

DOUBLY HEAVY BARYONS IN THE BORN-OPPENHEIMER APPROXIMATION

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The Born-Oppenheimer approximation, used to calculate the binding energy in the positively-charged ionized hydrogen molecule, is applied to calculating the mass spectrum in doubly heavy baryons. The problem of the binding energy of the hydrogen molecule ion is solved in the non-relativistic quantum mechanics by using the perturbation theory. In the case of static protons, this approach is called the Born-Oppenheimer approximation. The Hamiltonian-operator average for the ionized hydrogen molecule is found by applying the Ritz variational method. A numerical estimate of the equilibrium ion binding energy is obtained as well as the optimized distance between protons. This methods are applied to the doubly heavy baryon with heavy quarks of the same flavor. The binding energy of these baryons is found with account of additional interquark-potential-energy terms due to the quark confinement. The doubly charmed baryon with color antitriplet doubly charmed diquark is studied as an example and its binding energy in dependence on the distance between the charmed quarks is studied numerically and found to be a growing function without local minima.

1. INTRODUCTION

Ordinary baryons are colorless bound states of three quarks. Light baryons are formed from the light u -, d -, and s -quarks. Heavy baryons contain one heavy charmed c - or bottom b -quark inside. Doubly heavy baryons (DHBs) are bound states of two heavy and one light quarks. The most exotic among ordinary baryons are triply heavy baryons formed from

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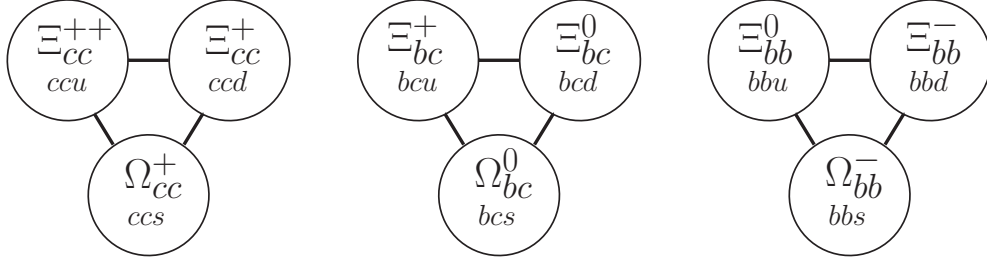


Figure 1. The doubly-charmed, bottom-charmed and doubly-bottom triplets of DHBs.

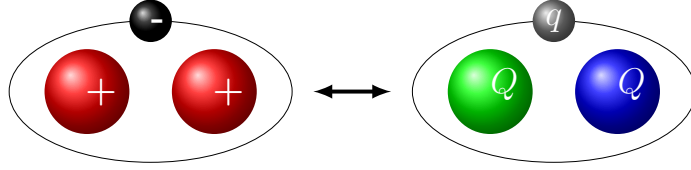


Figure 2. Contents of the positively-charged ionized hydrogen molecule and doubly heavy baryon. Heavy quarks are similar to protons while the light quark determines dynamics in DHB like the electron in the ion.

three heavy quarks.

DHBs, having one light quark only, are flavor triplets under the $SU(3)_F$ -group of light-quark flavors. The doubly-charmed, bottom-charmed and doubly-bottom triplets of DHBs are shown in Fig. 1.

DHBs have two different scales of which the small one is the scale of the doubly heavy diquark (DHD) — antitriplet color state from two heavy quarks Q_1 and Q_2 and the large scale is the baryon scale determined by the light-quark cloud. In the quark non-relativistic limit, dynamics of positively-charged ion of the hydrogen molecule and DHB under assumption that forces among the quarks are potential are very similar (see Fig. 2).

Heavy mesons — open-charmed D -mesons containing the c -quark, and open-bottom B -mesons containing the b -quark, were discovered in the 70s of the last century and since then a lot of information has been obtained about them [1]. Soon after, the open-charmed Λ_c - and open-bottom Λ_b -baryons were found but it tooks more than two decades for a signal of DHB. Among all of DHBs, doubly-charmed baryons, Ξ_{cc}^{++} and Ξ_{cc}^+ , only are found experimentally [1]. The lightest doubly-charmed baryons have the quark contents ccu or ccd . In 2002, the SELEX collaboration at Fermilab reported a signal that was interpreted as a doubly-charmed baryon, Ξ_{cc}^+ . It was initially observed in the $\Xi_{cc}^+ \rightarrow \Lambda_c^+ K^- \pi^+$ charged

hadron decay [2] and three years later its existence was confirmed by the same collaboration in the $\Xi_{cc}^+ \rightarrow pD^+K^-$ decay [3]. Its mass is as follows [1]:

$$M_{\Xi_{cc}^+} = (3518.9 \pm 0.9) \text{ MeV}. \quad (1)$$

Theoretical predictions of the DHB masses are substantially larger, i. e., $3627 \pm 12 \text{ MeV}$ [4] and $3480 \pm 50 \text{ MeV}$ [5]. The SELEX collaboration also determined an upper bound on its lifetime $\tau_{\Xi_{cc}^+} < 33 \times 10^{-15} \text{ s}$ [2] which is significantly shorter than existing theoretical predictions obtained in various approaches [6?] as well as estimates based on lattice QCD methods [7].

Attempts to detect the Ξ_{cc}^+ -baryon have been made in the $\Xi_{cc}^+ \rightarrow \Lambda_c^+ K^- \pi^+$ channel and many other allowed reactions by BaBar [8], Belle [9, 10] and LHCb [11–13] collaborations, as well as in the FOCUS photon production experiment at Fermilab [14]. None of these experiments confirmed yet the existence of this resonance.

In 2017, the LHCb Collaboration announced the discovery of an isospin partner of the Ξ_{cc}^+ -baryon — the doubly charmed Ξ_{cc}^{++} -baryon with the quark content ccu — in the four-particle decay, $\Xi_{cc}^{++} \rightarrow \Lambda_c^+ K^- \pi^+ \pi^+$ [15]. A year later, its existence was confirmed in the two-particle decay, $\Xi_{cc}^{++} \rightarrow \Sigma_c^+ \pi^+$, by the same collaboration [16]. Both measurements agree well with each other and result following Ξ_{cc}^{++} -baryon mass [1]:

$$M_{\Xi_{cc}^{++}} = (3621.6 \pm 0.4) \text{ MeV}, \quad (2)$$

which, unlike the Ξ_{cc}^+ -baryon mass (1), is in good agreement with theoretical predictions [6, 7]. The isospin splitting in the system of two experimentally detected states, Ξ_{cc}^+ and Ξ_{cc}^{++} , is estimated to be [15]:

$$M_{\Xi_{cc}^{++}} - M_{\Xi_{cc}^+} = (103 \pm 2) \text{ MeV}, \quad (3)$$

which significantly exceeds the similar splitting in other similar baryon systems with a typical value of several MeV. So, an identification of doubly charmed baryons as isospin partners is questionable.

In [17], searches of the Ξ_{cc}^{++} -baryon in the $\Xi_{cc}^{++} \rightarrow D^+ p K^- \pi^+$ decay are published by the LHCb Collaboration and no significant excess of background is detected in the energy range $\sqrt{s} = 3300 - 3800 \text{ MeV}$. In a difference to such a suppressed mode, two other decay channels are observed: $\Xi_{cc}^{++} \rightarrow \Sigma_c'^+ \pi^+$ [18] and $\Xi_{cc}^{++} \rightarrow \Xi_c^0 \pi^+ \pi^+$ [19].

The LHCb collaboration has measured also of the Ξ_{cc}^{++} -baryon lifetime [20]:

$$\tau_{\Xi_{cc}^{++}} = (2.56 \pm 0.27) \times 10^{-13} \text{ c}, \quad (4)$$

which agrees well with theoretical predictions [4, 5, 21] and is an order of magnitude larger than the limit on the Ξ_{cc}^{+} -baryon lifetime [2] obtained by the SELEX Collaboration.

In the future, the LHCb collaboration plans to measure the Ξ_{cc}^{++} spin and parity [22] as well as to continue searching for its isospin partner — Ξ_{cc}^{+} -baryon for the purpose to compare its mass and width with measurements by the SELEX collaboration. As for the other doubly charmed strange Ω_{cc}^{+} -baryon [22], its lifetime is expected to be comparable with the Ξ_{cc}^{+} -baryon lifetime, however, decay channels most favored for its detection contain more charged particles in the final state than similar Ξ_{cc}^{+} -decays. As a consequence, the efficiency of baryon reconstruction must be rather small which significantly complicates Ω_{cc}^{+} -detection. Searches for Ξ_{bc}^{-} , Ω_{bc}^{-} and Ξ_{bb} -baryons are also planned in future [22]. These baryons do not have any "golden" decay modes for their detection, so it is planned to perform a joint analysis of several modes simultaneously to identify a signal from these baryons.

The results of the SELEX collaboration [2, 3] stimulated not only experimental searches for doubly heavy baryons, but also theoretical studies of masses and decay widths. There is a discrepancy in predictions for both masses and lifetimes of DHBs, so a correctness of frameworks used for theoretical predictions can be determined only after the experimental detection of bottom DHBs.

In this paper, we presented an application of the Born-Oppenheimer approximation, first, to the positively-charged ionized hydrogen molecule and, second, extend it to DHBs. As an example of DHBS, the doubly charmed Ξ_{cc} -baryon is chosen and theoretical calculations of its mass in the Born-Oppenheimer approximation are discussed.

2. POSITIVELY CHARGED ION OF HYDROGEN MOLECULE

In this section, the Born-Oppenheimer approximation is applied to a positively charged ion H_2^{+} of the hydrogen molecule. The corresponding Schrödinger equation of this quantum system is as follows:

$$\hat{H} \Psi(\vec{r}, \vec{R}) = E_{\text{ion}} \Psi(\vec{r}, \vec{R}). \quad (5)$$

The Hamiltonian operator of the ion can be written as follows:

$$\hat{H} = -\frac{1}{M} \Delta_{\vec{R}} + \frac{e^2}{R} - \frac{1}{2m} \left(1 + \frac{m}{2M}\right) \Delta_{\vec{r}} - \frac{e^2}{r_a} - \frac{e^2}{r_b},$$

where e is the elementary charge, M and m ($M = 1836m$) are the proton and electron masses, respectively, \vec{R} is the distance between the protons, and \vec{r} is the distance from the electron to the protons' center of masses. It is possible to factorize variables in (5) by choosing the wave-function in the form:

$$\Psi(\vec{r}, \vec{R}) = \psi(\vec{r}, \vec{R}) \chi(\vec{R}), \quad (6)$$

where $\psi(\vec{r}, \vec{R})$ is the electron wave-function and $\chi(\vec{R})$ is the wave-function of the two proton system.

The Schrödinger equation for $\chi(\vec{R})$ is as follows:

$$-\frac{1}{M} \frac{\Delta_{\vec{R}} \chi(\vec{R})}{\chi(\vec{R})} + \frac{e^2}{R} + \mathcal{E}(R) - \frac{1}{M} \frac{\Delta_{\vec{R}} \psi(\vec{r}, \vec{R})}{\psi(\vec{r}, \vec{R})} - \frac{2}{M} \frac{\nabla_{\vec{R}} \chi(\vec{R}) \nabla_{\vec{R}} \psi(\vec{r}, \vec{R})}{\psi(\vec{r}, \vec{R}) \chi(\vec{R})} = E_{\text{ion}}, \quad (7)$$

where $\mathcal{E}(R)$ is the binding energy of the electron in the ion. The corresponding equation for $\psi(\vec{r}, \vec{R})$ has the form:

$$-\left[\frac{1}{2m} \left(1 + \frac{m}{2M}\right) \Delta_{\vec{r}} + \frac{e^2}{r_a} + \frac{e^2}{r_b} \right] \psi(\vec{r}, \vec{R}) = \mathcal{E}(R) \psi(\vec{r}, \vec{R}) \quad (8)$$

In the limit $M \rightarrow \infty$ the problem above is reduced to the one for the electron in the electric field of two static protons which is known as the Born-Oppenheimer approximation. The ion energy is the sum of Coulombic repulsive energy between protons and the effective energy of the electron:

$$E_{\text{ion}}(R) = \frac{e^2}{R} + \mathcal{E}(R). \quad (9)$$

In the approach considered, the ion exists when $E_{\text{ion}}(R)$ has a minimum, $E_{\text{ion}}(R_{\text{min}}) = E_{\text{min}}$, at finite R . Dynamics of protons is determined by the Schrödinger equation:

$$-\frac{1}{M} \Delta_{\vec{R}} \chi^{(0)}(R) + \left[\frac{e^2}{R} + \mathcal{E}(R) \right] \chi^{(0)}(R) = E_{\text{ion}}^{(0)}(R), \quad (10)$$

which is written in the leading order in $1/M$ power expansion. Because of a complicated dependence of $E_{\text{ion}}^{(0)}(R)$ on R , it can be solved only numerically.

Let us turn to Eq. (8) and solve it perturbatively by applying the Ritz variational method. Assume that the electron is in the ground state of both hydrogen atoms. A spin part of the

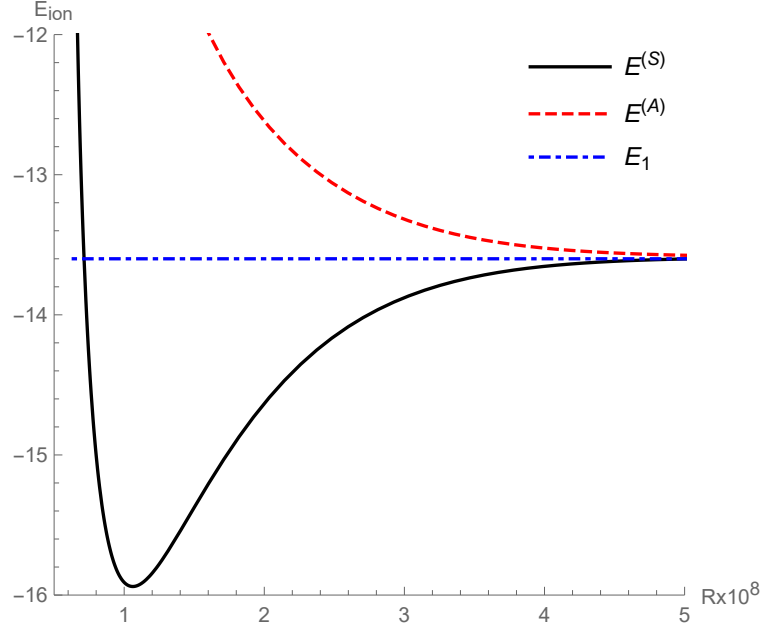


Figure 3. Ion energy E (in eV) in dependence on the distance ρ_R (in cm) between nuclei.

wave-function is factorized and is assumed implicitly. The basic functions are chosen in the exponential form:

$$\psi_{100}(r_a) = \frac{\gamma^{3/2}}{\sqrt{\pi a^3}} e^{-\gamma r_a/a}, \quad \psi_{100}(r_b) = \frac{\gamma^{3/2}}{\sqrt{\pi a^3}} e^{-\gamma r_b/a}, \quad (11)$$

where $a \simeq 0.53 \times 10^{-8}$ cm is the Bohr radius and γ is the Ritz variational parameter. With these functions, the Hamiltonian average is calculated. The unperturbative ion wave-function is the following superposition:

$$\psi(r_a, r_b) = \alpha \psi_{100}(r_a) + \beta \psi_{100}(r_b). \quad (12)$$

From the symmetry of the Hamiltonian operator follows two possibilities: at $\alpha = \beta$ the ion wave-function, $\psi^{(S)}(r_a, r_b)$, is symmetric under the nucleus position exchange and at $\alpha = -\beta$ it is antisymmetric, $\psi^{(A)}(r_a, r_b)$. The ion energies $E^{(S)}$ and $E^{(A)}$ in dependence on the distance R between nuclei are presented in Fig. 3. A bound state with static nuclei exists for the state with $\psi^{(S)}(r_a, r_b)$ only. Its binding energy is $E_{\min}^{(S)} = -15.9$ eV and the corresponding nucleus distance $R_{\text{ion}} = 1.06 \times 10^{-8}$ cm, a twice of the Bohr radius.

3. QUANTUM MECHANICS OF DOUBLY HEAVY BARYONS

In the Born-Oppenheimer approximation, the dynamics of DHBs is discussed. The DHB Hamiltonian operator in the non-relativistic limit of both heavy and light quarks can be written in a form very similar to the case of the hydrogen molecule ion (2):

$$\hat{H}_{\text{DHB}} = -\frac{\Delta}{2m_q} + \alpha_s \left[\frac{\lambda_A}{r_A} + \frac{\lambda_B}{r_B} + \frac{\lambda_{AB}}{R} \right] + \frac{3k}{4} (|\lambda_A| r_A + |\lambda_B| r_B + |\lambda_{AB}| R), \quad (13)$$

where m_q is the light quark mass. heavy quarks are marked by A and B indices. Potential energy operators describing interactions between quark pairs are chosen as Cornell potentials with $\alpha_s(\mu)$ to be a strong coupling at the energy scale μ . At the scales of doubly heavy diquarks is chosen as follows: $\alpha_s(2M_c) = 0.30$, $\alpha_s(M_c + M_b) = 0.24$, and $\alpha_s(2M_b) = 0.21$. $k = 0.15 \text{ GeV}^2$ is a string tension in the confining potential and λ_A , λ_B , and λ_{AB} are coefficients determined by the color $SU(3)_C$ -group of QCD [23]. From now on, the unit system with $\hbar = c = 1$ is used.

Let us discuss the quark-pair interactions in a baryon. A pair of quarks in a diquark forms either a color antitriplet or a color sextet ($3 \times 3 = \bar{3} + 6$). When interacting with the third quark in a baryon, only a color antitriplet couples with a quark color triplet and a singlet (colorless) state is obtained, since ($\bar{3} \times 3 = 1 + 8$) and ($6 \times 3 = 8 + 10$). As a consequence, any pairwise interaction of quarks in a baryon must be color antitriplet. So, all the coefficients determined by the QCD color group $SU(3)_C$ are equal: $\lambda_A = \lambda_B = \lambda_{AB} \equiv -\lambda = -2/3$.

To get an energy in DHB, the Born-Oppenheimer approximation is applied in which heavy quarks are assumed to be static source of a field for a light quark. Unperturbed wave-functions of heavy diquarks (HD) — two-particle systems from heavy and light quarks determined by Coulombic potential and coincide with the ground wave-functions of the hydrogen atom:

$$\psi_{100}(r_A) = \frac{\gamma^{3/2}}{\sqrt{\pi a_D^3}} e^{-\gamma r_A/a_D}, \quad \psi_{100}(r_B) = \frac{\gamma^{3/2}}{\sqrt{\pi a_D^3}} e^{-\gamma r_B/a_D}, \quad (14)$$

except the Bohr radius $a \simeq 0.53 \times 10^{-8} \text{ cm}$ is replaced by the HD radius

$$a_D^{-1} = 2\alpha_s m_q/3, \quad a_D \simeq 3 \text{ fm} \quad (m_q = 300 \text{ MeV}). \quad (15)$$

It is also convenient to define a reduced distance $\rho_R = \gamma R/a_D$ between heavy quarks. DHB wave-function are symmetric and antisymmetric superpositions of $\psi_{100}(r_A)$ and $\psi_{100}(r_B)$

under the heavy quark position exchange. As in the hydrogen molecule ion wave function, the spin degrees of freedom are factorized and assumed to be present implicitly.

Within the Ritz variational method, the energy $E_{\text{ion}} = E^{(S)}$ as a function of two Ritz parameters γ and the reduced distance ρ_R has the following general form:

$$E_{\text{ion}}(\rho_R, \gamma) = f(\rho_R) \gamma^2 + g(\rho_R) \gamma, \quad (16)$$

where $f(\rho_R)$ and $g(\rho_R)$ are known functions [24]. The energy of a bound state results after minimizing over both γ and ρ_R :

$$\frac{\partial E_{\text{ion}}(\rho_R, \gamma)}{\partial \gamma} = 0, \quad \frac{\partial E_{\text{ion}}(\rho_R, \gamma)}{\partial \rho_R} = 0. \quad (17)$$

It is easy to find the optimal value of γ : $\gamma_{\text{min}} = -g(\rho_R)/f(\rho_R)/2$ and, after it is substituted in (16), to get the energy as a function of ρ_R only. The function obtained is studied numerically on the local minimum existence.

Similar expression for the DHB energy is as follows:

$$E_{\text{DHB}}(\rho_R, \gamma) = F(\rho_R) \gamma^2 + G(\rho_R) \gamma + H(\rho_R) \frac{1}{\gamma}, \quad (18)$$

where $F(\rho_R)$, $G(\rho_R)$, and $H(\rho_R)$ are some functions [25]. In a difference to (16), the energy get an extra term $\sim 1/\gamma$. The minimizing procedure over γ results a cubic equation for DHB instead of a linear equation in the case of the ion H_2^+ :

$$2\gamma^3 F(\rho_R) + \gamma^2 G(\rho_R) - H(\rho_R) = 0. \quad (19)$$

This equation has three solutions: one is real and other two are complex. As far as the binding energy is real, the real solution only is physical:

$$\gamma_1 = \frac{G}{6F} \frac{Y^3 + 1}{Y(Y + 1)}, \quad (20)$$

where $Y(\rho_R)$ is a combination of $F(\rho_R)$, $G(\rho_R)$, and $H(\rho_R)$ [25].

4. DOUBLY CHARMED BARYON Ξ_{CC}^{++}

Consider doubly charmed baryon, Ξ_{cc}^{++} , as an example. It consist of two heavy c -quarks and one light u -quark. It was observed by the LHCb Collaboration at CERN and its mass is known very precisely now [1]:

$$M(\Xi_{cc}^{++})_{\text{Exp}} = (3621.6 \pm 0.4) \text{ MeV}. \quad (21)$$

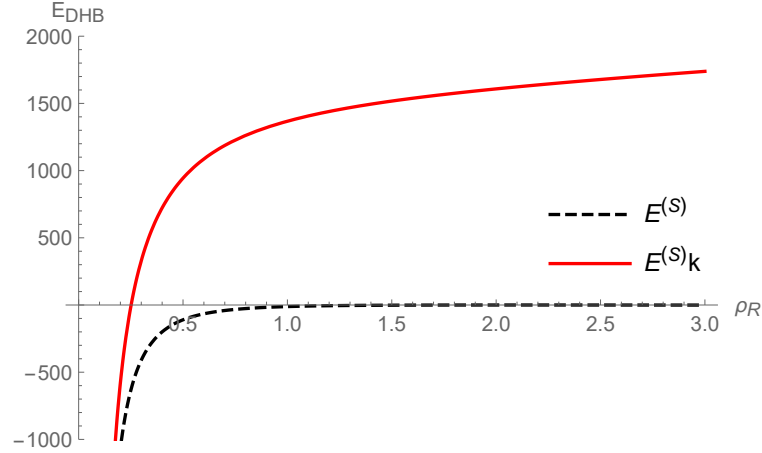


Figure 4. The energy $E^{(S)}(\rho_R)$ for the DHB with the antitriplet in dependence on reduced distance ρ_R between heavy quarks.

Theoretically, the mass of the Ξ_{cc}^{++} -baryon is the sum of constituent quark masses and the binding energy:

$$M(\Xi_{cc}^{++})_{\text{Th}} = 2M_c + m_u + E_{\text{DHB}} = 3782 \text{ MeV} + E_{\text{DHB}} \quad (22)$$

For the binding energy estimate, the following parameters are used:

$$\lambda = \frac{2}{3}, \quad \alpha_s(2M_c) = 0.3, \quad k = 0.15 \text{ GeV}^2. \quad (23)$$

After $F^{(S)}(\rho_R)$, $G^{(S)}(\rho_R)$, and $H^{(S)}(\rho_R)$ are substituted into the equation for the energy $E^{(S)}$, we obtain the dependence of the energy on ρ_R and its plot is presented in Fig. 4. It is seen that the energy $E^{(S)}$ has no minimum, so a static diquark does not exist. The dynamics of heavy quarks should be taken into account and this problem is postponed for a future publication [25].

5. SUMMARY

The methods developed for calculations of the binding energy in the positively-charged ionized hydrogen molecule are used for the DHB binding energy. Additional terms in the DTB energy due to the linear part in the interaction potential between quarks are calculated. The binding energy E_{DHB} is a growing function of the reduced distance ρ_R between heavy quarks, without a minimum. The bound state with two stationary heavy quarks is not realized within the Born-Oppenheimer approximation considered here. To get the bound state,

the dynamics of heavy quarks should be taken into account. The spin-spin interaction of quarks in the baryon should be also included in the binding energy. Doubly charmed baryons in the Born-Oppenheimer approximation were considered earlier [23], but the calculational procedure used there differs from that presented in this paper.

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