}(q)_{n,n'} = \zeta(n, n') \sum_l J(\tau_n, \tau_{n'} + R_l) e^{i q R_l} + \delta_{n,n'} \sum_{l,n''} J(\tau_n, \tau_{n''} + R_l) - \sum_{l,n''} J(\tau_n, \tau_{n''} + R_l), \quad \text{(3)}$$

$$\mathcal{J}'(q)_{n,n'} = \zeta'(n, n') \sum_l J(\tau_n, \tau_{n'} + R_l) e^{i q R_l}, \quad \text{(4)}$$

where $\delta_{n,n'}$ is the Kronecker delta function, $n''$ runs through the Cu ions with spins parallel to that of the $n$th Cu while $n'''$ runs through ions with spins antiparallel to that of the $n$th Cu. $\zeta(n, n')$ ($\zeta'(n, n')$) is equal to 1 when the spins for the $n$th and $n'$th Cu’s are parallel (antiparallel) otherwise equal to zero.

Note that $\sum_m \omega_m(q)^2 = tr(\mathcal{H}_{SW}^2)$, thus Eq. (1) can be written in the following form:

$$tr(\mathcal{H}_{SW}(\Gamma)^2 + \mathcal{H}_{SW}(H)^2 + 4\mathcal{H}_{SW}(P)^2 - 6\mathcal{H}_{SW}(N)^2) = 0. \quad \text{(5)}$$
Firstly we consider the 1st NN. For Cu ion labelled by \( n = 1 \), there are four 1st NNs, as shown in the first 4 rows of the Table II of the Appendix. Cu ions in this compound occupy the 24d Wyckoff positions, and there are in total 24 Cu-Cu 1st NN bonds as also listed in Table II of the Appendix. We use \((n, n', R_l)\) to denote the bond formed by the Cu ions labeled by \( \tau_n \) and \( \tau_n' + R_l \). With these data, we can obtain all the matrix elements of \( H_{SW} \) for any given \( \mathbf{q} \). For each pair \((n, n')\) of Cu ions, there is at most one nearest-neighbor exchange path connecting them as shown in Table II. For the mentioned four high symmetry points, the nondiagonal matrix elements of \( H_{SW} \) are found to be one of the following values \( \pm J_1 \), or \( \pm iJ_1 \), or 0. While the diagonal matrix elements are equal to a constant for any \( \mathbf{q} \). Therefore we prove that \( tr(H_{SW}(\Gamma)^2) = tr(H_{SW}(H)^2) = tr(H_{SW}(N)^2) \) and Eq. (5) is satisfied for the 1st NN. Similarly, we can prove that Eq. (5) holds from the 2th NN to the 11th NN. Further we can prove that Eq. (1) holds with the exchanges up to 11th NNs. However for the 12th NN, as shown in Table III of the Appendix, for each pair \((n, n')\), there may exist 4 exchange pathes connecting them, so the corresponding matrix element of \( H_{SW} \) are the summation of four terms by Eqs. (3) and (4). This situation is different from that for the 1st NN, and one can easily prove that Eq. (5) is no longer right for 12th NNs. Therefore the “sum rule” (i.e. Eq. (1)) holds only up to the 11th NNs.

It is worth mentioning that, though the Cu₃TeO₆ system has a global inversion center, most of the Cu-Cu bonds don’t own inversion symmetry. Within the distance of 7 Å, only the DMIs for 5th NN and 11th NN are required to be vanishing because their bonds have inversion center. Using the FPLR approach \[58\], we calculate the DMIs. Since the strength of DMI is proportional to the corresponding \( J \), we only calculate the \( D_1 \) and \( D_9 \) (we refer to the DMI of the ith NN as \( D_i \)). The \( D_1 \) for the Cu-Cu bond between \((0, 0.25, 0.969)\) and \((-0.031, 0.5, 0.75)\) in the coordinate system is estimated to be \((0.05, 0.25, 0.34)\) meV. The direction of \( D_1 \) is nearly parallel to the normal direction of the triangle formed by the three atoms in the Cu-O-Cu bond, which is consistent with the physical expectation. While our calculation show that \( D_9 \) is very small (|\( D_9 \)| = 0.06 meV) and have little effect on the magnetic configuration. Our numerical ratio of |\( D_1 \)|/\( J_1 \) is about 0.06, which is smaller than the pure theoretical model estimation (0.2) \[47\]. The calculated DMIs result in a canting angle about 1.3°, which is in agreement with the experimental value ~6° \[50\]. The size of the nodal line is proportional to square of the ratio of DMI and \( \mathbf{J} \) \[47\], thus it is hard to identify the nodal lines from the Dirac points for the current experiments.

IV. CONCLUSION

In conclusion, using first-principles calculation, we presented a comprehensive investigation of Cu₃TeO₆. The calculations show that Cu₃TeO₆ is an insulator with a band gap about 2.07 eV and the calculated magnetic moment of the Cu ions is 0.81 μ\( \text{B} \). Using magnetic force theorem and a first-principles linear-response approach, we estimate the spin exchange parameters. The calculated exchange parameters are short-range and can be neglected for the distance more than 7 Å. The strongest terms \( J_1 \) and \( J_9 \) are compatible with the magnetic ground state, while the terms \( J_2 \), \( J_4 \), and \( J_{10} \) are much smaller and not compatible with the magnetic ground states, which is consistent with the modest frustration in this compound. We calculated the magnon spectra using linear spin wave theory and the calculated spin wave is in good agreement with the experiment. We also prove analytically that the “sum rule” proposed in Ref. \[52\] only holds up to the 11th nearest-neighbour interactions. The calculated DMIs lead to a very small canting angle about 1.3° of non-collinear antiferromagnetic order. The weak DMIs are the possible reason why the previous experimental work did not observe the nodal lines.

V. ACKNOWLEDGEMENT

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VI. APPENDIX

In the Appendix, we list the coordinates of 12 Cu ions in Table I.

| n   | \( \tau_n \)               |
|-----|-----------------------------|
| 1   | \((x, 0, \frac{1}{2})\)     |
| 2   | \((\frac{1}{2}, -x, 0, \frac{1}{2})\) |
| 3   | \((\frac{1}{2}, x, 0)\)     |
| 4   | \((\frac{1}{2}, \frac{1}{2} - x, 0)\) |
| 5   | \((0, \frac{1}{2}, x)\)     |
| 6   | \((-x, 0, -\frac{1}{2})\)   |
| 7   | \((\frac{1}{2} + x, 0, \frac{1}{2})\) |
| 8   | \((-\frac{1}{2}, -x, 0)\)   |
| 9   | \((\frac{1}{2}, \frac{1}{2} + x, 0)\) |
| 10  | \((0, -\frac{1}{2}, -x)\)   |
| 11  | \((0, \frac{1}{2}, -\frac{1}{2} + x)\) |
| 12  | \((0, \frac{1}{2}, \frac{1}{2} + x)\) |

TABLE I. The coordinates of the 12 Cu ions in the conventional unit cell basis vectors. \( x = 0.96907 \).

According to Eqs. (2,3,4) of the main text, it is very easy to calculate the matrix \( H_q \) for any wave vector \( q \) when knowing the full information of all the bonds. We thus give the detailed information of all the bonds connecting Cu ions for the 1st NN and 12th NN in Tables II and III, respectively.

| n   | \( n' \) | \( R_{q} \)               |
|-----|----------|-----------------------------|
| 1   | 9        | \((1, 1, 0)\)               |
| 1   | 10       | \((\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 1   | 11       | \((1, 0, 1)\)               |
| 1   | 12       | \((1, 0, -1)\)              |
| 2   | 9        | \((0, 1, 1)\)               |
| 2   | 10       | \((-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\) |
| 2   | 11       | \((-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 2   | 12       | \((-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 3   | 7        | \((1, 1, 0)\)               |
| 3   | 8        | \((-1, 1, 0)\)              |
| 3   | 11       | \((0, 1, 1)\)               |
| 3   | 12       | \((\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 4   | 7        | \((\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 4   | 8        | \((-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 4   | 11       | \((1, 0, 1)\)               |
| 4   | 12       | \((\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 5   | 7        | \((1, 0, 1)\)               |
| 5   | 8        | \((-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 5   | 9        | \((0, 1, 1)\)               |
| 5   | 10       | \((0, -1, 1)\)              |
| 6   | 7        | \((1, 0, 1)\)               |
| 6   | 8        | \((-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 6   | 9        | \((\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 6   | 10       | \((-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |

TABLE II. The 24 bonds for the first NN: each bond is characterized by the positions of the two endings: \( \tau_n, \tau_{n'} + R_q \).

| \( n \) | \( n' \) | \( R_q \)               |
|---------|---------|-----------------------------|
| 1       | 8       | \((-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 1       | 8       | \((-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\) |
| 1       | 8       | \((-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 2       | 7       | \((\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 2       | 7       | \((\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 2       | 7       | \((\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 3       | 10      | \((-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 3       | 10      | \((-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 3       | 10      | \((-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 4       | 9       | \((\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})\) |
| 4       | 9       | \((\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 4       | 9       | \((\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 5       | 12      | \((-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 5       | 12      | \((-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 5       | 12      | \((-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 6       | 11      | \((\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |
| 6       | 11      | \((-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})\) |
| 6       | 11      | \((-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})\) |

TABLE III. The 24 bonds for the 12th NN: each bond is characterized by the positions of the two endings: \( \tau_n, \tau_{n'} + R_q \).
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