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Bremsstrahlung emission accompanying α-decay of deformed nuclei

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Abstract

A fully quantum model describing the angular distribution of the bremsstrahlung photon emission accompanying the α-decay of a deformed nucleus is presented for the first time. An analytical dependence of the bremsstrahlung probability on the quadrupole deformation parameter β_2 of the decaying nucleus has been found. Such a model and the detailed formalism allow us to calculate the stable spectra of the bremsstrahlung emission probability for different values of the angle between the direction of the α-particle motion and the symmetry axis of the decaying nucleus. We present the results of this new model by the calculation of the photon emission probability accompanying the α-decay of the ^{226}Ra nucleus which has the nuclear deformation parameter $\beta_2 = 0.151$. The results show by a clear way the role and the influence of the nuclear deformation of the decaying nucleus on the bremsstrahlung photon spectrum.

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1. Introduction

In recent years many experimental [1–8] and theoretical [7–25] efforts have been made to investigate on the nature of the bremsstrahlung emission in the α-decay of heavy nuclei, because the feature of the energy spectrum of photons is strongly related to the dynamics of the α-decay and alpha — nucleus potential. In some cases the energy spectrum of bremsstrahlung shows some slight oscillations [7], in other case authors observed a minimum [2,3], in some experiments [6, 25] authors did not observe any structure. To understand the peculiarities of the bremsstrahlung spectra and describe them accurately, it is necessary to develop a suitable model sensitive to different characteristics of the α-decay in order to describe accurately the process of tunneling of the α-particle through the Coulomb barrier.

If one compare the bremsstrahlung spectra relative to the α-decay of the ^{214}Po and ^{226}Ra nuclei presented in Ref. [8], for which nuclei there are similar shapes of the alpha — nucleus potential, one can see the relevant difference between them pointing out different photon emission distributions and probabilities during the α-decay of the ^{214}Po and ^{226}Ra nuclei. An explanation of such differences in the spectra can be found in the different Q-values for the α-decay of the two mentioned nuclei. Have such two nuclei other characteristics with different values which influence differently the photon emission? The Q-values for these two nuclei lead to different tunneling regions in their barriers. One can suppose that such difference leads to different contributions from the tunneling regions into the total photon spectra. This condition was confirmed in Ref. [8]. Moreover, one can suppose that the acceleration of the α-particle emits photons most strongly when it transits through the nuclear surface. From here, we naturally come to another possible characteristic that is the nuclear deformation. By comparing the two studied nuclei, we find different surface deformations for the two nuclei: while ^{214}Po is practically a spherically symmetric nucleus, ^{226}Ra is really deformed. It is relevant the question: how the deformation can influence the photon emission? Will such influence be small or large for the deformed nuclei? Will the photon emission from the region of the nuclear shape be essentially different for strongly deformed nuclei?

By such a way, we come to a new and difficult problem: to take the nuclear deformation into account in calculations of the bremsstrahlung spectra accompanying the α-decay. Such a question was never studied before. The aim of the present paper is to improve our model [7,8,21,23] with the inclusion of the deformation of the α-decaying nucleus.

2. Model of bremsstrahlung for deformed nuclei

We define the bremsstrahlung probability $W(w)$ during the α-decay so (like Eq. (1) in Ref. [23], also see Refs. [7,8,21]):

$$W(w) = N_0 w \left| p(w) \right|^2, \qquad k_{i,f} = \sqrt{2mE_{i,f}}, \qquad w = E_i - E_f, \tag{1}$$

where $p(w)$ has the form of Eq. (4) in Ref. [23] and N_0 is a normalization coefficient of the calculation to the experimental data at low energy. In expression of $p(w)$ the vector $\mathbf{k}$ represents an impulse of the photon, pointed out the direction of its propagation; the vector $\mathbf{r}$ is the radius-vector, marking the position of the α-particle relatively to the center-of-mass of the nuclear system. One can write (see Eq. (9) in Ref. [23])

$$\exp(-i\mathbf{kr}) = \exp(-ikr\cos\theta_{\alpha-\gamma}), \quad k = |\mathbf{k}|,\ r = |\mathbf{r}| \tag{2}$$

and we obtain:

$$p(w) = \sum_{\mu=-1,1} h_\mu \xi_\mu^* \int_0^{+\infty} r^2\,dr \int \psi_f^*(\mathbf{r}) e^{-ikr\cos\theta_{\alpha-\gamma}} \frac{\partial}{\partial \mathbf{r}} \psi_i(\mathbf{r})\,d\Omega, \tag{3}$$

where the angle $\theta_{\alpha-\gamma}$ between the vectors $\mathbf{k}$ and $\mathbf{r}$ is the angle between the direction $\mathbf{n}_r = \mathbf{r}/r$ of the motion (or tunneling) of the α-particle in the decaying nucleus and the direction $\mathbf{n}_{\mathrm{ph}} = \mathbf{k}/k$ of propagation of the emitted photon. Here, m is the reduced mass of the system, $E_{i,f}$ and $k_{i,f}$ are the total energy and wave vector of the system in the initial i-state (i.e. the state before the photon emission) or in the final f-state (i.e. the state after the photon emission), $\psi_i(\mathbf{r})$ and $\psi_f(\mathbf{r})$ are the wave functions of the system in the initial i- and final f-state, $w = k = |\mathbf{k}|$ is the frequency (energy) of the photon, ξ_{-1} and ξ_{+1} are the vectors of the circular polarization with opposite directions of rotation (see Ref. [26, p. 42]). We use the Coulomb calibration and the system of units where $\hbar = 1$ and $c = 1$.

To describe the interaction between the α-particle and daughter nucleus we use the α-nucleus potential in the general form:

$$V(r,\theta,l,Q) = v_C(r,\theta) + v_N(r,\theta,Q) + v_l(r), \tag{4}$$

where the Coulomb $v_C(r,\theta)$, nuclear $v_N(r,\theta,Q)$ and centrifugal $v_l(r)$ components are defined as in Ref. [27] (see relations (6)–(10) of the cited paper). We assume that the parameter of deformation β_2 used in the previous cited relations of Ref. [27], is enough small. Further, we shall need in expansion of the nuclear component by powers of β_2:

$$\begin{aligned} v_N(r,\theta,Q) = V_0(A,Z,Q)\cdot\bigl\{&v_{N0}(r) + v_{N1}(r)\cdot\beta_2 Y_{20}(\theta) \\ &+ \text{minor terms}\bigr\}, \end{aligned} \tag{5}$$

where are

$$\begin{aligned} v_{N0}(r) &= \left(1 + \exp\frac{r - r_0 - R}{d}\right)^{-1}, \\ v_{N1}(r) &= \frac{R}{d} v_{N0}^2(r) \exp\frac{r - r_0 - R}{d}. \end{aligned} \tag{6}$$

For many heavy nuclei the deformation parameter β_2 is sufficiently small. In such a case, we can apply the spherically symmetric approximation for the α-nucleus potential (4). At $\beta_2 = 0$ we have to know the wave functions (WFs) in the initial and final states (see formula (8) in Ref. [8]). We use the following boundary conditions: the i-state of the system before the photon emission is a pure decaying state, and therefore for its description we use WF for the α-decay; after the photon emission the state of the system is changed and it is more convenient to use WF as the scattering of the α-particle by the daughter nucleus for the description of the f-state (see Refs. [7,8]).

We shall find the wave function for the deformed α-nucleus potential by the perturbation theory. The small non-spherical correction to the spherical potential is

$$\hat{W} = w_C(r,\theta) + w_N(r,\theta,Q), \tag{7}$$

where are

$$w_C(r,\theta) = \begin{cases} \beta_2 \cdot \frac{6Ze^2R^2}{5r^3} \cdot Y_{20}(\theta), & \text{for } r \geqslant r_m, \\ \beta_2 \cdot \frac{6Ze^2R^2}{5r_m^3}\left(2 - \frac{r^3}{r_m^3}\right) \cdot Y_{20}(\theta), & \text{for } r < r_m \end{cases} \tag{8}$$

and

$$w_N(r,\theta,Q) = V_0(A,Z,Q)\cdot\{v_{N1}(r)\cdot\beta_2 Y_{20}(\theta) + \text{minor terms}\}. \tag{9}$$

For the determination of the unknown wave function $\psi(\mathbf{r})$ as a solution of the Schrödinger equation with the deformed potential (4) it needs to define a set of known for us functions, on the basis of which this function $\psi(\mathbf{r})$ could be expanded (see Appendix A). We separate the wave function $\psi(\mathbf{r})$ into three terms:

$$\psi(\mathbf{r}) = \psi_{\mathrm{sph},l_0m_0}(\mathbf{r}) + \Delta_r\psi_{\mathrm{sph}}(\mathbf{r}) + \Delta_\theta\psi_{\mathrm{sph}}(\mathbf{r}), \tag{10}$$

where $\psi_{\mathrm{sph},l_0m_0}(\mathbf{r})$ is the spherically symmetric unperturbed wave function, $\Delta_r\psi_{\mathrm{sph}}(\mathbf{r})$ and $\Delta_\theta\psi_{\mathrm{sph}}(\mathbf{r})$ are radial and angular corrections describing the radial and angular deformations of this unperturbed wave function, having expressions:

$$\begin{aligned}
\Delta_r\psi_{\mathrm{sph}}(\mathbf{r}) &= \beta_2\cdot\Delta_r\tilde{R}_{\mathrm{sph},l_0}(r)\cdot Y_{l_0m_0}(\theta,\varphi),\\
\Delta_\theta\psi_{\mathrm{sph}}(\mathbf{r}) &= \sum_{l,m\neq l_0,m_0}\{R_{\mathrm{sph},l}(r) + \beta_2\cdot\Delta_r\tilde{R}_{\mathrm{sph},l}(r)\}\cdot Y_{lm}(\theta,\varphi),
\end{aligned} \tag{11}$$

where are

$$\Delta_r\tilde{R}_{\mathrm{sph},l}(r) = \int\limits_{\theta'\neq\theta_{\mathrm{sph}}}\tilde{c}^{(1)}_{lm}(\theta')R_{\theta' l}(r)\sin\theta'\,d\theta', \tag{12}$$

$$\tilde{c}^{(1)}_{l'm'}(\theta') = \frac{1}{E}\sum_l I^{m'}_{ll'}\int\limits_0^{+\infty}R^*_{\theta',l'}(r)w^{(1)}(r)R_{\mathrm{sph},l}(r)r^2\,dr. \tag{13}$$

Here, $R_{\theta',l'}(r)$, $\tilde{c}^{(1)}_{l'm'}(\theta')$ and $I^{m'}_{ll'}$ are defined in Appendix A.

On the basis of relation (10) we come to the same separation for the matrix element:

$$p(w) = p_{\mathrm{sph}}(w) + \Delta_r p(w) + \Delta_\theta p(w), \tag{14}$$

where the matrix element p_{sph} of the spherically symmetric α-decay and its radial correction $\Delta_r p$ taking into account the radial deformation of the α-decay have the form:

$$\begin{aligned}
p_{\mathrm{sph}}(w) &= \delta_{l_f,1}\sqrt{\frac{2}{3}}\sum_{n=0}^{+\infty}i^{n+1}(-1)^n(2n+1)P_n(\cos\theta_{\alpha-\gamma})\cdot J_1(w;n),\\
\Delta_r p(w) &= \delta_{l_f,1}\beta_2\cdot\sqrt{\frac{2}{3}}\sum_{n=0}^{+\infty}i^{n+1}(-1)^n(2n+1)P_n(\cos\theta_{\alpha-\gamma})\cdot J_2(w;n),
\end{aligned} \tag{15}$$

where

$$\begin{aligned}
J_1(w;n) &= \int\limits_0^{+\infty}R^*_{\mathrm{sph},l_f=1}(r)\frac{\partial R_{\mathrm{sph},l_i=0}(r)}{\partial r}j_n(kr)r^2\,dr,\\
J_2(w;n) &= \int\limits_0^{+\infty}\biggl\{R^*_{\mathrm{sph},l_f=1}(r)\frac{\partial\Delta_r\tilde{R}_{\mathrm{sph},l_i=0}(r)}{\partial r}\\
&\quad + \Delta_r\tilde{R}^*_{\mathrm{sph},l_f=1}(r)\frac{\partial R_{\mathrm{sph},l_i=0}(r)}{\partial r}\biggr\}j_n(kr)r^2\,dr
\end{aligned} \tag{16}$$

and $P_l(\theta)$ is the term of the Legendre's polynomial of order l (for example, see Ref. [29, p. 752 (c.1)]). The angular correction $\Delta_\theta p(w)$ is defined on the basis of the angular deformation of the wave function, but in the present calculations we do not use this correction because it gives a smaller contribution in comparison with the radial correction. In obtaining Eq. (15) we choose the selection rules for the quantum numbers of the final f-state (when the integral is non-zero):

$$\begin{aligned} &l_i = 0,\ m_i = 0 \quad \text{for the initial state,} \\ &l_f = 1,\ m_f = -\mu = \pm 1 \quad \text{for the final state.} \end{aligned} \tag{17}$$

Now the total matrix element (14) (without taking into account the angular correction) obtains the form:

$$p(w) = \delta_{l_f,1} \cdot \sqrt{\frac{2}{3}} \sum_{n=0}^{+\infty} i^{n+1} (-1)^n (2n+1) P_n(\cos\theta_{\alpha-\gamma}) \cdot \bigl(J_1(w;n) + \beta_2 J_2(w;n)\bigr). \tag{18}$$

Using the expression (1) we find the probability $W_{l=0}$ in the first approximations at $l = 0$ and its correction $W^{(n=1)}$ in the second approximation at $l = 1$:

$$\begin{aligned} &W_{l=0}(w) = \frac{2}{3} N_0 k_f w \bigl| J_1(w;0) + \beta_2 J_2(w;0)\bigr|^2, \\ &W^{(n=1)}(w, \theta_{\alpha-\gamma}) = 6 N_0 k_f w \bigl| J_1(w;1) + \beta_2 J_2(w;1)\bigr|^2 \cos^2\theta_{\alpha-\gamma}. \end{aligned} \tag{19}$$

From here we obtain the total bremsstrahlung probability up to the second approximation at $l = 1$:

$$\begin{aligned} &W_{l=1}(w, \theta_{\alpha-\gamma}) = W_{l=0}(w) \bigl| 1 - N(w, \beta_2) \cos\theta_{\alpha-\gamma} \bigr|^2, \\ &N(w, \beta_2) = 3i \frac{J_1(w;1) + \beta_2 J_2(w;1)}{J_1(w;0) + \beta_2 J_2(w;0)}. \end{aligned} \tag{20}$$

3. Comparison between theory and experiment by the analysis of the bremsstrahlung spectrum of the deformed ^{226}Ra nucleus

The main question which can be asked to the development of the new formalism that includes the deformation of the α-decaying nucleus into the model of the bremsstrahlung emission is how much such a nuclear deformation influences the bremsstrahlung spectrum. We shall find the bremsstrahlung spectrum for the ^{226}Ra nucleus which has non-zero value of the β_2 quadrupole deformation parameter. At the present stage we shall take into account only the first important radial correction of the wave function. We calculate the bremsstrahlung probability by Eq. (20) and determine two radial integrals $J_1(w;n)$ and $J_2(w;n)$ by Eq. (16). The α-nucleus potential is defined by Eq. (4) with parameters from Ref. [8]. The Q-value for the α-decay of ^{226}Ra is 4.904 MeV (see Ref. [30]), and the β_2 parameter is 0.151 (see Ref. [31]). For a concrete analysis of the influence of the nuclear deformation on the shape of the bremsstrahlung spectrum, we select the angle $\theta_{\alpha-\gamma}$ between the direction of the α-particle motion (with possible tunneling) and the one of the photon emission to be equal to $90^\circ \pm 25^\circ$ because this was the configuration of the detectors in the experiment Ref. [8], taking into account the angular resolution of the detectors.

The calculated photon emission probabilities of the bremsstrahlung accompanying the α-decay of ^{226}Ra, at different values of the angle θ_α between the direction of the α-particle motion and its tunneling in the barrier region and the direction of the symmetry axis of the decaying

^{226}Ra nucleus, are presented in Fig. 1. As Fig. 1(a) shows, the result obtained at the angle $\theta_\alpha = 180^\circ$ or 0° (dashed line) is higher than the one at $\theta_\alpha = 90^\circ$ (dash-dotted line). The difference between these two results is evident and stable in the whole energy region of the emitted photons; it increases by increasing the photon energy E_γ. This fact theoretically confirms that the shape of the bremsstrahlung spectrum is sensitive to the deformation of the nucleus in the α-decay and such a result (obtained for the first time) is stable. Since in the experiment [7,8] the α-detector cannot select a particular direction θ_α of the α-particle motion with respect to the direction of the symmetry axis, the obtained probability has been integrated over the angle θ_α from 0 to π, in order to take into account all possible orientations of the axial symmetry axis of the deformed decaying nucleus in the center-of-mass system. This result which includes the nuclear deformation β_2 is presented in the figure by the full line and it well describes the experimental results (Ref. [8]) also at higher photon energies $E_\gamma > 350$ keV. The result of the bremsstrahlung spectrum calculation confirms the role and the sensitivity of the nuclear deformation on the photon emission probability. The bremsstrahlung probability calculated for the spherical and symmetric decay (at limit for $\beta_2 \to 0$) leads to a lower result as showed in the cited Fig. 1(a) by the dash-double dotted line.

For a comparison we report in Fig. 1(b) the final result (full line) of the present model which takes into account the nuclear deformation of the ^{226}Ra nucleus together with the result (dotted line) given in our previous paper [8]. For photons of high energies ($E_\gamma > 350$ keV) the inclusion of the nuclear deformation in the model strongly improves the description of the bremsstrahlung spectrum. Such an intuition was already suggested in conclusion of our previous paper [8].

4. Conclusions

We developed a fully quantum model to investigate the role and influence of the nuclear deformation of the nucleus on the emitted bremsstrahlung spectrum. In this model we take into account the α-nucleus potential for the deformed nucleus and the expansion of wave function of the α-particle. For the determination of the matrix element of the photon emission at the deformed α-nucleus potential we also take into account the corrections of the deformed wave function. We studied the case of the ^{226}Ra nucleus which is a deformed nucleus. The results discussed in this paper and presented in the figure show by a clear way that the photon emission probability accompanying the α-decay is sensitive to the angle θ_α of the α-emission with respect to the symmetry axis of the deformed nucleus. The final results integrated over all values of θ_α are in very good agreement with the experimental data, and also evidence the relevant effect due to the nuclear deformation parameter β_2. If we disregard the nuclear deformation in the model, the calculation (dotted line in Fig. 1(b)) of the photon emission probability is lower than the integrated calculation and experimental data at energies $E_\gamma > 350$ keV.

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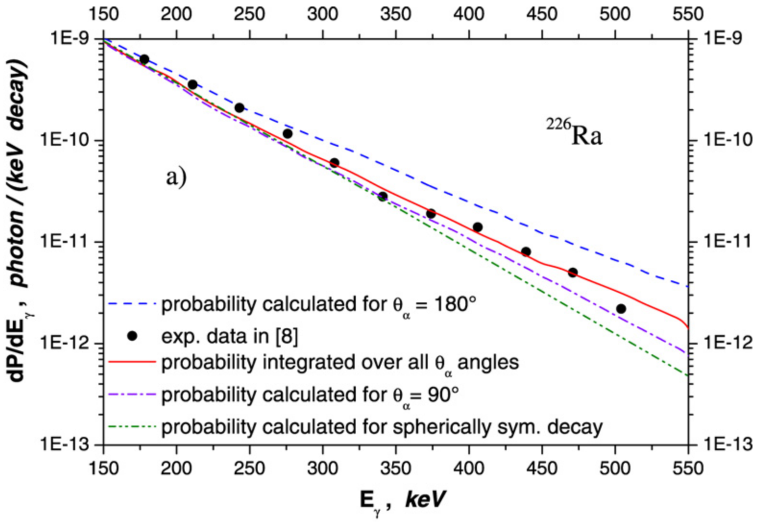

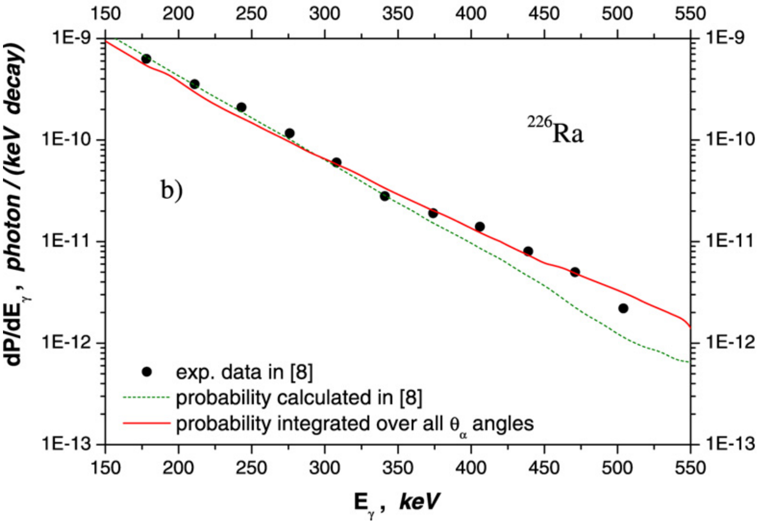

Fig. 1. The bremsstrahlung photon emission probability in the α-decay of the ^{226}Ra nucleus. (a) Dashed line is the probability calculated with the new model for $\theta_\alpha = 180^\circ$; full circles are the experimental data given in Ref. [8]; full line is the total probability integrated over all θ_α angles; dash-dotted line is the probability calculated with the new model for $\theta_\alpha = 90^\circ$; dash-double dotted line is the probability calculated for the spherically symmetric decay (at limit for $\beta_2 \to 0$). (b) Full circles are the experimental data given in panel (a); full line is the total probability given in panel (a); dotted line is the previous total probability given in Ref. [8].

Appendix A

(1) We shall expand the unknown function $\psi(\mathbf{r})$ over basis of functions ψ_θ:

$$\psi(\mathbf{r}) = \int c(\theta)\psi_\theta(\mathbf{r})\,d\theta, \qquad \psi_\theta(\mathbf{r}) = R_{\theta,l}(r) \cdot Y_{lm}(\mathbf{n}_r), \tag{A.1}$$

where the function ψ_θ is a solution of the Schrödinger equation with potential $V(r,\theta)$ for a fixed angle θ. In particular, at $\theta_{\rm sph} = \arccos 1/\sqrt{3}$ the potential $V(r,\theta_{\rm sph})$ coincides with Eq. (4) at $\beta_2 = 0$. Substituting expansion (A.1) into the Schrödinger equation with potential (4), we obtain:

$$E \int c(\theta)\psi_\theta\, d\theta - E c(\theta_{\rm sph})\psi_{\theta_{\rm sph}} = \int c(\theta)\hat{W}\psi_\theta\, d\theta. \tag{A.2}$$

Multiplying this equality from the left by $\psi^*_{\theta',l',m'}$, then integrating it over the volume $\mathbf{dr}$, we find:

$$E\big[c(\theta') - c(\theta_{\rm sph})\delta(\theta' - \theta_{\rm sph})\big] = \int d\theta\, c(\theta) \int \psi^*_{\theta',l',m'}\hat{W}\psi_\theta\, \mathbf{dr}. \tag{A.3}$$

We shall find coefficients $c(\theta)$ in the form $c(\theta) = c^{(0)}(\theta) + c^{(1)}(\theta) + c^{(2)}(\theta) + \cdots$ where the value $c^{(1)}(\theta)$ is of the same order of the perturbation $\hat{W}$. We shall find corrections to the wave function $\psi_{\rm sph}$ at $\theta_{\rm sph}$ of the spherically symmetric decay, according to which we assume: $c^{(0)}(\theta_{\rm sph}) = 1$, and $c^{(0)}(\theta) = 0$ at $\theta \ne \theta_{\rm sph}$. In order to obtain the first approximation, we substitute $c(\theta) = c^{(0)}(\theta) + c^{(1)}(\theta)$ into Eq. (A.3) taking into account values of the first order only. At $\theta \ne \theta_{\rm sph}$ we have:

$$c^{(1)}_{l',m'}(\theta) = \frac{1}{E}\int \psi^*_{\theta,l',m'}\hat{W}\psi_{\rm sph}\, \mathbf{dr}. \tag{A.4}$$

Using the found solution (7)–(9) of the operator $\hat{W}$ and taking into account the property expressed in Eq. (4) of Ref. [28] (see p. 131), we obtain:

$$\begin{aligned} c^{(1)}_{l'm'}(\theta) &= \beta_2 \cdot \tilde{c}^{(1)}_{l'm'}(\theta), \\ \tilde{c}^{(1)}_{l'm'}(\theta) &= \frac{1}{E}\sum_l I^{m'}_{ll'} \int\limits_0^{+\infty} R^*_{\theta,l'}(r) w^{(1)}(r) R_{{\rm sph},l}(r) r^2\, dr, \end{aligned} \tag{A.5}$$

where is

$$I^{m'}_{ll'} = \sqrt{\frac{5\cdot(2l+1)}{4\pi(2l'+1)}}\, C^{l'0}_{l020} C^{l'm'}_{lm'20}. \tag{A.6}$$

(2) Assuming that in the initial i-state the system has numbers $l = m = 0$, and using the *gradient formula* (2.56) of Ref. [26], we obtain the gradient from the undeformed wave function, the gradient from the radial correction of the wave function

$$\begin{aligned} \frac{\partial}{\partial \mathbf{r}}\psi_{{\rm sph},l_i=0}(\mathbf{r}) &= -\sqrt{\frac{1}{3}}\frac{dR_{{\rm sph},l_i=0}(r)}{dr} \sum_{\mu'=-1,1} Y_{1,-\mu'}\big(\mathbf{n}^i_r\big)\xi_{\mu'}, \\ \frac{\partial}{\partial \mathbf{r}}\Delta_r\psi_{{\rm sph},l_i=0}(\mathbf{r}) &= -\beta_2\cdot\sqrt{\frac{1}{3}}\frac{d\Delta_r\tilde{R}_{{\rm sph},l_0=0}(r)}{dr} \sum_{\mu'=-1,1} Y_{1,-\mu'}\big(\mathbf{n}^i_r\big)\xi_{\mu'}, \end{aligned} \tag{A.7}$$

and the gradient from the angular corrections of the wave function at $l = 1$

$$\begin{aligned} &\frac{\partial}{\partial \mathbf{r}}\Delta_\theta\psi(\mathbf{r}) \\ &\quad = \sqrt{\frac{1}{3}}\left(\frac{dR_{{\rm sph},l=1}(r)}{dr} + \frac{2}{r}R_{{\rm sph},l=1}(r) + \beta_2\frac{d\Delta_r\tilde{R}_{{\rm sph},l=1}(r)}{dr} + \beta_2\frac{2}{r}\Delta_r\tilde{R}_{{\rm sph},l=1}(r)\right) \end{aligned}$$

$$
\begin{aligned}
&\times \sum_{\mu=-1,1} (0,1,1 \mid 0,\mu,\mu)\xi_\mu \\
&- \sqrt{\frac{2}{3}}\left(\frac{dR_{\mathrm{sph},l=1}(r)}{dr} - \frac{1}{r}R_{\mathrm{sph},l=1}(r) + \beta_2 \frac{d\Delta_r \tilde{R}_{\mathrm{sph},l=1}(r)}{dr} - \beta_2 \frac{1}{r}\Delta_r \tilde{R}_{\mathrm{sph},l=1}(r)\right) \\
&\times \sum_{m=-1,0,1}\sum_{\mu=-1,1} (2,1,1 \mid m-\mu,\mu,m) Y_{2,m-\mu}(\mathbf{n}_r)\xi_\mu. \qquad \text{(A.8)}
\end{aligned}
$$

Here, $(l1j \mid m-\mu\mu m)$ are *Clebsch–Gordan's coefficients* (see Table I in Ref. [26, p. 317]), and $Y_{1,\mu}(\mathbf{n}_r^{i,f})$ are normalized spherical functions (see Eq. (28.7) of Ref. [29, pp. 118–121, and pp. 752–755]).

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