

$^{12}\text{C} + ^{12}\text{C}$ resonances by a molecular model

E Uegaki$^1$ and Y Abe$^2$

$^1$Graduate School of Engineering and Resource Science, Akita University, Akita 010-8502, Japan
$^2$Research Center for Nuclear Physics, Osaka University, Ibaraki 567-0047, Japan
E-mail: uegaki@phys.akita-u.ac.jp

Abstract. Resonances observed in the $^{12}\text{C} + ^{12}\text{C}$ collisions are studied with a molecular model. At high spins $J = 12–16$, a stable dinuclear configuration is found to be an equator-equator touching one as is obtained in the $^{28}\text{Si} + ^{28}\text{Si}$ system. With $K$-quantum number being specified as rotation-vibration model, normal modes have been solved around the equilibrium, firstly. Furthermore, Coriolis coupling has been investigated by diagonalization among low-lying normal-mode states with $K = 0$ and $K$-excitation. It is found that the Coriolis coupling introduces about 30% of $K$-mixing into the $K = 0$ molecular ground states of $J = 12–16$. The analyses of the angular momentum coupling show up a dominance of the lowest $L$ in the inelastic channel of the molecular ground state newly obtained. Thus alignments appear strongly in the inelastic channel, which is in agreement with the explanation by the band crossing model. Discussion is given on “why disalignments appear in the $^{28}\text{Si} + ^{28}\text{Si}$ system, in contrast to the above results”.

1. Introduction
The first discovery of the sub-barrier resonances in the $^{12}\text{C} + ^{12}\text{C}$ system is the starting point of the heavy-ion resonances [1]. Well above the Coulomb barrier, series of resonances have been found with high spins of $J = 12–16$ [2, 3]. Coupled channel calculations have been applied with the elastic and inelastic channels such as $2^+$ excitation of $^{12}\text{C}$ nuclei, which are expected to play an important role in the resonances. Band Crossing Model, based on the double resonance mechanism, has successfully explained resonance mechanism and resonance states with the aligned configurations of the orbital angular momentum and the spins of the excited states of $^{12}\text{C}$ [4]. On the other hand, for high-spin resonances observed in $^{24}\text{Mg} + ^{24}\text{Mg}$ and $^{28}\text{Si} + ^{28}\text{Si}$, we have developed a new molecular model [5, 6, 7]. In particular, for $^{28}\text{Si} + ^{28}\text{Si}$, the molecular model naturally explains peculiar disalignments observed between the orbital angular momentum and the spins of $^{28}\text{Si}$ fragments. The resonances in both $^{12}\text{C} + ^{12}\text{C}$ and $^{28}\text{Si} + ^{28}\text{Si}$ systems are thought to have dinuclear configurations of oblate constituent nuclei, but they have completely different structures, i.e., aligned in the former while disaligned in the latter, concerning angular momentum coupling. The contrasting features are observed experimentally and well explained by the two models, respectively. Thus, it is keenly interesting to know how they can be understood consistently. In other words, the question is how or in what conditions angular momentum coupling is determined in the resonance states. For the purpose, we take up $^{12}\text{C} + ^{12}\text{C}$ system with the new molecular model, and show how the aligned configuration arises in the resonances, not the disaligned one.
2. Dinuclear molecular structure of $^{12}$C -- $^{12}$C

2.1. Dynamical property and Normal modes

Assuming a constant deformation and axial symmetry of the constituent nuclei for simplicity, we have seven degrees of freedom ($q_i$) = ($\theta_1, \theta_2, \theta_3, R, \alpha, \beta_1, \beta_2$), as illustrated in fig. 1. The relative vector of two $^{12}$C nuclei ($R, \theta_2, \theta_1$) defines molecular $z'$-axis. The orientations of the symmetry axes of the $^{12}$C nuclei are considered as internal degrees of freedom, and are described with Euler angles ($\alpha_i, \beta_i$) referring to the molecular axes. With $\alpha_1$ and $\alpha_2$, $\theta_3 = (\alpha_1 + \alpha_2)/2$ of the total $K$-rotation around $z'$-axis and $\alpha = (\alpha_1 - \alpha_2)/2$ of twisting motion are defined.

The kinetic energy is given classically in terms of angular velocities, and then the quantization is done to describe the rotation of the whole system with the total angular momentum operator $\hat{K}$ and the internal motions referring to the molecular axes. The nucleus-nucleus interaction is given with folding potential using the nucleon-nucleon interaction DDM3Y. Expecting a stable state of $^{2}\Sigma$ configuration, the interaction potential is described with geometrical configurations specified by the internal degrees ($R, \alpha, \beta_1, \beta_2$). Consistently with the coordinate system, at first we introduce a rotation-vibration type wave function specified with $K$-quantum number as basis one, $\Psi_{\lambda} \sim D_{MK}^{J}(\theta_i)\chi_K(R, \alpha, \beta_1, \beta_2)$, where $\chi_K$ describes the internal motions. Correspondingly with specified $J$ and $K$, we define a multidimensional centrifugal potential

$$T'_{\text{rot}}(J, K; R, \alpha, \beta_1, \beta_2) = \frac{\hbar^2}{2} \left[ \frac{1}{\mu R^2}\left\{ J(J+1) - \frac{3}{2} K^2 + \frac{1}{2} \cos 2\alpha \cot \beta_1 \cot \beta_2 (K^2 - 1) \right\} + \left( \frac{1}{I} + \frac{1}{\mu R^2} \right) \left( \frac{K^2 - 1}{4 \sin^2 \beta_1} + \frac{K^2 - 1}{4 \sin^2 \beta_2} - \frac{1}{2} \right) \right],$$

(1)

where $I$ denotes the moment of inertia of the constituent nuclei $^{12}$C, the value of which is estimated from the excitation energy of the $2\Sigma^+$ state of $^{12}$C. In order to know dynamical aspects of multi-dimensional internal motion, we calculate the effective potential for given $J$ and $K$,

$$V_{JK}(R, \alpha, \beta_1, \beta_2) = V_{\text{interaction}}(R, \alpha, \beta_1, \beta_2) + T'_{\text{rot}}(J, K; R, \alpha, \beta_1, \beta_2).$$

(2)

In fig. 2, a multidimensional energy surface is displayed. A local minimum is obtained around $\beta = 90^\circ$ and $R = 5.6$ fm, which is called as equator-equator (E-E) configuration. The barrier height is 5.7 MeV located at $R \sim 7.5$ fm.

Couplings among various molecular configurations are taken into account by the method of normal mode around the equilibrium at $\beta_1 = 90^\circ$, which gives rise to the molecular modes of

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**Figure 1.** Dinuclear molecular coordinates; seven degrees of freedom of $^{12}$C + $^{12}$C (oblate-oblative system) are described with ($q_i$) = ($\theta_1, \theta_2, \theta_3, R, \alpha, \beta_1, \beta_2$).

**Figure 2.** Contour map of the effective potential energy $V_{JK}$ with $J = 14$ and $K = 0$ for the $R - \beta(\beta_1 = \beta_2)$ degrees at $\alpha = \pi/2$. Contours are displayed by 2 MeV.
excitation. Combining the kinetic energy operator and the expanded effective potential, the total hamiltonian is written as

\[ H = H_0 + T'_C + (\text{higher order}), \]

where \( H_0 \) and \( T'_C \) denote the normal-mode hamiltonian and the Coriolis coupling, respectively. \( H_0 \) is separated into each internal degree of freedom, which means the internal degrees of freedom \((R, \alpha, \beta_1, \beta_2)\) are the normal modes themselves, as follows,

\[ H_0 = H(R) + H(\alpha) + H(\Delta \beta_1) + H(\Delta \beta_2) + H_{\text{coupl}}(\alpha, \beta_1, \beta_2) \]

where \( \Delta \beta_i \) denote \( \beta_i - \pi/2 \). Additional \( H_{\text{coupl}} \) includes coupling among \( \beta_i \) and \( \alpha \) such as \( \beta_1 \beta_2 \cos 2\alpha \) as well as corrections for confinement of \( \beta_i \) on weak \( K \)-dependence. Thus we use basis wave functions, \( \Psi_{JMK}(\theta_i; R, \alpha, \beta_1, \beta_2) \sim D^{JK}_{MK}(\theta_i) f_n(R) \phi_\nu(\alpha) \varphi_{n1}(\beta_1) \varphi_{n2}(\beta_2) \), where \( f_n, \varphi_{n1}, \) and \( \varphi_{n2} \) are H.O. functions, while \( \phi_\nu \) is a rotational function \( e^{i\nu\alpha} \) or \( \cos \nu \alpha \), since the confinement in \( \alpha \)-motion is very weak. The energy of the basis state is given as

\[ E_{JK}(n, \nu, n_1, n_2) = E_0(R_e) + \{J(J + 1) - K^2 - 1\} h^2 / 2\mu R_e^2 + \{K^2 - 2\} h^2 / 4I \]
\[ + (n + 1/2)\hbar \omega_R + (n_1 + n_2 + 1)\hbar \omega_\beta + \nu^2 h^2 / 4I, \]

where \( \hbar \omega_\beta \approx 5 \text{ MeV} \). \( H_{\text{coupl}} \) and coupling by \( H(\alpha) \) have been diagonalized. Since \( H_0 \) is almost separable, the eigenenergy of \( H_0 \) is very close to eq. (5) except for the following case: \( H_{\text{coupl}} \) couples strongly between the basis states with \((n_1, n_2, \nu) = (2, 0, 0), (1, 1, 2)\), in which butterfly and anti-butterfly modes appear as likely described with \( \beta_\pm = (\Delta \beta_1 \pm \Delta \beta_2) / \sqrt{2} \) [6, 7]. Note that a selection rule exists as \( K = \nu = \text{even} \) in general. In addition, we have rules \((-1)^{n_1} = (-1)^{(K+\nu)/2} \) and \((-1)^{n_2} = (-1)^{(K-\nu)/2} \). In fig. 3, molecular normal modes of \(^{12}\text{C} + ^{12}\text{C}\) with spin 14 are displayed, classified with quantum numbers as \( K = 0, 1, 2 \). The first excited state of \( K = 0 \) is twisting excitation with \( \nu \approx 4 \) of \( \alpha \)-rotation, and the next levels are of the butterfly modes. The lowest \( K = 1 \) state starts with \( \beta \) excitation of \((n_1, n_2, \nu) = (1, 0, 1)\) due to the selection rule.

2.2. Coriolis coupling

Generally in the rotating system, we have Coriolis coupling, which is denoted as \( T'_C \) in eq. (3). It is obtained as many terms described with differential operators of \( \theta_i \) and those of the internal variables \((\alpha, \beta_1, \beta_2)\), but we can make them into a simple form such as a product \(-J' \cdot (S'_1 + S'_2) / \mu R_e^2 \) between the total angular momentum operator \( J' \) and spins of the constituent nuclei \( S'_\ell \) which refer to the molecular axes. We consider it as residual coupling, which causes \( K \)-mixing with \( \Delta K = 1 \). In \(^{12}\text{C} + ^{12}\text{C}\), in which alignments are expected to be important, we have to take this coupling into account, as it favors alignments. Actually, in the molecular ground state, \((K = 1, \nu = 1)\) mixed component appears to bring strong alignments in the single \( 2^+ \) channel.

Figure 3. Energy spectra of molecular normal modes of \(^{12}\text{C} + ^{12}\text{C}\) for \( J = 14 \). From the left, levels with \( K = 0, 1, 2 \) are displayed. Diagonalization of the Coriolis coupling with 3 low lying states of \( K = 0, 1, 2 \) gives a new spectrum in the r.h.s.
Since we specify $K$-quantum number at the first stage, the angular momentum coupling has its own characteristics of each specified $K$. In fig. 4, a configuration of $^{12}\text{C} + ^{12}\text{C}$ is displayed. Spin vectors are illustrated as an example, upward ones (black) of which are aligned with the orbital angular momentum $\mathbf{L}$, while downward ones (red) are anti-aligned with $\mathbf{L}$. The downward spins originate from the upward ones by $\pi$-rotation around $z'$-axis. followed with the phase $\exp(iK\theta_3)$. Thus characteristics of the angular momentum coupling are inferred: 1) amplitudes $A_{J\pm S}$ are almost in the same magnitudes, 2) relative phase between $A_{J-S}$ and $A_{J+S}$ is $(-1)^{K}$, which is confirmed later in table 1.

Usually the spins $S'_{i}$ are described with differential operators of Euler angles $\beta_i$. It is noted here that $\beta_i$ can describe not only rotational motions but also vibrational motions of the poles of the constituent nuclei, depending on the potential. In our molecular model, with respect to confinements around the equilibrium configurations, the normal modes of $\beta_i$-motions are vibrational. For the H.O. states, the differential operators of $\beta_i$ are written as $-\partial/\partial\beta_i = -\partial/\partial\Delta\beta_i = \sqrt{m\omega_\beta}2\hbar(b_i^*-b_i)$, and $\Delta\beta_i = \sqrt{\hbar/2m\omega_\beta}(b_i^*+b_i)$, respectively, where $b_i^*$ and $b_i$ denote the creation and annihilation operators of bosons for $\beta_i$, respectively. Note that $m$ is defined as $(1/I+1/\mu_\beta^2)^{-1}$, and $\hbar/m\omega_\beta$ is nondimensional. The Coriolis coupling operator $J'(S'_1+S'_2)$ connect different $K$ states, namely $J'$ gives lowering and raising operators of $K$, $J'_\pm = J'_1 \pm iJ'_2$, respectively. Thus the Coriolis coupling is written with those operators and we can calculate its matrix elements among $K$-states.

Low lying three states of $K = 0, 1$ and $2$ are taken for basis states, and the Coriolis coupling between them are solved. In fig. 3, energy levels before the diagonalization are connected by red lines and the resulting levels are displayed in the r.h.s for $J = 14$. The molecular ground state of $J = 14$ is obtained with energy gain 1.8 MeV from the $K = 0$ state, in which mixed probability with $K \neq 0$ is $30\%$. In fig. 5(a), the energy spectrum of basis states for $J = 12 - 16$ are displayed, and in (b), the spectrum obtained after $K$-mixing are displayed, classified into resultant three bands. For comparison, experimental resonance levels with spin assignments [3] are indicated in the r.h.s. Level energies of the first band are in good agreement with the experiment. Note that for the states of the second and third bands to be reliable solutions, they need more extended basis states than three low-lying basis ones for the diagonalization, as the energies of the states of those excited bands are close to those of the other basis states.

**Figure 4.** A configuration of $^{12}\text{C} + ^{12}\text{C}$ is displayed. Upward spin vectors (black) are aligned with $\mathbf{L}$, and downward ones (red) are anti-aligned with $\mathbf{L}$, both of which are included in the states with specified $K$.

**Figure 5.** (a) Each energy spectrum of $J = 12 - 16$ for the low lying $K = 0,1,2$ states, (b) Whole spectrum after $K$-mixing are displayed, where thin lines are an eye-guide for $J = 14$. Experimental resonance levels with spin assignments [3] are given.
3. Analyses of angular momentum coupling

We examine the angular momentum coupling of the molecular wave functions, before and after \(K\)-mixing, by calculating overlapping between those functions and the channel wave functions. We define a generalized channel wave function, with a given orbital angular momentum \(l\) for the relative motion as

\[
\mathcal{Y}(I_1I_2)LJM = \sum_{M_J,m} (H_{M_J}m|JM) \mathcal{S}_{12} |\psi^J(I_1I_2)JM_l|^2 m(\theta_2,\theta_1),
\]

where \(\psi^J(I_1I_2)JM_l\) denotes a channel wave function composed with D-functions, i.e., rotational functions for the constituent nuclei with spins \((I_1, I_2)\) and a specified channel spin \(I\). \(\mathcal{S}_{12}\) denotes the symmetry operator between two identical constituent nuclei. The overlapping integral is defined as follows, to obtain the distribution on \([\langle I_1, I_2\rangle, L]\),

\[
A_{JK;\langle I_1, I_2\rangleL} = \int d\Omega \int \left[ \sum_I \mathcal{Y}(I_1I_2)IL;JM \right] \Psi'_{JMJK}(\theta_1, \alpha, \beta_1, \beta_2) \sqrt{\sin \beta_1 \sin \beta_2} d\alpha d\beta_1 d\beta_2,
\]

where \(\Psi'_{JMJK}\) is defined as \(\Psi_{JMJK}/f_n(R)\), dropping the radial wave function out, from the eigenstate of \(H_0\). \(\Omega\) denotes the solid angle of \((\theta_1)\). As we can transform the generalized channel wave function into a kind of molecular wave function, with the rotational function of the whole system \(D_{JMJK}(\theta_1)\) in a series of \(K\), we easily calculate overlapping integrals [8]. Note that \(\sqrt{\sin \beta_1 \sin \beta_2}\) of the integral volume elements in eq. (6) is due to the definition of the volume element \(dV = dRd\alpha d\beta_1 d\beta_2\) for the model wave function with vibrational description.

In table 1, the amplitudes \(A_{JK;\langle I_1, I_2\rangleL}\) are shown for each \(K\)-state of the low-lying series of \(J = 14\) and for the resultant molecular ground state with \(K\)-mixing by the Coriolis coupling. Only single 2\(^+\) channel is examined, because the amplitudes of the mutual one are small for the low lying \(K\)-states adopted. In each \(K\)-state, we see almost the same magnitudes of the amplitudes for \(L = 12\) and \(L = 16\), as expected by the consideration with fig. 5, and thus the states with specified \(K\) have not spin alignments. However, after \(K\)-mixing by the Coriolis coupling, the components of \(L = 14\) and 16 in the single 2\(^+\) channel extremely diminish as given in the rightmost column, and we obtain strong spin alignments.

| Table 1. Analyses of alignments by the distribution of the amplitudes \(A_{JK;\langle I_1, I_2\rangleL}\) in the elastic and single 2\(^+\) channels of the states of \(J = 14\). \(A_{JK;\langle I_1, I_2\rangleL}\) of three states, \(K = 0, 1\) and 2 are indicated in the left, and the total amplitudes of the mixed results with the coefficients (the values in the parentheses) obtained by the Coriolis diagonalization are given in the r.h.s. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| \(K = 0(0.836)\) | \(K = 1(-0.465)\) | \(K = 2(-0.289)\) | total(\(K\)-mixed state) |
| elastic channel | 0.86 | 0 | 0 | 0.72 |
| single 2\(^+\) channel | 0.86 | 0 | 0 | 0.72 |
| \(L = 12\) | -0.29 | 0.65 | 0.36 | -0.65 |
| \(L = 14\) | 0.24 | -0.06 | 0.80 | -1 \times 10^{-3} |
| \(L = 16\) | -0.31 | -0.65 | 0.30 | -0.04 |

4. Discussion — Different characteristics in disalignments of \(^{28}\text{Si} + ^{28}\text{Si}\) —

The resonances in \(^{28}\text{Si} + ^{28}\text{Si}\) system are expected to be similar to \(^{12}\text{C} + ^{12}\text{C}\), with dinuclear configurations of oblate constituent nuclei, but those systems have completely different structures. Namely, disalignments in \(^{28}\text{Si} + ^{28}\text{Si}\) are observed experimentally and well explained by the molecular model [8]. Thus, it is very interesting to know how they can be understood consistently, i.e., to know what determines the angular momentum coupling of the resonance states.
As explained in [7], we have found an equilibrium configuration like two pancakes sitting on the plane, as is displayed in fig. 6, the shape of which is axially asymmetric as a whole. With tight binding between two $^{28}$Si, the whole compound system is expected to behave like an axial-asymmetric rotator, which rotates wobblingly on the plane with a high spin. In the high-spin limit ($|K|/J \sim 0$), we obtain analytical wobbling ($K$-mixing) solutions of the asymmetric rotator as $F_n(K) = H_n(K/b) \exp(-K^2/2b^2)$ with the Hermite polynomial $H_n$, where $K$ is taken to be $K = \text{even}$. Since the intrinsic deformation axes of $^{28}$Si are almost orthogonal to the plane, the spin vectors are in the plane, which is the origin of disalignments.

In this context, we have assumed that the axis of the largest moment is along $X$-axis in fig. 6, due to the density distribution of the whole system of fig. 6. Namely, in the quantum mechanical understanding, we have assumed new moments of inertia along $X$-axis, which are expected to come out with induced deformations of the constituent $^{28}$Si nuclei. Of course, at decays, the induced deformations vanish and $^{28}$Si nuclei return to be normal ones. Note that in the sticking limit, the spins $S'_i$ of $^{28}$Si nuclei along $X$-axis are frozen and are constrained to be proportional to $J'_i$, and thus the the energy of the Coriolis coupling turns to $J'_i^2$, as a part of rotator energy. This is the reason why the system turns to be like an axial-asymmetric rotator [7]. Thus the necessary condition is enough binding of the constituent nuclei to be a compound system like an axial-asymmetric rotator.

![Figure 6. A configuration of $^{28}$Si + $^{28}$Si is displayed. Spin vectors in the wobbling motions and those at decays are illustrated respectively, as an example, the latter of which are in the reaction plane and are disaligned with $L$.](image)

5. Conclusions
Molecular model has been applied to $^{12}$C + $^{12}$C system, where the double resonance mechanism is known to be successful. With respect to the Coriolis coupling, $K$-mixing is calculated. Alignments between the orbital angular momentum and the fragment spin in the single $2^+$ channel have been obtained, which is qualitatively in agreement with band crossing model.

In conclusion, description of the molecular model includes various angular momentum couplings, both alignments and disalignments. The answer for “which coupling scheme appears?” depends on strength of nucleus-nucleus interactions. Actually, in the heavier system such as $^{28}$Si + $^{28}$Si, the interaction between the constituent nuclei is stronger than $^{12}$C + $^{12}$C case, which is exhibited by the deep potential energy surface around the equilibrium. Moreover, the heavier constituent nuclei are expected to deform easily from their original deformation, to form a total compound system. Thus we can naturally understand the mechanism for the contrasting features of angular momentum couplings between the two systems.

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