t-J model on the effective brick-wall lattice for newly discovered high temperature superconducting Ba$_2$CuO$_{3+\delta}$

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Layered copper oxides have highest superconducting transition temperatures at ambient pressure. Its mechanism remains a grand challenge in condensed matter physics. The essential physics lying in 2-dimensional copper-oxygen layers is well described by a single band Hubbard model or its strong coupling limit t-J model in 2-dimensional square lattice. Recently discovered high temperature superconductor Ba$_2$CuO$_{3+\delta}$ with $\delta \sim 0.2$ has different crystal structure with large portion of in-plane oxygen vacancies. We observe that an oxygen vacancy breaks the bond of its two neighboring copper atoms, and propose ordered vacancies in Ba$_2$CuO$_{3+\delta}$ lead to extended t-J model on an effective brick-wall lattice. For the nearest neighbor hopping, the brick-wall model can be mapped onto t-J model on honeycomb lattice. Our theory explains the superconductivity of the new compound at high charge carrier density, and predict a time reversal symmetry broken pairing state.

Introduction.—Understanding of high Tc copper oxides remains a grand challenge in condensed matter physics despite intensive studies in the past over thirty years. It is generally accepted that the basic physics of high $T_c$ cuprates is on CuO$_2$ planes, and the half-filled $d_{x^2-y^2}$ holes of formal Cu$^{2+}$ form Mott insulator or charge transfer insulator. Chemical doping to the parent compounds introduces additional holes and leads to the $d$-wave superconductivity with the highest transition temperatures at ambient pressure. Recently discovered superconductor of Ba$_2$CuO$_{3+\delta}$ with $\delta \approx 0.2$ is a new family of high $T_c$ cuprate. The Meissner effect measurement shows that the compound has transition temperature $T_c = 73K$, which is much higher than that of the similar structure high $T_c$ cuprate Ba$_x$La$_{1-x}$CuO$_4$. It is then interesting and important to examine the electronic structure and superconductivity of the newly discovered Ba$_2$CuO$_{3+\delta}$, which may also shed new light to our understanding of high $T_c$ cuprates in general.

Ba$_2$CuO$_{3+\delta}$ has compressed octahedron with the apical oxygen atoms closer to the central Cu-atoms, the Cu-O bond length for the apical O is about 1.9 Å, shorter than the Cu-O bond length on the Cu-O plane. This is different from other known cuprates, where the Cu-O bond along the apical O is longer. There are a large number of O-vacancies in Ba$_2$CuO$_{3+\delta}$, which are located on the CuO$_2$ plane as neutron data showed.¹ These vacancies are expected to play important role in the electron structure and possibly superconductivity. First principles calculations have been reported by Liu et al.,² who considered various possible crystal structures. For $\delta = 0.25$, they have found crystal structures corresponding to lower total energies. There have been a number of proposed theories for its electronic structure and superconductivity. In the usual cuprates, the formal valence of Cu is less than +2.2, corresponding to the hole concentration on the CuO$_2$ plane less than 20%. In Ba$_2$CuO$_{3+\delta}$, the average valence of Cu is +2(1 + $\delta$), corresponding to average hole concentration of 2$\delta$ $> 0.2$ for the value of given $\delta \sim 0.2$. This has led to the proposal of 2-band Hubbard model to describe the new compound.¹ Large number of O vacancies has led to the proposal of weakly linked 2-chain ladder for the superconductivity,² whose related physics has been previously examined extensively in study of Hubbard or t-J ladder.³

In this paper, we take the viewpoint that the observed superconductivity in Ba$_2$CuO$_{3+\delta}$ is resulted from an ordered crystal structure and the O-vacancy effectively transforms the original square lattice of CuO$_2$ to a new lattice. We propose a crystal structure for Ba$_2$CuO$_{3+\delta}$, where layers of 1-dimensional CuO chains and layers of 2-dimensional CuO$_1$5 plane are alternating as illustrated in Fig. 1(a). We expect the CuO chains to serve as charge reservoir, in analogy to the CuO chains in YBCO, and the CuO$_1$5 planes to contain the essential physics for the superconductivity in Ba$_2$CuO$_{3+\delta}$. We argue that the effective Hamiltonian of a CuO$_1$5 plane is described by a single band $t$-$t'$-$J$ model on a new brick-wall lattice, which is described by a single band $t$-$t'$-$J$ model on an underlying brick-wall lattice, which is shown in fig. 1(b), with $t$ and $t'$ the nearest neighbor (n.n.) and next n.n. hopping integrals and $J$ the n.n. spin-spin coupling of the spin-1/2 Cu-holes.

We use renormalized mean field theory to study the $t$-$t'$-$J$ model on the brick-wall lattice. We find that the superconductivity extends to hole density of as high as 40%, and the maximum of the pairing order parameter appears at a larger hole concentration than the other cuprates due to the shift of the van Hove singularity for the density of states in the brick-wall lattice. The pairing symmetry depends on the value of $t'/t$ and the hole concentration, and may break time reversal symmetry, which can be tested in muon spin rotation ($\mu$SR) experiment. The effects of bond disorder is also studied, and...
the superconductivity is expected to survive a weak bond disorder that deviates the structure from perfect brick-wall lattice.

Our theory appears to be consistent with the available experiments and explains the superconductivity of Ba$_2$CuO$_{3.25}$ with relatively large hole concentration. We attribute the change of the electronic structure in the planar layer of the compound to the O-vacancy, which in turn changes the effective lattice. This may provide a new route to study high $T_c$ in future.

Model and effective lattice.—As mentioned above, we consider a crystal structure shown in Fig. 1 (a), with alternative layers of CuO chain and CuO$_{1.5}$ plane (x-y plane). The average $\delta$ is 0.25 in such a structure. The O-vacancies (missing O-atoms) in CuO$_{1.5}$ layer form a square lattice and there are three O-atoms around each Cu-atom on the plane. The energy of the crystal structure has not been calculated, but should be similar to the one of the lowest energy crystal structure calculated for Ba$_2$CuO$_{3.25}$ by Liu et al [6], with the difference that in the latter case the O-vacancies form an alternative chains along the x-direction. We will focus on the electronic structure of CuO$_{1.5}$ plane and consider CuO chains to serve as charge reservoir. While the average of the formal valence of Cu in Ba$_2$CuO$_{3.25}$ is Cu$^{2.5+}$, the formal valence of Cu-atom on the CuO$_{1.5}$ layer can be significantly smaller because of the compensation from the CuO chains.

For each Cu-atom on the CuO$_{1.5}$ plane, there are five nearest neighbor O atoms including two apical O-atoms, two on the x-axis and one on the y-axis. The possible anti-bonding Cu-3d orbitals here are 3$d_{3z^2-r^2}$ or 3$d_{x^2-y^2}$, whose relative energies depend on the dimension or ratio of the bond lengths between the short apical Cu-O bond and the in-plane Cu-O bond. Here we assume orbital 3$d_{3z^2-r^2}$ to have higher energy, which is consistent with a density functional calculation for proper parameter[15]. Then the lowest-energy of the atomic 3d hole state is $d_{3z^2-r^2}$, which replaces $3d_{x^2-y^2}$ in other cuprates as the relevant orbital. Considering Cu-3d$^{10}$ and O-2p$^6$ as the vacuum configuration, the formal Cu$^{2+}$ thus has one hole primarily on Cu-3$d_{3z^2-r^2}$. Because of the large repulsive interaction $U$ for two holes on the same Cu-site, the ground state at the half filled, namely one hole per Cu-atom in average, will be a Mott insulator, similar to that of La$_2$CuO$_4$.

We next consider additional holes to the half filled case. As soft-X ray absorption experiment[6] shows, the additional hole largely goes to the O-2p orbitals, which implies that the formal Cu$^{3+}$ has one hole on Cu-3$d_{3z^2-r^2}$ and the other on O-2p. We expect them to form a spin singlet, similar to the Zhang-Rice spin singlet[16] formed in other cuprates, and moves through the lattice as a charge carrier.

Since the hopping of the hole between the two neighboring Cu-atoms is essentially mediated by oxygen 2p orbitals in between, it is strongly suppressed if the oxygen between the two Cu-atoms is missing. Therefore, the nearest neighbor Cu-Cu bond may be effectively removed from the lattice if the O-atom between them is missing. This leads to an effective brick-wall lattice as shown in fig.1(b).

As we discussed above, the physics in Ba$_2$CuO$_{3.25}$ may be similar to that in other cuprates and we may consider the material as a doped Mott insulator within a single orbital model, although the relevant Cu-3d orbital and the underlying lattice due to the missing O ions will be different from the other cuprates. The low energy physics of Ba$_2$CuO$_{3.25}$ is thus described by a 2-dimensional t-J model on a brick-wall lattice,

$$H = -\sum_{ij} \left( t_{ij} P_G c_{i\sigma}^\dagger c_{j\sigma} P_G + h.c. \right) + J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $c_{i\sigma}$ and $c_{j\sigma}^\dagger$ are the annihilation and creation operator of electrons with spin $\sigma$ at site $i$ respectively, $t_{ij}$ is the hopping integral of electrons between site $i$ and $j$, $P_G$ is the Gutzwiller projection operator to project out doubly occupied electron states on the Cu-sites and $(ij)$ means n.n. pairs of $i$ and $j$. Repeated spin indices are summed. As we analyzed above, the dominant orbital is 3$d_{3z^2-r^2}$, thus the hopping integrals are isotropic along the x- and y- axes. And we consider only the case with n.n. and next n.n. hoppings, whose hopping integrals are $t_{nn} = t$ and $t_{nnn} = t'$ respectively.

Mean field results.—As shown in Fig. 1 (b), the superconducting order parameters of the brick-wall lattice are denoted by $\Delta_\alpha$ with $\alpha = 1, 2, 3$. Usually, the symmetry of a system will impose some constraints on the order parameters. The point group symmetry of the brick-wall lattice is $D_2$ which has four irreducible representations as listed in Table I. Since we are only interested in spin singlet pairing, only the $A$ and $B_1$ representations are relevant. For $A$ representation, We have real pairings with

![FIG. 1. (a) Proposed crystal structure for Ba$_2$CuO$_{3.25}$ with alternating Cu-O chain layer (middle layer) and Cu-O$_{1.5}$ plane (top and bottom layers). The apical O-atoms are all occupied. The Cu-O$_{1.5}$ plane forms a brick-wall structure due to the missing O-atoms. (b)The brick-wall lattice formed by Cu (light blue for A sublattice and dark blue for B sublattice) and O (red) atoms. $\Delta_2, \Delta_2, \Delta_2$ are the superconducting order parameters on the corresponding bonds. The unit cell vectors are depicted as green dashed lines with length $a$.](image-url)
\[ \Delta_1 = \Delta_2. \] For \( B_1 \) representation (will be denoted as \( B \) hereafter), we have real pairings with \( \Delta_1 = -\Delta_2, \Delta_3 = 0. \)

\( t' = 0 \) is a special case, where the Hamiltonian has a higher symmetry than the lattice, the \( D_6 \) symmetry. This can be understood as the following. The brick-wall lattice can be treated as a squeezed honeycomb lattice. If one considers only the n.n. coupling, the model can be mapped onto a t-J model with the n.n. hopping on an honeycomb lattice, and has a \( D_6 \) symmetry. Previous studies on t-J model on honeycomb lattice have suggested a \( d + id \)-wave topological superconducting phase which corresponds to a two-dimensional representation of \( D_6 \) group. Although the \( D_6 \) symmetry is reduced to \( D_2 \) as one turns on the next n.n. hopping, it is possible that the pairing symmetry may still be \( d + id \), or more precisely \( A + iB \) in the \( D_2 \) case, where the 2D representation reduces to \( A \oplus B \), for small \( t' \). In the following calculations, we will take the \( A + iB \) ansatz \( \Delta_1 = \Delta_2^* = \Delta_{xA} + i\Delta_{xB} \) and \( \Delta_3 = \Delta_y \) where \( \Delta_{xA}, \Delta_{xB}, \) and \( \Delta_y \) are all real, as shown in Fig. 2(d). \( \Delta_{xA} \) and \( \Delta_{xB} \) tracks the contribution from \( A \) and \( B \) respectively, a case with finite \( \Delta_{xA} \) and vanished \( \Delta_{xB} \) corresponds to pure \( A \) phase, while a case with finite \( \Delta_{xB} \) and \( \Delta_{xA} = \Delta_y = 0 \) corresponds to pure \( B \) phase.

Then we solve the superconducting order parameters with the standard renormalized mean field theory approch (see the details in appendix A), and the results for \( t' = 0, t' = 0.1, \) and \( t' = -0.1 \) are depicted in Fig. 2 (a), (b) and (c) respectively. The result for \( t' = 0 \) shows a time-reversal symmetry breaking \( A + iB \)-wave \((d+id)\)-wave phase in large doping regime, which is consistent with the previous studies on honeycomb lattice. The optimal doping of the superconducting dome corresponds to the van Hove singularities as shown in the inset of Fig. 2(a). For small but finite \( t' = \pm 0.1t \), we still have the \( A + iB \) phase at low doping \((p < 0.25)\). But with increasing doping, the \( A + iB \) phase is replaced by a pure \( B \) phase \((t' = 0.1t) \) or a pure \( A \) phase \((t' = -0.1t)\).

In each phase, we find that the doping with maximum superconducting order parameter corresponds to the peak in density of states, i.e. the van Hove singularities.

We also perform the calculations for various dopings and \( t' \), the resultant phase diagram is shown in Fig. 3. One can find a robust \( A + iB \) phase in rather large parameter regime and a phase transition from \( A + iB \) phase to \( A \) phase in \( t' < 0 \) region and a transition from \( A + iB \) to \( B \) phase in \( t' > 0 \) region. The different behavior between positive and negative \( t' \) can be understood from the Fermi surface geometry. In Fig. 3 we depict the typical Fermi surface for each phases. In large doping regime, the underlying Fermi surface for \( t' > 0 \) has a very good nesting along \( k_x \) direction that favors one dimensional instability, while the Fermi surface for \( t' < 0 \) does not have such a nesting and favors a two dimensional instability. On the other hand, the superconducting pairing in \( B \) phase is one dimensional (because \( \Delta_y = 0 \)), while the pairing in \( A \) phase is more two dimensional. Thus one have the \( B \) phase at \( t' > 0 \) and \( A \) phase at \( t' < 0 \) in

FIG. 2. Spin singlet pairing order parameters \( \Delta_{xA}, \Delta_{xB} \) and \( \Delta_3 \) of Hamiltonian (a) obtained from the renormalized mean field theory for \( t' = 0 \) (a), \( t'/t = 0.1 \) (b) and \( t'/t = -0.1 \) (c) with \( J/t = 0.4 \) for all cases. \( \Delta_{xA} (\Delta_{xB}) \) indicates the contribution from \( A(B) \) representation, respectively. The pairing order parameters on three distinct bonds are indicated in (d). The insets in (a-c) are the DOS and the corresponding Fermi energy at the optimal dopings marked by the arrows.

![FIG. 2](image)

FIG. 3. Phase diagram of different pairing symmetry obtained from RMFT calculation. The yellow, green, and purple Regions corresponding to \( A + iB \), pure \( B \), and pure \( A \) phase, respectively. We also depict the typical Fermi surface topology and quasi particle gap in Brillouine zone for each phase \((t' = 0 p = 0.15 \) for \( A + iB \) phase, \( t' = 0.1t p = 0.31 \) for \( B \) phase, and \( t' = -0.1 \) \( p = 0.36 \) for \( A \) phase\)). The orange dotted lines are the boundary of the reduced Brillouin Zone, while the symbol h indicates the region occupied by holes. The \( A + iB \) and \( B \) phases are gapped, while \( A \) phase is gapless with its nodes depicted as red spots in the figure.

![FIG. 3](image)

| TABLE I. character table of group \( D_2 \) |
|------------------|------------------|------------------|------------------|
| Reps \( e \) | \( C_2(z) \) | \( \sigma_x \) | \( \sigma_y \) |
| \( A \) | +1 | +1 | +1 | +1 |
| \( B_1 \) | +1 | -1 | -1 | -1 |
| \( B_2 \) | +1 | -1 | +1 | -1 |
| \( B_3 \) | +1 | -1 | +1 | +1 |
large doping regime.

As we analyzed above, the $A + iB$ phase at $t' = 0$ corresponds to the $d + id$ superconductivity, thus the $A + iB$ phase should also be a topological superconducting phase. To confirm that, we calculated the Chern number $\nu_{\text{Ch}}$ associated with each phase. We find that the $A + iB$ phase has a Chern number $\nu_{\text{Ch}} = 2$, while the pure $A$ and $B$ phase is topologically trivial and has Chern number $\nu_{\text{Ch}} = 0$. Thus, the phase transition between them is indeed a topological phase transition associated with a gap closing behavior.

Effects of bond disorder. — It is natural to expect the existence of bond disorder in the system that deviates the structure from a perfect brick-wall lattice, and its effects on the superconductivity need to be investigated.

We start with a $N = 32 \times 32$ brick-wall lattice of periodic boundary condition, in which there are $3N/2$ n.n. bonds with nonzero hopping integral $t$ and superexchange $J$, forming the structure depicted in Fig. 1(b). Note that, as compared with the square lattice, there are $N/2$ n.n. bonds missing in the brick-wall lattice. To introduce bond disorder, $N_{\text{dis}}$ n.n. bonds are redistributed randomly. Explicitly, we take out $N_{\text{dis}}$ bonds randomly from the $3N/2$ n.n. bonds of the brick-wall lattice and then distribute them randomly to the place of $N/2$ previously missing bonds. Clearly, $N_{\text{dis}}$ takes an integer value between 0 and $N/2$, and the strength of bond disorder is measured by the value of $\eta = 2N_{\text{dis}}/N$. At a given $\eta$, we generate 20 disorder realizations and obtain the ground state of each realization self-consistently. We stay with $t' = 0$ and doping concentration $\rho = 0.25$ where the superconducting brick-wall lattice is in the $A + iB$ phase.

The average renormalized pairing of each disorder realization, $\Delta = \frac{1}{N} \sum_{\langle i,j \rangle} g_{ij} |\Delta_{ij}|$, at zero temperature is plotted in Fig. 4(a) as crosses at various disorder strength $\eta$, with the solid line represent their ensemble averages. The ensemble averaged $\Delta$ decreases linearly as the disorder strength $\eta$ increases, and saturates to a nonzero minimum value at $\eta \approx 0.09$. We thus expect the superconductivity on the perfect brick-wall lattice to survive weak bond disorders. To estimate the effects of bond disorder on the superconducting transition temperature $T_c$, the temperature dependence of $\Delta$ is plotted in Fig. 4(b) for $\eta \approx 0.038$ and $\eta \approx 0.078$, with the result in the absence of disorder ($\eta = 0$) is also shown for comparison. Clearly, the suppression of the mean-field critical temperature by bond disorder is much weaker than the suppression of the ensemble averaged $\Delta$ at zero-temperature.

Summary. — In summary, we have proposed an effective brick-wall $t - t' - J$ model for the newly discovered high Tc superconductor. By using renormalized mean field theory, we have demonstrated that the superconductivity extends to very large hole concentration, and the pairing order parameter is peaked at larger hole concentration. The pairing symmetry can be complex and breaks time reversal invariance, similar to the superconductivity theoretically studied for the $t - J$ model on the honeycomb lattice. It will be interesting to test this in $\mu$SR experiment. We note that Hubbard model on square lattice has recently been studied using more sophisticated numerical methods. Our study based on renormalized mean field theory on the brick-wall lattice may be viewed as a starting point for these more advanced numerical methods. Our mean field result on the bond disorder effect suggests a relatively weaker reduction to the superconductivity transition temperature.

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Appendix A: Renormalized Mean Field Theory

The basic idea of renormalized mean field theory (RMFT) is to approximate the Gutzwiller projection \( P_G \) in (1) by Gutzwiller factors, and the Hamiltonian becomes

\[
\mathcal{H} = - \sum_{ij} (g^t_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + \sum_{ij} g^f_{ij} \mathbf{S}_i \cdot \mathbf{S}_j , \tag{A1}\]

where \( g^t_{ij} = \sqrt{4\rho_i \rho_j/(1+\rho_i)(1+\rho_j)} \) and \( g^f_{ij} = 4/(1+\rho_i)(1+\rho_j) \), with \( \rho_i \) the local doping concentration on site \( i \). The exchange term is then decoupled in terms of the mean fields of hopping \( \chi^0_{ij} = \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle \) and pairing \( \Delta^0_{ij} = \langle c^\dagger_{i\sigma} c_{j\sigma'} \rangle \). The mean-field Hamiltonian reads

\[
\mathcal{H} = - \sum_{ij} (g^t_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + \frac{3J}{8} \sum_{ij} g^f_{ij} \tag{A2}\]

\[
\times \left[ \chi^0_{ij} c^\dagger_{i\sigma} c_{j\sigma'} + \Delta^0_{ij} c^\dagger_{i\sigma} c_{j\sigma'} + \text{h.c.} - |\chi^0_{ij}|^2 - |\Delta^0_{ij}|^2 \right].
\]

The ground state is obtained by solving the hopping and pairing parameters in Eq. (A2) self-consistently.

In uniform solutions, \( \rho_i = \rho \), and the Gutzwiller factors \( g^t_{ij} = g_t = 2\rho/(1+\rho) \) and \( g^f_{ij} = g_f = 4/(1+\rho) \). The three independent n.n. bonds are denoted as \( \alpha = 1, 2, 3 \), as shown in Fig. (b). In the momentum space, the mean-field Hamiltonian reads

\[
\mathcal{H}^{MF} = \sum_{k} C^k \left( \begin{array}{ccc}
\epsilon(k) & f(k) & 0 \\
f^\dagger(k) & \epsilon(k) & g^f_{2}(k) \\
0 & g^f_{1}(k) & f(k) \\
g^f_{2}(k) & 0 & -f^\dagger(k) & -\epsilon(k)
\end{array} \right) C^k , \tag{A3}\]

where \( C_k = (C_{kA^\dagger}, C_{kB^\dagger}, C^{\dagger}_{-kA}, C^{\dagger}_{-kB})^T \), and the matrix element is given by

\[
\epsilon(k) = - \sum_{\delta} g^t_{\delta} \exp[\text{i}k \cdot \mathbf{r}_\delta] - \mu
\]

\[
f(k) = \sum_{\alpha} (-g^t_{\delta} - \frac{3}{8} g_t J \chi^0_{\alpha}) \exp[\text{i}k \cdot \mathbf{r}_\alpha]
\]

\[
g^f_{1}(k) = \sum_{\alpha} (-\frac{3}{8} g_f J \Delta^0_{\alpha}) \exp[\text{i}k \cdot \mathbf{r}_\alpha]
\]

\[
g^f_{2}(k) = \sum_{\alpha} (-\frac{3}{8} g_f J \Delta^0_{\alpha}) \exp[-\text{i}k \cdot \mathbf{r}_\alpha],
\]

where \( \alpha = 1, 2, 3 \) is the index of the n.n. site while \( \delta = 1, 2, 3, 4 \) is the index of the next n.n. site. \( H^{MF} \) can be diagonalized via Bogolyubov transformation at each \( k \) point

\[
\begin{pmatrix}
C_{kA^\dagger} \\
C_{kB^\dagger} \\
C^{\dagger}_{-kA} \\
C^{\dagger}_{-kB}
\end{pmatrix} = U^k
\begin{pmatrix}
\alpha_{k^\dagger} \\
\beta_{k^\dagger} \\
\alpha^{\dagger}_{-k} \\
\beta^{\dagger}_{-k}
\end{pmatrix} \tag{A4}
\]

And the self-consistent equations are given by

\[
\Delta^0_{\alpha} = \frac{1}{N_S} \sum_k \exp[i \mathbf{k} \cdot \mathbf{r}_\alpha] (u^k_{13} u_{23}^k + u^k_{14} u_{24}^k) \tag{A5}
\]

\[
\chi^0_{\alpha} = \frac{1}{N_S} \sum_k \exp[-i \mathbf{k} \cdot \mathbf{r}_\alpha] (u^k_{13} u_{23}^k + u^k_{14} u_{24}^k) \tag{A6}
\]

where \( N_S \) is the number of unit cells. The value of the mean fields can be obtained by solving the self-consistent equation. The physical superconducting order parameters are given by

\[
\Delta_\alpha = g_t \Delta^0_{\alpha}. \tag{A7}
\]