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Research Article

Semiclassical Potential Function of B–B Interaction: Reduction to Integrable Form

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Abstract

The paper represents Part 1 of 2 of the study aimed at constructing a semiclassical interaction potential between a pair of boron atoms in an analytical form, thus allowing one *ab initio* determination of the key ground state parameters of the diboron molecule B_2. Based on semiclassical expressions for the electron orbitals of the B atom, the B–B potential function is reduced to a linear combination of exponential integrals, which can be calculated in elementary functions.

Introduction

Previously, a relatively simple quasiclassical theory of the molecules and condensed matter ground state was proposed (the foundations of the theory were set out in the monograph [1]), which in the initial, i.e. semiclassical, approximation allows one to introduce the concept of the effective electric charge of nuclei and, on its basis, to construct expressions for radial distributions of self-consistent electron density and electric field potential in the atoms that constitute the system [2,3].

This approach made it possible to determine some parameters of the electronic structure [4-8] (and even the isotope effect) in elemental boron and boron-rich materials with relative errors of several percent, which is quite acceptable for materials science.

A more sophisticated semiclassical approach to the problem of the electronic structure of condensed matter was developed in [9]. It was proved that atoms are semiclassical electron systems in the sense of the closeness of their exact quantum electron energy spectrum to the spectrum calculated within the semiclassical approximation. The wave functions of electrons bound in an atom were presented in the form of hydrogen-like atomic orbitals with certain effective charge numbers. On their basis, the matrix elements of the secular equation determining the electronic structure of molecules and condensed matter were calculated. Test estimates were made for the boron atom B and the diboron molecule B_2.

Note that, in view of recent advances in the description of all-boron nanosystems within the modified diatomic model [10], the *ab initio* construction of the B–B pair interaction potential is of not only academic but also practical importance. In the introductory part of the paper [11], devoted to the construction of the semiclassical B–B potential, several references to theoretical methods for determining diatomic potentials were already given. In order not to repeat them, we will mention here only some similar studies not reflected in that review.

Tietz-type potentials, describing the solution of the Thomas–Fermi equation, yielded from a simple semiclassical statistical model of an atom, can be successfully applied for studying the vibrational states of diatomic molecules as well. In particular, the Tietz potential form with four parameters (equilibrium bond length, potential depth and width, and the parameter controlling the values as a ratio of the well depth) of the spectroscopic fitting was used [12] to five different molecules/dimers. Generally, the derived formula of such a Tietz potential works for multiple molecules/dimers.

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Solutions to the D-dimensional Schrodinger equation were investigated via the modified Rosen–Morse potential and employed for numerous diatomic molecules [13] to reproduce their potential energy curves. Based on the multiparameter exponential-type potential, its extended version was suggested [14] to improve the calculation accuracy near the equilibrium and in the asymptotic region. This study also provided a reference for the construction of potential energy functions for diatomic molecules.

In [15], a model potential developed for the ammonia molecule was extended to the planar-geometry water molecule in a single-center partial-wave approximation in analogy with a self-consistent field method and used to calculate DC Stark resonance parameters. Using full and multi-reference configuration interaction methods, reliable energetic references for B_n, $n = 1 - 4$, clusters were found in [16]. These methods provided results for structural parameters with a mean absolute error of 0.020 Å. The best performance in predicting the relative energies of clusters was 12.8 kJ/mol.

Using a diatomic model, the anharmonic zero-point vibrations of a crystal were studied [17], and their amplitude was shown to be not able to exceed a limiting value, a certain fraction of the interatomic distance. Compressing/stretching of the crystal has to decrease/increase the amplitude of such vibrations. A monolayer triangular lattice model consisting of two types of particles was studied [18] by Monte Carlo simulations within a mesoscopic theory, assuming the short-range attraction and long-range repulsion between particles of the same kind and short-range repulsion and long-range attraction for the cross-interactions.

According to the *ab initio* molecular dynamics study [19], the atomic structures of liquid and amorphous boron have notably different microstructures and, consequently, average coordination numbers. Not isolated atoms, but almost ideal and defective pentagonal pyramidal clusters B_6 are the building blocks of liquid boron, while the packing of pure amorphous boron is somewhat close to that of the α-rhombohedral phase, i.e., mainly consists of slightly deformed B_{12} icosahedra. This means that during the rapid solidification, pentagonal pyramids develop, resulting in the formation of icosahedra. Calculating the physical characteristics of non-crystalline solids (polycrystals, composites, and multi-phase systems) is challenging due to the high computational cost of *ab initio* methods and the low accuracy of empirical potentials. To respond to this problem, it was proposed [20] an efficient technique for atomistic simulations with high accuracy and reasonable computational cost. In particular, the elastic moduli of polycrystalline diamond and their dependence on grain size were determined using the approach based on machine learning interatomic potentials trained on local fragments of the polycrystalline system.

We aim to construct a semiclassical interaction potential between a pair of boron atoms in an analytical form. In this paper, representing Part 1 of 2 of the study, the semiclassical B–B potential function is reduced to a linear combination of exponential integrals, which can be calculated in elementary functions.

Method

Semiclassical construction of B–B interaction potential

Previously, in the semiclassical approximation, we have derived [11] an integral expression for the boron–boron interatomic pair potential u as a function $u(a)$ of the distance a between the nuclei of two interacting B-atoms:

$$u(a)=5e^2\left(\left(\frac{2}{a}+\frac{2Z_{12}}{r_B}\right)\exp\left(-\frac{2Z_{12}a}{r_B}\right)+\left(\frac{2}{a}+\frac{3Z_{34}}{2r_B}+\frac{Z_{34}^2a}{2r_B^2}+\frac{Z_{34}^3a^2}{4r_B^3}\right)\exp\left(-\frac{Z_{34}a}{r_B}\right)+\left(\frac{1}{a}+\frac{3Z_5}{4r_B}+\frac{Z_5^2a}{4r_B^2}+\frac{Z_5^3a^2}{24r_B^3}\right)\exp\left(-\frac{Z_5a}{r_B}\right)\right)$$
$$-\frac{e^2}{r_Ba}\int_0^\infty dr\, r\left(\left(\frac{2}{r}+\frac{2Z_{12}}{r_B}\right)\exp\left(-\frac{2Z_{12}r}{r_B}\right)+\left(\frac{2}{r}+\frac{3Z_{34}}{2r_B}+\frac{Z_{34}^2r}{2r_B^2}+\frac{Z_{34}^3r^2}{4r_B^3}\right)\exp\left(-\frac{Z_{34}r}{r_B}\right)+\left(\frac{1}{r}+\frac{3Z_5}{4r_B}+\frac{Z_5^2r}{4r_B^2}+\frac{Z_5^3r^2}{24r_B^3}\right)\exp\left(-\frac{Z_5r}{r_B}\right)\right), \quad (1)$$
$$\left(J_{12}(r)+J_{34}(r)+J_5(r)\right)$$

where r is the integration variable,

$$0 \le r\ \infty, \quad (2)$$

of the distance dimension, and

$$J_{12}(r)=Z_{12}\left(\left(1+\frac{2Z_{12}|r-a|}{r_B}\right)\exp\left(-\frac{2Z_{12}|r-a|}{r_B}\right)-\left(1+\frac{2Z_{12}(r+a)}{r_B}\right)\exp\left(-\frac{2Z_{12}(r+a)}{r_B}\right)\right), \quad (3)$$

$$J_{34}(r)=\frac{Z_{34}}{4}\left(\left(1+\frac{Z_{34}|r-a|}{r_B}-\frac{Z_{34}^2|r-a|^2}{2r_B^2}+\frac{Z_{34}^3|r-a|^3}{2r_B^3}\right)\exp\left(-\frac{Z_{34}|r-a|}{r_B}\right)-\left(1+\frac{Z_{34}(r+a)}{r_B}-\frac{Z_{34}^2(r+a)^2}{2r_B^2}+\frac{Z_{34}^3(r+a)^3}{2r_B^3}\right)\exp\left(-\frac{Z_{34}(r+a)}{r_B}\right)\right), \quad (4)$$

$$J_5(r)=\frac{Z_5}{8}\left(\left(1+\frac{Z_5|r-a|}{r_B}+\frac{Z_5^2|r-a|^2}{2r_B^2}+\frac{Z_5^3|r-a|^3}{6r_B^3}\right)\exp\left(-\frac{Z_5|r-a|}{r_B}\right)-\left(1+\frac{Z_5(r+a)}{r_B}+\frac{Z_5^2(r+a)^2}{2r_B^2}+\frac{Z_5^3(r+a)^3}{6r_B^3}\right)\exp\left(-\frac{Z_5(r+a)}{r_B}\right)\right), \quad (5)$$

are the explicitly defined functions of r argument. Parameters, $Z_{12} \approx 4.69$, $Z_{34} \approx 2.76$, and $Z_5 \approx 1.48$, are the effective nuclear charge numbers for B-atom 1s, 2s, and 2p-shell electrons, respectively. As for the constant

$$r_B=\frac{\hbar^2}{e^2 m}\approx 0.529\ \text{Å}\ , \quad (6)$$

it is the Bohr radius related to the Bohr energy

$$E_B=\frac{e^2}{2r_B}\approx 13.6\ \text{eV}\ . \quad (7)$$

The advantages of introducing the effective charge numbers of the nucleus, Z_{12}, Z_{34} and Z_5 as parameters that respectively describe the states of the 1s-, 2s-, and 2p-shells of the B atom are associated with the possibility in this case of representing the radial distributions of the electron density and potential of atoms by hydrogen-like electron orbitals, which ultimately leads to an analytical expression of the potential energy of the B–B interatomic interaction.

By introducing the dimensionless quantities,

$$U\equiv\frac{u}{E_B}, \quad (8)$$

$$A\equiv\frac{a}{r_B}, \quad (9)$$

$$R\equiv\frac{r}{r_B}, \quad (10)$$

we rewrite the B–B semiclassical potential function in a dimensionless form (in which R stands for the dimensionless integration variable):

$$U(A)=U_{12}(A)+U_{34}(A)+U_5(A)-F_{12}(A)-F_{34}(A)-F_5(A)-F_{12-34}(A)-F_{12-5}(A)-F_{34-5}(A), \quad (11)$$

$$U_{12}(A)=\left(\frac{20}{A}+20Z_{12}\right)\exp(-2Z_{12}A), \quad (12)$$

$$U_{34}(A)=\left(\frac{20}{A}+15Z_{34}+5Z_{34}^2A+\frac{5Z_{34}^3A^2}{2}\right)\exp(-Z_{34}A), \quad (13)$$

$$U_5(A)=\left(\frac{10}{A}+\frac{15Z_5}{2}+\frac{5Z_5^2A}{2}+\frac{5Z_5^3A^2}{12}\right)\exp(-Z_5A), \quad (14)$$

are the explicitly defined functions of the A parameter, while

$$F_{12}(A)=\int_0^\infty dR I_{12}(A,R)J_{12}, \quad (15)$$

$$F_{34}(A)=\int_0^\infty dR I_{34}(A,R)J_{34}, \quad (16)$$

$$F_5(A)=\int_0^\infty dR I_5(A,R)J_5, \quad (17)$$

$$F_{12-34}(A)=\int_0^\infty dR\left(I_{12}(A,R)J_{34}(A,R)+J_{12}(A,R)I_{34}(A,R)\right), \quad (18)$$

$$F_{12-5}(A)=\int_0^\infty dR\left(I_{12}(A,R)J_5(A,R)+J_{12}(A,R)I_5(A,R)\right), \quad (19)$$

$$F_{34-5}(A)=\int_0^\infty dR\left(I_{34}(A,R)J_5(A,R)+J_{34}(A,R)I_5(A,R)\right) \quad (20)$$

are the given integral functions

Here are introduced the following integrand functions:

$$I_{12}(A,R)=\left(\alpha^{(0)}(A)+\alpha^{(1)}(A)(2Z_{12}R)\right)\exp(-2Z_{12}R)\,, \quad (21)$$

$$\alpha^{(0)}(A)=\frac{4}{A}\,, \quad (21\text{-}0)$$

$$\alpha^{(1)}(A)=\frac{2}{A}\,; \quad (21\text{-}1)$$

$$I_{34}(A,R)=\left(\beta^{(0)}(A)+\beta^{(1)}(A)(Z_{34}R)+\beta^{(2)}(A)(Z_{34}R)^2+\beta^{(3)}(A)(Z_{34}R)^3\right)\exp(-Z_{34}R)\,, \quad (22)$$

$$\beta^{(0)}(A)=\frac{4}{A}\,, \quad (22\text{-}0)$$

$$\beta^{(1)}(A)=\frac{3}{A}\,, \quad (22\text{-}1)$$

$$\beta^{(2)}(A)=\frac{1}{A}\,, \quad (22\text{-}2)$$

$$\beta^{(3)}(A)=\frac{1}{2A}\,; \quad (22\text{-}3)$$

$$I_{5}(A,R)=\left(\gamma^{(0)}(A)+\gamma^{(1)}(A)(Z_5R)+\gamma^{(2)}(A)(Z_5R)^2+\gamma^{(3)}(A)(Z_5R)^3\right)\exp(-Z_5R)\,, \quad (23)$$

$$\gamma^{(0)}(A)=\frac{2}{A}\,, \quad (23\text{-}0)$$

$$\gamma^{(1)}(A)=\frac{3}{2A}\,, \quad (23\text{-}1)$$

$$\gamma^{(2)}(A)=\frac{1}{2A}\,, \quad (23\text{-}2)$$

$$\gamma^{(3)}(A)=\frac{1}{12A}\,; \quad (23\text{-}3)$$

$0 \le R < A$:

$$J_{12}(A,R)=\delta^{(0)}\left(A_>^+\right)\exp(+2Z_{12}R)+\delta^{(1)}\left(A_>^+\right)(2Z_{12}R)\exp(+2Z_{12}R)+\delta^{(0)}\left(A_>^-\right)\exp(-2Z_{12}R)+\delta^{(1)}\left(A_>^-\right)(2Z_{12}R)\exp(-2Z_{12}R)\,, \quad (24\text{-}\ A_>^\pm)$$

$$\delta^{(0)}\left(A_>^+\right)=Z_{12}(1+2Z_{12}A)\exp(-2Z_{12}A)\,, \quad (24\text{-}0\text{-}\ A_>^+)$$

$$\delta^{(1)}\left(A_>^+\right)=-Z_{12}\exp(-2Z_{12}A)\,, \quad (24\text{-}1\text{-}\ A_>^+)$$

$$\delta^{(0)}\left(A_>^-\right)=-Z_{12}(1+2Z_{12}A)\exp(-2Z_{12}A)\,, \quad (24\text{-}0\text{-}\ A_>^-)$$

$$\delta^{(1)}\left(A_>^-\right)=-Z_{12}\exp(-2Z_{12}A)\,; \quad (24\text{-}1\text{-}\ A_>^-)$$

$A \le R \le \infty$:

$$J_{12}(A,R)=\delta^{(0)}\left(A_\le^-\right)\exp(-2Z_{12}R)+\delta^{(1)}\left(A_\le^-\right)(2Z_{12}R)\exp(-2Z_{12}R)\,, \quad (24\text{-}\ A_\le^-)$$

$$\delta^{(0)}\left(A_\le^-\right)=Z_{12}\left(-(1+2Z_{12}A)\exp(-2Z_{12}A)+(1-2Z_{12}A)\exp(+2Z_{12}A)\right)\,, \quad (24\text{-}0\text{-}\ A_\le^-)$$

$$\delta^{(1)}\left(A_\le^-\right)=Z_{12}\left(-\exp(-2Z_{12}A)+\exp(+2Z_{12}A)\right)\,; \quad (24\text{-}1\text{-}\ A_\le^-)$$

$0 \le R < A$:

$$\begin{aligned}J_{34}(A,R)=\;&\varepsilon^{(0)}\left(A_>^+\right)\exp(+Z_{34}R)+\varepsilon^{(1)}\left(A_>^+\right)(Z_{34}R)\exp(+Z_{34}R)+\varepsilon^{(2)}\left(A_>^+\right)(Z_{34}R)^2\exp(+Z_{34}R)+\\&\varepsilon^{(3)}\left(A_>^+\right)(Z_{34}R)^3\exp(+Z_{34}R)+\varepsilon^{(0)}\left(A_>^-\right)\exp(-Z_{34}R)+\varepsilon^{(1)}\left(A_>^-\right)(Z_{34}R)\exp(-Z_{34}R)+\\&\varepsilon^{(2)}\left(A_>^-\right)(Z_{34}R)^2\exp(-Z_{34}R)+\varepsilon^{(3)}\left(A_>^-\right)(Z_{34}R)^3\exp(-Z_{34}R)\end{aligned} \quad (25\text{-}\ A_>^\pm)$$

$$\varepsilon^{(0)}\left(A_>^+\right)=\frac{Z_{34}}{4}\left(1+(Z_{34}A)-\frac{(Z_{34}A)^2}{2}+\frac{(Z_{34}A)^3}{2}\right)\exp(-Z_{34}A)\,, \quad (25\text{-}0\text{-}\ A_>^+)$$

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$$\varepsilon^{(1)}\left(A_{>}^{+}\right)=-\frac{Z_{34}}{4}\left(1+\left(Z_{34}A\right)+\frac{3\left(Z_{34}A\right)^{2}}{2}\right)\exp\left(-Z_{34}A\right), \qquad (25\text{-}1\text{-}A_{>}^{+})$$

$$\varepsilon^{(2)}\left(A_{>}^{+}\right)=-\frac{Z_{34}}{8}\left(1-3\left(Z_{34}A\right)\right)\exp\left(-Z_{34}A\right), \qquad (25\text{-}2\text{-}A_{>}^{+})$$

$$\varepsilon^{(3)}\left(A_{>}^{+}\right)=-\frac{Z_{34}}{8}\exp\left(-Z_{34}A\right), \qquad (25\text{-}3\text{-}A_{>}^{+})$$

$$\varepsilon^{(0)}\left(A_{>}^{-}\right)=-\frac{Z_{34}}{4}\left(1+\left(Z_{34}A\right)-\frac{\left(Z_{34}A\right)^{2}}{2}+\frac{\left(Z_{34}A\right)^{3}}{2}\right)\exp\left(-Z_{34}A\right), \qquad (25\text{-}0\text{-}A_{>}^{-})$$

$$\varepsilon^{(1)}\left(A_{>}^{-}\right)=-\frac{Z_{34}}{4}\left(1-\left(Z_{34}A\right)+\frac{3\left(Z_{34}A\right)^{2}}{2}\right)\exp\left(-Z_{34}A\right), \qquad (25\text{-}1\text{-}A_{>}^{-})$$

$$\varepsilon^{(2)}\left(A_{>}^{-}\right)=\frac{Z_{34}}{8}\left(1-3\left(Z_{34}A\right)\right)\exp\left(-Z_{34}A\right), \qquad (25\text{-}2\text{-}A_{>}^{-})$$

$$\varepsilon^{(3)}\left(A_{>}^{-}\right)=-\frac{Z_{34}}{8}\exp\left(-Z_{34}A\right); \qquad (25\text{-}3\text{-}A_{>}^{-})$$

$A\le R\le\infty$:

$$J_{34}\left(A,R\right)=\varepsilon^{(0)}\left(A_{\le}^{-}\right)\exp\left(-Z_{34}R\right)+\varepsilon^{(1)}\left(A_{\le}^{-}\right)(Z_{34}R)\exp\left(-Z_{34}R\right)+\varepsilon^{(2)}\left(A_{\le}^{-}\right)(Z_{34}R)^{2}\exp\left(-Z_{34}R\right)+\varepsilon^{(3)}\left(A_{\le}^{-}\right)(Z_{34}R)^{3}\exp\left(-Z_{34}R\right), \qquad (25\text{-}A_{\le}^{-})$$

$$\varepsilon^{(0)}\left(A_{\le}^{-}\right)=\frac{Z_{34}}{4}\left(\left(1-(Z_{34}A)-\frac{(Z_{34}A)^{2}}{2}-\frac{(Z_{34}A)^{3}}{2}\right)\exp\left(+Z_{34}A\right)-\left(1+(Z_{34}A)-\frac{(Z_{34}A)^{2}}{2}+\frac{(Z_{34}A)^{3}}{2}\right)\exp\left(-Z_{34}A\right)\right), \qquad (25\text{-}0\text{-}A_{\le}^{-})$$

$$\varepsilon^{(1)}\left(A_{\le}^{-}\right)=\frac{Z_{34}}{4}\left(\left(1+(Z_{34}A)+\frac{3(Z_{34}A)^{2}}{2}\right)\exp\left(+Z_{34}A\right)-\left(1-(Z_{34}A)+\frac{3(Z_{34}A)^{2}}{2}\right)\exp\left(-Z_{34}A\right)\right), \qquad (25\text{-}1\text{-}A_{\le}^{-})$$

$$\varepsilon^{(2)}\left(A_{\le}^{-}\right)=\frac{Z_{34}}{8}\left(-\left(1+3(Z_{34}A)\right)\exp\left(+Z_{34}A\right)+\left(1-3(Z_{34}A)\right)\exp\left(-Z_{34}A\right)\right), \qquad (25\text{-}2\text{-}A_{\le}^{-})$$

$$\varepsilon^{(3)}\left(A_{\le}^{-}\right)=\frac{Z_{34}}{8}\left(\exp\left(+Z_{34}A\right)-\exp\left(-Z_{34}A\right)\right); \qquad (25\text{-}3\text{-}A_{\le}^{-})$$

$0\le R<A$:

$$J_{5}\left(A,R\right)=\zeta^{(0)}\left(A_{>}^{+}\right)\exp\left(+Z_{5}R\right)+\zeta^{(1)}\left(A_{>}^{+}\right)\left(Z_{5}R\right)\exp\left(+Z_{5}R\right)+\zeta^{(2)}\left(A_{>}^{+}\right)\left(Z_{5}R\right)^{2}\exp\left(+Z_{5}R\right)+\zeta^{(3)}\left(A_{>}^{+}\right)(Z_{5}R)^{3}\exp\left(+Z_{5}R\right)+\zeta^{(0)}\left(A_{>}^{-}\right)\exp\left(-Z_{5}R\right)+\zeta^{(1)}\left(A_{>}^{-}\right)\left(Z_{5}R\right)\exp\left(-Z_{5}R\right)+\zeta^{(2)}\left(A_{>}^{-}\right)(Z_{5}R)^{2}\exp\left(-Z_{5}R\right)+\zeta^{(3)}\left(A_{>}^{-}\right)(Z_{5}R)^{3}\exp\left(-Z_{5}R\right), \qquad (26\text{-}A_{>}^{\pm})$$

$$\zeta^{(0)}\left(A_{>}^{+}\right)=\frac{Z_{5}}{8}\left(1+(Z_{5}A)+\frac{(Z_{5}A)^{2}}{2}+\frac{(Z_{5}A)^{3}}{6}\right)\exp\left(-Z_{5}A\right), \qquad (26\text{-}0\text{-}A_{>}^{+})$$

$$\zeta^{(1)}\left(A_{>}^{+}\right)=-\frac{Z_{5}}{8}\left(1+\left(Z_{5}A\right)+\frac{\left(Z_{5}A\right)^{2}}{2}\right)\exp\left(-Z_{5}A\right), \qquad (26\text{-}1\text{-}A_{>}^{+})$$

$$\zeta^{(2)}\left(A_{>}^{+}\right)=\frac{Z_{5}}{16}\left(1+\left(Z_{5}A\right)\right)\exp\left(-Z_{5}A\right), \qquad (26\text{-}2\text{-}A_{>}^{+})$$

$$\zeta^{(3)}\left(A_{>}^{+}\right)=-\frac{Z_{5}}{48}\exp\left(-Z_{5}A\right), \qquad (26\text{-}3\text{-}A_{>}^{+})$$

$$\zeta^{(0)}\left(A_{>}^{-}\right)=-\frac{Z_{5}}{8}\left(1+\left(Z_{5}A\right)+\frac{\left(Z_{5}A\right)^{2}}{2}+\frac{\left(Z_{5}A\right)^{3}}{6}\right)\exp\left(-Z_{5}A\right), \qquad (26\text{-}0\text{-}A_{>}^{-})$$

$$\zeta^{(1)}\left(A_{>}^{-}\right)=-\frac{Z_{5}}{8}\left(1+\left(Z_{5}A\right)+\frac{\left(Z_{5}A\right)^{2}}{2}\right)\exp\left(-Z_{5}A\right), \qquad (26\text{-}1\text{-}A_{>}^{-})$$

$$\zeta^{(2)}\left(A_{>}^{-}\right)=-\frac{Z_5}{16}\left(1+(Z_5A)\right)\exp\left(-Z_5A\right), \qquad (26\text{-}2\text{-}A_{>}^{-})$$

$$\zeta^{(3)}\left(A_{>}^{-}\right)=-\frac{Z_5}{48}\exp\left(-Z_5A\right); \qquad (26\text{-}3\text{-}A_{>}^{-})$$

$A\le R\le\infty$:

$$J_5(A,R)=\zeta^{(0)}\left(A_{\le}^{-}\right)\exp\left(-Z_5R\right)+\zeta^{(1)}\left(A_{\le}^{-}\right)(Z_5R)\exp\left(-Z_5R\right)+\zeta^{(2)}\left(A_{\le}^{-}\right)(Z_5R)^2\exp\left(-Z_5R\right)+\zeta^{(3)}\left(A_{\le}^{-}\right)(Z_5R)^3\exp\left(-Z_5R\right) \qquad (26\text{-}A_{\le}^{-})$$

$$\zeta^{(0)}\left(A_{\le}^{-}\right)=\frac{Z_5}{8}\left(\left(1-(Z_5A)+\frac{(Z_5A)^2}{2}-\frac{(Z_5A)^3}{6}\right)\exp\left(+Z_5A\right)+\left(1+(Z_5A)+\frac{(Z_5A)^2}{2}+\frac{(Z_5A)^3}{6}\right)\exp\left(-Z_5A\right)\right), \qquad (26\text{-}0\text{-}A_{\le}^{-})$$

$$\zeta^{(1)}\left(A_{\le}^{-}\right)=\frac{Z_5}{8}\left(\left(1-(Z_5A)+\frac{(Z_5A)^2}{2}\right)\exp\left(+Z_5A\right)+\left(1+(Z_5A)+\frac{(Z_5A)^2}{2}\right)\exp\left(-Z_5A\right)\right), \qquad (26\text{-}1\text{-}A_{\le}^{-})$$

$$\zeta^{(2)}\left(A_{\le}^{-}\right)=\frac{Z_5}{16}\left(\left(1-(Z_5A)\right)\exp\left(+Z_5A\right)+\left(1+(Z_5A)\right)\exp\left(-Z_5A\right)\right), \qquad (26\text{-}2\text{-}A_{\le}^{-})$$

$$\zeta^{(3)}\left(A_{\le}^{-}\right)=\frac{Z_5}{48}. \qquad (26\text{-}3\text{-}A_{\le}^{-})$$

Reducing this integral expression of the interatomic B–B pair potential to an explicit function of the distance between the nuclei of two interacting B atoms is an important task due to the physical significance of interatomic interactions in general.

At sufficiently small internuclear distances, the electron clouds of two boron atoms (as well as any pair of interacting atoms) overlap, leading to an intense exchange of their valence electrons. Furthermore, the electrons and nuclei of different atoms are attracted/repulsed by Coulomb forces. The effective potential energy corresponding to the superposition of all these B–B interactions as a function of the B–B internuclear distance has a minimum, the absolute value of whose depth (relative to the potential energy of non-interacting atoms, i.e., at an infinitely large distance) determines the binding energy of the diboron molecule B_2.

When the kinetic energy of relative motion is less than the binding energy, inelastic scattering of two boron atoms can occur, leading to their unification into a diatomic molecule due to the conversion of that kinetic energy into the energy of relative vibrations of two bound boron atoms.

Results

Reduction to integrable form

Now, using exponential arguments as the integral variable *x*, we can transform the integral functions introduced above into a linear combination of definite integrals of the integrands in the form of elementary functions – products of polynomials and exponents with positive or negative arguments. As is well known, such integrals can be calculated directly by partial integration, reducing them to a linear combination of tabulated integrals (the corresponding derivation procedure, while simple in nature, is too cumbersome to include in the paper):

$$F_{12}(A)=\int_0^{4Z_{12}A}dx\left(\eta^{(0)}\left(A_{>}^{+}\right)+\eta^{(1)}\left(A_{>}^{+}\right)x+\eta^{(2)}\left(A_{>}^{+}\right)x^2+\eta^{(0)}\left(A_{>}^{-}\right)\exp(-x)+\eta^{(1)}\left(A_{>}^{-}\right)x\exp(-x)+\eta^{(2)}\left(A_{>}^{-}\right)x^2\exp(-x)\right)+\int_{4Z_{12}A}^{\infty}dx\left(\eta^{(0)}\left(A_{\le}^{-}\right)\exp(-x)+\eta^{(1)}\left(A_{\le}^{-}\right)x\exp(-x)+\eta^{(2)}\left(A_{\le}^{-}\right)x^2\exp(-x)\right), \qquad (27)$$

$$\eta^{(0)}\left(A_{>}^{+}\right)=\frac{\alpha^{(0)}(A)\delta^{(0)}\left(A_{>}^{+}\right)}{4Z_{12}}, \qquad (27\text{-}0\text{-}A_{>}^{+})$$

$$\eta^{(1)}\left(A_{>}^{+}\right)=\frac{\alpha^{(0)}(A)\delta^{(1)}\left(A_{>}^{+}\right)+\alpha^{(1)}(A)\delta^{(0)}\left(A_{>}^{+}\right)}{8Z_{12}}, \qquad (27\text{-}1\text{-}A_{>}^{+})$$

$$\eta^{(2)}\left(A_{>}^{+}\right)=\frac{\alpha^{(1)}(A)\delta^{(1)}\left(A_{>}^{+}\right)}{16Z_{12}}, \qquad (27\text{-}2\text{-}A_{>}^{+})$$

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$$\eta^{(0)}\left(A_>^-\right)=\frac{\alpha^{(0)}(A)\delta^{(0)}\left(A_>^-\right)}{4Z_{12}}, \qquad (27\text{-}0\text{-}A_>^-)$$

$$\eta^{(1)}\left(A_>^-\right)=\frac{\alpha^{(0)}(A)\delta^{(1)}\left(A_>^-\right)+\alpha^{(1)}(A)\delta^{(0)}\left(A_>^-\right)}{8Z_{12}}, \qquad (27\text{-}1\text{-}A_>^-)$$

$$\eta^{(2)}\left(A_>^-\right)=\frac{\alpha^{(1)}(A)\delta^{(1)}\left(A_>^-\right)}{16Z_{12}}, \qquad (27\text{-}2\text{-}A_>^-)$$

$$\eta^{(0)}\left(A_\le^-\right)=\frac{\alpha^{(0)}(A)\delta^{(0)}\left(A_\le^-\right)}{4Z_{12}}, \qquad (27\text{-}0\text{-}A_\le^-)$$

$$\eta^{(1)}\left(A_\le^-\right)=\frac{\alpha^{(0)}(A)\delta^{(1)}\left(A_\le^-\right)+\alpha^{(1)}(A)\delta^{(0)}\left(A_\le^-\right)}{8Z_{12}}, \qquad (27\text{-}1\text{-}A_\le^-)$$

$$\eta^{(2)}\left(A_\le^-\right)=\frac{\alpha^{(1)}(A)\delta^{(1)}\left(A_\le^-\right)}{16Z_{12}}; \qquad (27\text{-}2\text{-}A_\le^-)$$

and

$$F_{34}(A)=\int_0^{2Z_{34}A}dx\begin{pmatrix}\theta^{(0)}\left(A_>^+\right)+\theta^{(1)}\left(A_>^+\right)x+\theta^{(2)}\left(A_>^+\right)x^2+\theta^{(3)}\left(A_>^+\right)x^3+\theta^{(4)}\left(A_>^+\right)x^4+\theta^{(5)}\left(A_>^+\right)x^5+\theta^{(6)}\left(A_>^+\right)x^6+\\ \theta^{(0)}\left(A_>^-\right)\exp(-x)+\theta^{(1)}\left(A_>^-\right)x\exp(-x)+\theta^{(2)}\left(A_>^-\right)x^2\exp(-x)+\theta^{(3)}\left(A_>^-\right)x^3\exp(-x)+\theta^{(4)}\left(A_>^-\right)x^4\exp(-x)+\\ \theta^{(5)}\left(A_>^-\right)x^5\exp(-x)+\theta^{(6)}\left(A_>^-\right)x^6\exp(-x)\end{pmatrix}+$$
$$\int_{2Z_{34}A}^{\infty}dx\begin{pmatrix}\theta^{(0)}\left(A_\le^-\right)\exp(-x)+\theta^{(1)}\left(A_\le^-\right)x\exp(-x)+\\ \theta^{(2)}\left(A_\le^-\right)x^2\exp(-x)+\theta^{(3)}\left(A_\le^-\right)x^3\exp(-x)+\theta^{(4)}\left(A_\le^-\right)x^4\exp(-x)+\theta^{(5)}\left(A_\le^-\right)x^5\exp(-x)+\theta^{(6)}\left(A_\le^-\right)x^6\exp(-x)\end{pmatrix}, \qquad (28)$$

$$\theta^{(0)}\left(A_>^+\right)=\frac{\beta^{(0)}(A)\varepsilon^{(0)}\left(A_>^+\right)}{2Z_{34}}, \qquad (28\text{-}0\text{-}A_>^+)$$

$$\theta^{(1)}\left(A_>^+\right)=\frac{\beta^{(0)}(A)\varepsilon^{(1)}\left(A_>^+\right)+\beta^{(1)}(A)\varepsilon^{(0)}\left(A_>^+\right)}{4Z_{34}}, \qquad (28\text{-}1\text{-}A_>^+)$$

$$\theta^{(2)}\left(A_>^+\right)=\frac{\beta^{(0)}(A)\varepsilon^{(2)}\left(A_>^+\right)+\beta^{(1)}(A)\varepsilon^{(1)}\left(A_>^+\right)+\beta^{(2)}(A)\varepsilon^{(0)}\left(A_>^+\right)}{8Z_{34}}, \qquad (28\text{-}2\text{-}A_>^+)$$

$$\theta^{(3)}\left(A_>^+\right)=\frac{\beta^{(0)}(A)\varepsilon^{(3)}\left(A_>^+\right)+\beta^{(1)}(A)\varepsilon^{(2)}\left(A_>^+\right)+\beta^{(2)}(A)\varepsilon^{(1)}\left(A_>^+\right)+\beta^{(3)}(A)\varepsilon^{(0)}\left(A_>^+\right)}{16Z_{34}}, \qquad (28\text{-}3\text{-}A_>^+)$$

$$\theta^{(4)}\left(A_>^+\right)=\frac{\beta^{(1)}(A)\varepsilon^{(3)}\left(A_>^+\right)+\beta^{(2)}(A)\varepsilon^{(2)}\left(A_>^+\right)+\beta^{(3)}(A)\varepsilon^{(1)}\left(A_>^+\right)}{32Z_{34}}, \qquad (28\text{-}4\text{-}A_>^+)$$

$$\theta^{(5)}\left(A_>^+\right)=\frac{\beta^{(2)}(A)\varepsilon^{(3)}\left(A_>^+\right)+\beta^{(3)}(A)\varepsilon^{(2)}\left(A_>^+\right)}{64Z_{34}}, \qquad (28\text{-}5\text{-}A_>^+)$$

$$\theta^{(6)}\left(A_>^+\right)=\frac{\beta^{(3)}(A)\varepsilon^{(3)}\left(A_>^+\right)}{128Z_{34}}, \qquad (28\text{-}6\text{-}A_>^+)$$

$$\theta^{(0)}\left(A_>^-\right)=\frac{\beta^{(0)}(A)\varepsilon^{(0)}\left(A_>^-\right)}{2Z_{34}}, \qquad (28\text{-}0\text{-}A_>^-)$$

$$\theta^{(1)}\left(A_>^-\right)=\frac{\beta^{(0)}(A)\varepsilon^{(1)}\left(A_>^-\right)+\beta^{(1)}(A)\varepsilon^{(0)}\left(A_>^-\right)}{4Z_{34}}, \qquad (28\text{-}1\text{-}A_>^-)$$

$$\theta^{(2)}\left(A_{>}^{-}\right)=\frac{\beta^{(0)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)+\beta^{(1)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)+\beta^{(2)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)}{8Z_{34}}, \quad (28\text{-}2\text{-}A_{>}^{-})$$

$$\theta^{(3)}\left(A_{>}^{-}\right)=\frac{\beta^{(0)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)+\beta^{(1)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)+\beta^{(2)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)+\beta^{(3)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)}{16Z_{34}}, \quad (28\text{-}3\text{-}A_{>}^{-})$$

$$\theta^{(4)}\left(A_{>}^{-}\right)=\frac{\beta^{(1)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)+\beta^{(2)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)+\beta^{(3)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)}{32Z_{34}}, \quad (28\text{-}4\text{-}A_{>}^{-})$$

$$\theta^{(5)}\left(A_{>}^{-}\right)=\frac{\beta^{(2)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)+\beta^{(3)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)}{64Z_{34}}, \quad (28\text{-}5\text{-}A_{>}^{-})$$

$$\theta^{(6)}\left(A_{>}^{-}\right)=\frac{\beta^{(3)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)}{128Z_{34}}, \quad (28\text{-}6\text{-}A_{>}^{-})$$

$$\theta^{(0)}\left(A_{\le}^{-}\right)=\frac{\beta^{(0)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{2Z_{34}}, \quad (28\text{-}0\text{-}A_{\le}^{-})$$

$$\theta^{(1)}\left(A_{\le}^{-}\right)=\frac{\beta^{(0)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)+\beta^{(1)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{4Z_{34}}, \quad (28\text{-}1\text{-}A_{\le}^{-})$$

$$\theta^{(2)}\left(A_{\le}^{-}\right)=\frac{\beta^{(0)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)+\beta^{(1)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)+\beta^{(2)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{8Z_{34}}, \quad (28\text{-}2\text{-}A_{\le}^{-})$$

$$\theta^{(3)}\left(A_{\le}^{-}\right)=\frac{\beta^{(0)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)+\beta^{(1)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)+\beta^{(2)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)+\beta^{(3)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{16Z_{34}}, \quad (28\text{-}3\text{-}A_{\le}^{-})$$

$$\theta^{(4)}\left(A_{\le}^{-}\right)=\frac{\beta^{(1)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)+\beta^{(2)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)+\beta^{(3)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)}{32Z_{34}}, \quad (28\text{-}4\text{-}A_{\le}^{-})$$

$$\theta^{(5)}\left(A_{\le}^{-}\right)=\frac{\beta^{(2)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)+\beta^{(3)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)}{64Z_{34}}, \quad (28\text{-}5\text{-}A_{\le}^{-})$$

$$\theta^{(6)}\left(A_{\le}^{-}\right)=\frac{\beta^{(3)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)}{128Z_{34}}; \quad (28\text{-}6\text{-}A_{\le}^{-})$$

and

$$F_5(A)=\int_0^{2Z_5A}dx\begin{pmatrix}\iota^{(0)}\left(A_{>}^{+}\right)+\iota^{(1)}\left(A_{>}^{+}\right)x+\iota^{(2)}\left(A_{>}^{+}\right)x^2+\iota^{(3)}\left(A_{>}^{+}\right)x^3+\iota^{(4)}\left(A_{>}^{+}\right)x^4+\iota^{(5)}\left(A_{>}^{+}\right)x^5+\iota^{(6)}\left(A_{>}^{+}\right)x^6+\\ \iota^{(0)}\left(A_{>}^{-}\right)\exp(-x)+\iota^{(1)}\left(A_{>}^{-}\right)x\exp(-x)+\iota^{(2)}\left(A_{>}^{-}\right)x^2\exp(-x)+\iota^{(3)}\left(A_{>}^{-}\right)x^3\exp(-x)+\iota^{(4)}\left(A_{>}^{-}\right)x^4\exp(-x)+\\ \iota^{(5)}\left(A_{>}^{-}\right)x^5\exp(-x)+\iota^{(6)}\left(A_{>}^{-}\right)x^6\exp(-x)\end{pmatrix}+$$
$$\int_{2Z_5A}^{\infty}dx\begin{pmatrix}\iota^{(0)}\left(A_{\le}^{-}\right)\exp(-x)+\iota^{(1)}\left(A_{\le}^{-}\right)x\exp(-x)+\iota^{(2)}\left(A_{\le}^{-}\right)x^2\exp(-x)+\\ \iota^{(3)}\left(A_{\le}^{-}\right)x^3\exp(-x)+\iota^{(4)}\left(A_{\le}^{-}\right)x^4\exp(-x)+\iota^{(5)}\left(A_{\le}^{-}\right)x^5\exp(-x)+\iota^{(6)}\left(A_{\le}^{-}\right)x^6\exp(-x)\end{pmatrix}, \quad (29)$$

$$\iota^{(0)}\left(A_{>}^{+}\right)=\frac{\gamma^{(0)}(A)\zeta^{(0)}\left(A_{>}^{+}\right)}{2Z_5}, \quad (29\text{-}0\text{-}A_{>}^{+})$$

$$\iota^{(1)}\left(A_{>}^{+}\right)=\frac{\gamma^{(0)}(A)\zeta^{(1)}\left(A_{>}^{+}\right)+\gamma^{(1)}(A)\zeta^{(0)}\left(A_{>}^{+}\right)}{4Z_5}, \quad (29\text{-}1\text{-}A_{>}^{+})$$

$$\iota^{(2)}\left(A_{>}^{+}\right)=\frac{\gamma^{(0)}(A)\zeta^{(2)}\left(A_{>}^{+}\right)+\gamma^{(1)}(A)\zeta^{(1)}\left(A_{>}^{+}\right)+\gamma^{(2)}(A)\zeta^{(0)}\left(A_{>}^{+}\right)}{8Z_5}, \quad (29\text{-}2\text{-}A_{>}^{+})$$

$$\iota^{(3)}\left(A_{>}^{+}\right)=\frac{\gamma^{(0)}(A)\zeta^{(3)}\left(A_{>}^{+}\right)+\gamma^{(1)}(A)\zeta^{(2)}\left(A_{>}^{+}\right)+\gamma^{(2)}(A)\zeta^{(1)}\left(A_{>}^{+}\right)+\gamma^{(3)}(A)\zeta^{(0)}\left(A_{>}^{+}\right)}{16Z_5}, \qquad (29\text{-}3\text{-}A_{>}^{+})$$

$$\iota^{(4)}\left(A_{>}^{+}\right)=\frac{\gamma^{(1)}(A)\zeta^{(3)}\left(A_{>}^{+}\right)+\gamma^{(2)}(A)\zeta^{(2)}\left(A_{>}^{+}\right)+\gamma^{(3)}(A)\zeta^{(1)}\left(A_{>}^{+}\right)}{32Z_5}, \qquad (29\text{-}4\text{-}A_{>}^{+})$$

$$\iota^{(5)}\left(A_{>}^{+}\right)=\frac{\gamma^{(2)}(A)\zeta^{(3)}\left(A_{>}^{+}\right)+\gamma^{(3)}(A)\zeta^{(2)}\left(A_{>}^{+}\right)}{64Z_5}, \qquad (29\text{-}5\text{-}A_{>}^{+})$$

$$\iota^{(6)}\left(A_{>}^{+}\right)=\frac{\gamma^{(3)}(A)\zeta^{(3)}\left(A_{>}^{+}\right)}{128Z_5}, \qquad (29\text{-}6\text{-}A_{>}^{+})$$

$$\iota^{(0)}\left(A_{>}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)}{2Z_5}, \qquad (29\text{-}0\text{-}A_{>}^{-})$$

$$\iota^{(1)}\left(A_{>}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)}{4Z_5}, \qquad (29\text{-}1\text{-}A_{>}^{-})$$

$$\iota^{(2)}\left(A_{>}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)}{8Z_5}, \qquad (29\text{-}2\text{-}A_{>}^{-})$$

$$\iota^{(3)}\left(A_{>}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)}{16Z_5}, \qquad (29\text{-}3\text{-}A_{>}^{-})$$

$$\iota^{(4)}\left(A_{>}^{-}\right)=\frac{\gamma^{(1)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)}{32Z_5}, \qquad (29\text{-}4\text{-}A_{>}^{-})$$

$$\iota^{(5)}\left(A_{>}^{-}\right)=\frac{\gamma^{(2)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)}{64Z_5}, \qquad (29\text{-}5\text{-}A_{>}^{-})$$

$$\iota^{(6)}\left(A_{>}^{-}\right)=\frac{\gamma^{(3)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)}{128Z_5}, \qquad (29\text{-}6\text{-}A_{>}^{-})$$

$$\iota^{(0)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)}{2Z_5}, \qquad (29\text{-}0\text{-}A_{\le}^{-})$$

$$\iota^{(1)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)}{4Z_5}, \qquad (29\text{-}1\text{-}A_{\le}^{-})$$

$$\iota^{(2)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)}{8Z_5}, \qquad (29\text{-}2\text{-}A_{\le}^{-})$$

$$\iota^{(3)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(0)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)}{16Z_5}, \qquad (29\text{-}3\text{-}A_{\le}^{-})$$

$$\iota^{(4)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(1)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)}{32Z_5}, \qquad (29\text{-}4\text{-}A_{\le}^{-})$$

$$\iota^{(5)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(2)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)}{64Z_5} \qquad (29\text{-}5\text{-}A_{\le}^{-})$$

$$\iota^{(6)}\left(A_{\le}^{-}\right)=\frac{\gamma^{(3)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)}{128Z_5}; \qquad (29\text{-}6\text{-}A_{\le}^{-})$$

and

$$F_{12-34}(A)=\int_0^{(2Z_{12}-Z_{34})A}dx\begin{pmatrix}\kappa^{(0)}\left(A_>^+\right)\exp(-x)+\kappa^{(1)}\left(A_>^+\right)x\exp(-x)+\kappa^{(2)}\left(A_>^+\right)x^2\exp(-x)+\\ \kappa^{(3)}\left(A_>^+\right)x^3\exp(-x)+\kappa^{(4)}\left(A_>^+\right)x^4\exp(-x)+\lambda^{(0)}\left(A_>^+\right)\exp(+x)+\lambda^{(1)}\left(A_>^+\right)x\exp(+x)+\lambda^{(2)}\left(A_>^+\right)x^2\exp(+x)+\\ \lambda^{(3)}\left(A_>^+\right)x^3\exp(+x)+\lambda^{(4)}\left(A_>^+\right)x^4\exp(+x)\end{pmatrix}+$$
$$\int_0^{(2Z_{12}+Z_{34})A}dx\left(\kappa^{(0)}\left(A_>^-\right)\exp(-x)+\kappa^{(1)}\left(A_>^-\right)x\exp(-x)+\kappa^{(2)}\left(A_>^-\right)x^2\exp(-x)+\kappa^{(3)}\left(A_>^-\right)x^3\exp(-x)+\kappa^{(4)}\left(A_>^-\right)x^4\exp(-x)\right)+$$
$$\int_{(2Z_{12}+Z_{34})A}^{\infty}dx\left(\kappa^{(0)}\left(A_\le^-\right)\exp(-x)+\kappa^{(1)}\left(A_\le^-\right)x\exp(-x)+\kappa^{(2)}\left(A_\le^-\right)x^2\exp(-x)+\kappa^{(3)}\left(A_\le^-\right)x^3\exp(-x)+\kappa^{(4)}\left(A_\le^-\right)x^4\exp(-x)\right) \quad (30)$$

$$\kappa^{(0)}\left(A_>^+\right)=\frac{\alpha^{(0)}(A)\varepsilon^{(0)}\left(A_>^+\right)}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)}, \quad (30\text{-}0\text{-}\ A_>^+)$$

$$\kappa^{(1)}\left(A_>^+\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)}\left(\frac{\alpha^{(0)}(A)\varepsilon^{(1)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_{34}}-1}+\frac{\alpha^{(1)}(A)\varepsilon^{(0)}\left(A_>^+\right)}{1-\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}1\text{-}\ A_>^+)$$

$$\kappa^{(2)}\left(A_>^+\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)^2}\left(\frac{\alpha^{(0)}(A)\varepsilon^{(2)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_{34}}-1}+\frac{\alpha^{(1)}(A)\varepsilon^{(1)}\left(A_>^+\right)}{1-\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}2\text{-}\ A_>^+)$$

$$\kappa^{(3)}\left(A_>^+\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)^3}\left(\frac{\alpha^{(0)}(A)\varepsilon^{(3)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_{34}}-1}+\frac{\alpha^{(1)}(A)\varepsilon^{(2)}\left(A_>^+\right)}{1-\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}3\text{-}\ A_>^+)$$

$$\kappa^{(4)}\left(A_>^+\right)=\frac{\alpha^{(1)}(A)\varepsilon^{(3)}\left(A_>^+\right)}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)^4\left(1-\frac{Z_{34}}{2Z_{12}}\right)}, \quad (30\text{-}4\text{-}\ A_>^+)$$

$$\lambda^{(0)}\left(A_>^+\right)=\frac{\beta^{(0)}(A)\delta^{(0)}\left(A_>^+\right)}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)}, \quad (30\text{-}0'\text{-}\ A_>^+)$$

$$\lambda^{(1)}\left(A_>^+\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)}\left(\frac{\beta^{(1)}(A)\delta^{(0)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_{34}}-1}+\frac{\beta^{(0)}(A)\delta^{(1)}\left(A_>^+\right)}{1-\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}1'\text{-}\ A_>^+)$$

$$\lambda^{(2)}\left(A_>^+\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)^2}\left(\frac{\beta^{(2)}(A)\delta^{(0)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_{34}}-1}+\frac{\beta^{(1)}(A)\delta^{(1)}\left(A_>^+\right)}{1-\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}2'\text{-}\ A_>^+)$$

$$\lambda^{(3)}\left(A_>^+\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)^3}\left(\frac{\beta^{(3)}(A)\delta^{(0)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_{34}}-1}+\frac{\beta^{(2)}(A)\delta^{(1)}\left(A_>^+\right)}{1-\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}3'\text{-}\ A_>^+)$$

$$\lambda^{(4)}\left(A_{>}^{+}\right)=\frac{\beta^{(3)}(A)\delta^{(1)}\left(A_{>}^{+}\right)}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}-1\right)^{4}\left(1-\frac{Z_{34}}{2Z_{12}}\right)}, \quad (30\text{-}4'\text{-}\ A_{>}^{+})$$

$$\kappa^{(0)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)+\beta^{(0)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_{34}}{2Z_{12}}\right)}, \quad (30\text{-}0\text{-}\ A_{>}^{-})$$

$$\kappa^{(1)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)+\alpha^{(1)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)+\beta^{(0)}(A)\delta^{(1)}\left(A_{>}^{-}\right)+\beta^{(1)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_{34}}{2Z_{12}}\right)^{2}}, \quad (30\text{-}1\text{-}\ A_{>}^{-})$$

$$\kappa^{(2)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)+\alpha^{(1)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)+\beta^{(1)}(A)\delta^{(1)}\left(A_{>}^{-}\right)+\beta^{(2)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_{34}}{2Z_{12}}\right)^{3}}, \quad (30\text{-}2\text{-}\ A_{>}^{-})$$

$$\kappa^{(3)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)+\alpha^{(1)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)+\beta^{(2)}(A)\delta^{(1)}\left(A_{>}^{-}\right)+\beta^{(3)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_{34}}{2Z_{12}}\right)^{4}}, \quad (30\text{-}3\text{-}\ A_{>}^{-})$$

$$\kappa^{(4)}\left(A_{>}^{-}\right)=\frac{\alpha^{(1)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)+\beta^{(3)}(A)\delta^{(1)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_{34}}{2Z_{12}}\right)^{5}}, \quad (30\text{-}4\text{-}\ A_{>}^{-})$$

$$\kappa^{(0)}\left(A_{\le}^{-}\right)=\frac{\alpha^{(0)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)+\beta^{(0)}(A)\delta^{(0)}\left(A_{\le}^{-}\right)}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}+1\right)}, \quad (30\text{-}0\text{-}\ A_{>}^{-})$$

$$\kappa^{(1)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}+1\right)}\left(\frac{\alpha^{(0)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)+\beta^{(1)}(A)\delta^{(0)}\left(A_{\le}^{-}\right)}{\frac{2Z_{12}}{Z_{34}}+1}+\frac{\alpha^{(1)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)+\beta^{(0)}(A)\delta^{(1)}\left(A_{\le}^{-}\right)}{1+\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}1\text{-}\ A_{\le}^{-})$$

$$\kappa^{(2)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}+1\right)^{2}}\left(\frac{\alpha^{(0)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)+\beta^{(2)}(A)\delta^{(0)}\left(A_{\le}^{-}\right)}{\frac{2Z_{12}}{Z_{34}}+1}+\frac{\alpha^{(1)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)+\beta^{(1)}(A)\delta^{(1)}\left(A_{\le}^{-}\right)}{1+\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}2\text{-}\ A_{\le}^{-})$$

$$\kappa^{(3)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}+1\right)^{3}}\left(\frac{\alpha^{(0)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)+\beta^{(3)}(A)\delta^{(0)}\left(A_{\le}^{-}\right)}{\frac{2Z_{12}}{Z_{34}}+1}+\frac{\alpha^{(1)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)+\beta^{(2)}(A)\delta^{(1)}\left(A_{\le}^{-}\right)}{1+\frac{Z_{34}}{2Z_{12}}}\right), \quad (30\text{-}3\text{-}\ A_{\le}^{-})$$

$$\kappa^{(4)}\left(A_{\le}^{-}\right)=\frac{\alpha^{(1)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)+\beta^{(3)}(A)\delta^{(1)}\left(A_{\le}^{-}\right)}{Z_{34}\left(\frac{2Z_{12}}{Z_{34}}+1\right)^{4}\left(1+\frac{Z_{34}}{2Z_{12}}\right)} \quad (30\text{-}4\text{-}\ A_{\le}^{-})$$

and

$$F_{12-5}(A)=\int_0^{(2Z_{12}-Z_5)A}dx\begin{pmatrix}\mu^{(0)}\left(A_>^+\right)\exp(-x)+\mu^{(1)}\left(A_>^+\right)x\exp(-x)+\mu^{(2)}\left(A_>^+\right)x^2\exp(-x)+\\ \mu^{(3)}\left(A_>^+\right)x^3\exp(-x)+\mu^{(4)}\left(A_>^+\right)x^4\exp(-x)+\nu^{(0)}\left(A_>^+\right)\exp(+x)+\nu^{(1)}\left(A_>^+\right)x\exp(+x)+\nu^{(2)}\left(A_>^+\right)x^2\exp(+x)+\\ \nu^{(3)}\left(A_>^+\right)x^3\exp(+x)+\nu^{(4)}\left(A_>^+\right)x^4\exp(+x)\end{pmatrix}+$$

$$\int_0^{(2Z_{12}+Z_5)A}dx\begin{pmatrix}\mu^{(0)}\left(A_>^-\right)\exp(-x)+\mu^{(1)}\left(A_>^-\right)x\exp(-x)+\mu^{(2)}\left(A_>^-\right)x^2\exp(-x)+\\ \mu^{(3)}\left(A_>^-\right)x^3\exp(-x)+\mu^{(4)}\left(A_>^-\right)x^4\exp(-x)\end{pmatrix}+ \quad ,\ (31)$$

$$\int_{(2Z_{12}+Z_5)A}^{\infty}dx\left(\mu^{(0)}\left(A_\leq^-\right)\exp(-x)+\mu^{(1)}\left(A_\leq^-\right)x\exp(-x)+\mu^{(2)}\left(A_\leq^-\right)x^2\exp(-x)+\mu^{(3)}\left(A_\leq^-\right)x^3\exp(-x)+\mu^{(4)}\left(A_\leq^-\right)x^4\exp(-x)\right)$$

$$\mu^{(0)}\left(A_>^+\right)=\frac{\alpha^{(0)}(A)\zeta^{(0)}\left(A_>^+\right)}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)}, \quad (31\text{-}0\text{-}\ A_>^+)$$

$$\mu^{(1)}\left(A_>^+\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)}\left(\frac{\alpha^{(0)}(A)\zeta^{(1)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_5}-1}+\frac{\alpha^{(1)}(A)\zeta^{(0)}\left(A_>^+\right)}{1-\frac{Z_5}{2Z_{12}}}\right), \quad (31\text{-}1\text{-}\ A_>^+)$$

$$\mu^{(2)}\left(A_>^+\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)^2}\left(\frac{\alpha^{(0)}(A)\zeta^{(2)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_5}-1}+\frac{\alpha^{(1)}(A)\zeta^{(1)}\left(A_>^+\right)}{1-\frac{Z_5}{2Z_{12}}}\right), \quad (31\text{-}2\text{-}\ A_>^+)$$

$$\mu^{(3)}\left(A_>^+\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)^3}\left(\frac{\alpha^{(0)}(A)\zeta^{(3)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_5}-1}+\frac{\alpha^{(1)}(A)\zeta^{(2)}\left(A_>^+\right)}{1-\frac{Z_5}{2Z_{12}}}\right), \quad (31\text{-}3\text{-}\ A_>^+)$$

$$\mu^{(4)}\left(A_>^+\right)=\frac{\alpha^{(1)}(A)\zeta^{(3)}\left(A_>^+\right)}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)^4\left(1-\frac{Z_5}{2Z_{12}}\right)}, \quad (31\text{-}4\text{-}\ A_>^+)$$

$$\nu^{(0)}\left(A_>^+\right)=\frac{\gamma^{(0)}(A)\delta^{(0)}\left(A_>^+\right)}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)}, \quad (31\text{-}0'\text{-}\ A_>^+)$$

$$\nu^{(1)}\left(A_>^+\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)}\left(\frac{\gamma^{(1)}(A)\delta^{(0)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_5}-1}+\frac{\gamma^{(0)}(A)\delta^{(1)}\left(A_>^+\right)}{1-\frac{Z_5}{2Z_{12}}}\right), \quad (31\text{-}1'\text{-}\ A_>^+)$$

$$\nu^{(2)}\left(A_>^+\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)^2}\left(\frac{\gamma^{(2)}(A)\delta^{(0)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_5}-1}+\frac{\gamma^{(1)}(A)\delta^{(1)}\left(A_>^+\right)}{1-\frac{Z_5}{2Z_{12}}}\right), \quad (31\text{-}2'\text{-}\ A_>^+)$$

$$\nu^{(3)}\left(A_>^+\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)^3}\left(\frac{\gamma^{(3)}(A)\delta^{(0)}\left(A_>^+\right)}{\frac{2Z_{12}}{Z_5}-1}+\frac{\gamma^{(2)}(A)\delta^{(1)}\left(A_>^+\right)}{1-\frac{Z_5}{2Z_{12}}}\right), \quad (31\text{-}3'\text{-}\ A_>^+)$$

$$\nu^{(4)}\left(A_{>}^{+}\right)=\frac{\gamma^{(3)}(A)\delta^{(1)}\left(A_{>}^{+}\right)}{Z_5\left(\frac{2Z_{12}}{Z_5}-1\right)^4\left(1-\frac{Z_{34}}{2Z_{12}}\right)}, \qquad (31\text{-}4'\text{-}\ A_{>}^{+})$$

$$\mu^{(0)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)+\gamma^{(0)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_5}{2Z_{12}}\right)}, \qquad (31\text{-}0\text{-}\ A_{>}^{-})$$

$$\mu^{(1)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\alpha^{(1)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)+\gamma^{(0)}(A)\delta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_5}{2Z_{12}}\right)^2}, \qquad (31\text{-}1\text{-}\ A_{>}^{-})$$

$$\mu^{(2)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\alpha^{(1)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\delta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_5}{2Z_{12}}\right)^3}, \qquad (31\text{-}2\text{-}\ A_{>}^{-})$$

$$\mu^{(3)}\left(A_{>}^{-}\right)=\frac{\alpha^{(0)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\alpha^{(1)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\delta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\delta^{(0)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_5}{2Z_{12}}\right)^4}, \qquad (31\text{-}3\text{-}\ A_{>}^{-})$$

$$\mu^{(4)}\left(A_{>}^{-}\right)=\frac{\alpha^{(1)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\delta^{(1)}\left(A_{>}^{-}\right)}{2Z_{12}\left(1+\frac{Z_5}{2Z_{12}}\right)^5}, \qquad (31\text{-}4\text{-}\ A_{>}^{-})$$

$$\mu^{(0)}\left(A_{\leq}^{-}\right)=\frac{\alpha^{(0)}(A)\zeta^{(0)}\left(A_{\leq}^{-}\right)+\gamma^{(0)}(A)\delta^{(0)}\left(A_{\leq}^{-}\right)}{Z_5\left(\frac{2Z_{12}}{Z_5}+1\right)}, \qquad (31\text{-}0\text{-}\ A_{\leq}^{-})$$

$$\mu^{(1)}\left(A_{\leq}^{-}\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}+1\right)}\left(\frac{\alpha^{(0)}(A)\zeta^{(1)}\left(A_{\leq}^{-}\right)+\gamma^{(1)}(A)\delta^{(0)}\left(A_{\leq}^{-}\right)}{\frac{2Z_{12}}{Z_5}+1}+\frac{\alpha^{(1)}(A)\zeta^{(0)}\left(A_{\leq}^{-}\right)+\gamma^{(0)}(A)\delta^{(1)}\left(A_{\leq}^{-}\right)}{1+\frac{Z_5}{2Z_{12}}}\right), \qquad (31\text{-}1\text{-}\ A_{\leq}^{-})$$

$$\mu^{(2)}\left(A_{\leq}^{-}\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}+1\right)^2}\left(\frac{\alpha^{(0)}(A)\zeta^{(2)}\left(A_{\leq}^{-}\right)+\gamma^{(2)}(A)\delta^{(0)}\left(A_{\leq}^{-}\right)}{\frac{2Z_{12}}{Z_5}+1}+\frac{\alpha^{(1)}(A)\zeta^{(1)}\left(A_{\leq}^{-}\right)+\gamma^{(1)}(A)\delta^{(1)}\left(A_{\leq}^{-}\right)}{1+\frac{Z_5}{2Z_{12}}}\right), \qquad (31\text{-}2\text{-}\ A_{\leq}^{-})$$

$$\mu^{(3)}\left(A_{\leq}^{-}\right)=\frac{1}{Z_5\left(\frac{2Z_{12}}{Z_5}+1\right)^3}\left(\frac{\alpha^{(0)}(A)\zeta^{(3)}\left(A_{\leq}^{-}\right)+\gamma^{(3)}(A)\delta^{(0)}\left(A_{\leq}^{-}\right)}{\frac{2Z_{12}}{Z_5}+1}+\frac{\alpha^{(1)}(A)\zeta^{(2)}\left(A_{\leq}^{-}\right)+\gamma^{(2)}(A)\delta^{(1)}\left(A_{\leq}^{-}\right)}{1+\frac{Z_5}{2Z_{12}}}\right), \qquad (31\text{-}3\text{-}\ A_{\leq}^{-})$$

$$\mu^{(4)}\left(A_{\leq}^{-}\right)=\frac{\alpha^{(1)}(A)\zeta^{(3)}\left(A_{\leq}^{-}\right)+\gamma^{(3)}(A)\delta^{(1)}\left(A_{\leq}^{-}\right)}{Z_5\left(\frac{2Z_{12}}{Z_5}+1\right)^4\left(1+\frac{Z_5}{2Z_{12}}\right)}; \qquad (31\text{-}4\text{-}\ A_{\leq}^{-})$$

and

$$F_{34-5}(A)=\int_0^{(Z_{34}-Z_5)A}dx\begin{pmatrix}\xi^{(0)}(A_>^+)\exp(-x)+\xi^{(1)}(A_>^+)x\exp(-x)+\xi^{(2)}(A_>^+)x^2\exp(-x)+\xi^{(3)}(A_>^+)x^3\exp(-x)+\\ \xi^{(4)}(A_>^+)x^4\exp(-x)+\xi^{(5)}(A_>^+)x^5\exp(-x)+\xi^{(6)}(A_>^+)x^6\exp(-x)+o^{(0)}(A_>^+)\exp(+x)+o^{(1)}(A_>^+)x\exp(+x)+\\ o^{(2)}(A_>^+)x^2\exp(+x)+o^{(3)}(A_>^+)x^3\exp(+x)+o^{(4)}(A_>^+)x^4\exp(+x)+o^{(5)}(A_>^+)x^5\exp(+x)+o^{(6)}(A_>^+)x^6\exp(+x)\end{pmatrix}+$$

$$\int_0^{(Z_{34}+Z_5)A}dx\begin{pmatrix}\xi^{(0)}(A_>^-)\exp(-x)+\xi^{(1)}(A_>^-)x\exp(-x)+\xi^{(2)}(A_>^-)x^2\exp(-x)+\xi^{(3)}(A_>^-)x^3\exp(-x)+\\ \xi^{(4)}(A_>^-)x^4\exp(-x)+\xi^{(5)}(A_>^-)x^5\exp(-x)+\xi^{(6)}(A_>^-)x^6\exp(-x)\end{pmatrix}+$$

$$+\int_{(Z_{34}+Z_5)A}^{\infty}dx\begin{pmatrix}\xi^{(0)}(A_\le^-)\exp(-x)+\xi^{(1)}(A_\le^-)x\exp(-x)+\xi^{(2)}(A_\le^-)x^2\exp(-x)+\xi^{(3)}(A_\le^-)x^3\exp(-x)+\\ \xi^{(4)}(A_\le^-)x^4\exp(-x)+\xi^{(5)}(A_\le^-)x^5\exp(-x)+\xi^{(6)}(A_\le^-)x^6\exp(-x)\end{pmatrix},\quad (32)$$

$$\xi^{(0)}(A_>^+)=\frac{\beta^{(0)}(A)\zeta^{(0)}(A_>^+)}{Z_{34}-Z_5},\quad (32\text{-}0\text{-}A_>^+)$$

$$\xi^{(1)}(A_>^+)=\frac{1}{Z_{34}-Z_5}\left(\frac{\beta^{(0)}(A)\zeta^{(1)}(A_>^+)}{\frac{Z_{34}}{Z_5}-1}+\frac{\beta^{(1)}(A)\zeta^{(0)}(A_>^+)}{1-\frac{Z_5}{Z_{34}}}\right),\quad (32\text{-}1\text{-}A_>^+)$$

$$\xi^{(2)}(A_>^+)=\frac{1}{Z_{34}-Z_5}\left(\frac{\beta^{(0)}(A)\zeta^{(2)}(A_>^+)}{\left(\frac{Z_{34}}{Z_5}-1\right)^2}+\frac{\beta^{(1)}(A)\zeta^{(1)}(A_>^+)}{\left(\frac{Z_{34}}{Z_5}-1\right)\left(1-\frac{Z_5}{Z_{34}}\right)}+\frac{\beta^{(2)}(A)\zeta^{(0)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^2}\right),\quad (32\text{-}2\text{-}A_>^+)$$

$$\xi^{(3)}(A_>^+)=\frac{1}{Z_{34}-Z_5}\left(\frac{\beta^{(0)}(A)\zeta^{(3)}(A_>^+)}{\left(\frac{Z_{34}}{Z_5}-1\right)^3}+\frac{\beta^{(1)}(A)\zeta^{(2)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)\left(\frac{Z_{34}}{Z_5}-1\right)^2}+\frac{\beta^{(2)}(A)\zeta^{(1)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^2\left(\frac{Z_{34}}{Z_5}-1\right)}+\frac{\beta^{(3)}(A)\zeta^{(0)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^3}\right),\quad (32\text{-}3\text{-}A_>^+)$$

$$\xi^{(4)}(A_>^+)=\frac{1}{Z_{34}-Z_5}\left(\frac{\beta^{(1)}(A)\zeta^{(3)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)\left(\frac{Z_{34}}{Z_5}-1\right)^3}+\frac{\beta^{(2)}(A)\zeta^{(2)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^2\left(\frac{Z_{34}}{Z_5}-1\right)^2}+\frac{\beta^{(3)}(A)\zeta^{(1)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^3\left(\frac{Z_{34}}{Z_5}-1\right)}\right),\quad (32\text{-}4\text{-}A_>^+)$$

$$\xi^{(5)}(A_>^+)=\frac{1}{Z_{34}-Z_5}\left(\frac{\beta^{(2)}(A)\zeta^{(3)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^2\left(\frac{Z_{34}}{Z_5}-1\right)^3}+\frac{\beta^{(3)}(A)\zeta^{(2)}(A_>^+)}{\left(1-\frac{Z_5}{Z_{34}}\right)^3\left(\frac{Z_{34}}{Z_5}-1\right)^2}\right),\quad (32\text{-}5\text{-}A_>^+)$$

$$\xi^{(6)}(A_>^+)=\frac{\beta^{(3)}(A)\zeta^{(3)}(A_>^+)}{(Z_{34}-Z_5)\left(1-\frac{Z_5}{Z_{34}}\right)^3\left(\frac{Z_{34}}{Z_5}-1\right)^3},\quad (32\text{-}6\text{-}A_>^+)$$

$$o^{(0)}(A_>^+)=\frac{\gamma^{(0)}(A)\varepsilon^{(0)}(A_>^+)}{Z_{34}-Z_5},\quad (32\text{-}0'\text{-}A_>^+)$$

$$o^{(1)}(A_>^+)=\frac{1}{Z_{34}-Z_5}\left(\frac{\gamma^{(0)}(A)\varepsilon^{(1)}(A_>^+)}{1-\frac{Z_5}{Z_{34}}}+\frac{\gamma^{(1)}(A)\varepsilon^{(0)}(A_>^+)}{\frac{Z_{34}}{Z_5}-1}\right),\quad (32\text{-}1'\text{-}A_>^+)$$

$$o^{(2)}\left(A_{>}^{+}\right)=\frac{1}{Z_{34}-Z_{5}}\left(\frac{\gamma^{(0)}(A)\varepsilon^{(2)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{2}}+\frac{\gamma^{(1)}(A)\varepsilon^{(1)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)\left(\frac{Z_{34}}{Z_5}-1\right)}+\frac{\gamma^{(2)}(A)\varepsilon^{(0)}\left(A_{>}^{+}\right)}{\left(\frac{Z_{34}}{Z_5}-1\right)^{2}}\right), \qquad (32\text{-}2'\text{-}\ A_{>}^{+})$$

$$o^{(3)}\left(A_{>}^{+}\right)=\frac{1}{Z_{34}-Z_{5}}\left(\frac{\gamma^{(0)}(A)\varepsilon^{(3)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{3}}+\frac{\gamma^{(1)}(A)\varepsilon^{(2)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{2}\left(\frac{Z_{34}}{Z_5}-1\right)}+\frac{\gamma^{(2)}(A)\varepsilon^{(1)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)\left(\frac{Z_{34}}{Z_5}-1\right)^{2}}+\frac{\gamma^{(3)}(A)\varepsilon^{(0)}\left(A_{>}^{+}\right)}{\left(\frac{Z_{34}}{Z_5}-1\right)^{3}}\right), \qquad (32\text{-}3'\text{-}\ A_{>}^{+})$$

$$o^{(4)}\left(A_{>}^{+}\right)=\frac{1}{Z_{34}-Z_{5}}\left(\frac{\gamma^{(1)}(A)\varepsilon^{(3)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{3}\left(\frac{Z_{34}}{Z_5}-1\right)}+\frac{\gamma^{(2)}(A)\varepsilon^{(2)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{2}\left(\frac{Z_{34}}{Z_5}-1\right)^{2}}+\frac{\gamma^{(3)}(A)\varepsilon^{(1)}}{\left(1-\frac{Z_5}{Z_{34}}\right)\left(\frac{Z_{34}}{Z_5}-1\right)^{3}}\left(A_{>}^{+}\right)\right), \qquad (32\text{-}4'\text{-}\ A_{>}^{+})$$

$$o^{(5)}\left(A_{>}^{+}\right)=\frac{1}{Z_{34}-Z_{5}}\left(\frac{\gamma^{(2)}(A)\varepsilon^{(3)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{3}\left(\frac{Z_{34}}{Z_5}-1\right)^{2}}+\frac{\gamma^{(3)}(A)\varepsilon^{(2)}\left(A_{>}^{+}\right)}{\left(1-\frac{Z_5}{Z_{34}}\right)^{2}\left(\frac{Z_{34}}{Z_5}-1\right)^{3}}\right), \qquad (32\text{-}5'\text{-}\ A_{>}^{+})$$

$$o^{(6)}\left(A_{>}^{+}\right)=\frac{\gamma^{(3)}(A)\varepsilon^{(3)}\left(A_{>}^{+}\right)}{(Z_{34}-Z_{5})\left(1-\frac{Z_5}{Z_{34}}\right)^{3}\left(\frac{Z_{34}}{Z_5}-1\right)^{3}}, \qquad (32\text{-}6'\text{-}\ A_{>}^{+})$$

$$\xi^{(0)}\left(A_{>}^{-}\right)=\frac{\beta^{(0)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)}{Z_{34}+Z_{5}}, \qquad (32\text{-}0\text{-}\ A_{>}^{-})$$

$$\xi^{(1)}\left(A_{>}^{-}\right)=\frac{1}{Z_{34}+Z_{5}}\left(\frac{\beta^{(0)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)}{\frac{Z_{34}}{Z_5}+1}+\frac{\beta^{(1)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)}{1+\frac{Z_5}{Z_{34}}}\right), \qquad (32\text{-}1\text{-}\ A_{>}^{-})$$

$$\xi^{(2)}\left(A_{>}^{-}\right)=\frac{1}{Z_{34}+Z_{5}}\left(\frac{\beta^{(0)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^{2}}+\frac{\beta^{(1)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)\left(1+\frac{Z_5}{Z_{34}}\right)}+\frac{\beta^{(2)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{2}}\right), \qquad (32\text{-}2\text{-}\ A_{>}^{-})$$

$$\xi^{(3)}\left(A_{>}^{-}\right)=\frac{1}{Z_{34}+Z_{5}}\left(\frac{\beta^{(0)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(0)}\left(A_{>}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^{3}}+\frac{\beta^{(1)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^{2}\left(1+\frac{Z_5}{Z_{34}}\right)}+\frac{\beta^{(2)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{2}\left(\frac{Z_{34}}{Z_5}+1\right)}+\frac{\beta^{(3)}(A)\zeta^{(0)}\left(A_{>}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{3}}\right), \qquad (32\text{-}3\text{-}\ A_{>}^{-})$$

$$\xi^{(4)}\left(A_{>}^{-}\right)=\frac{1}{Z_{34}+Z_{5}}\left(\frac{\beta^{(1)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(1)}\left(A_{>}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^{3}\left(1+\frac{Z_5}{Z_{34}}\right)}+\frac{\beta^{(2)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{2}\left(\frac{Z_{34}}{Z_5}+1\right)^{2}}+\frac{\beta^{(3)}(A)\zeta^{(1)}\left(A_{>}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{3}\left(\frac{Z_{34}}{Z_5}+1\right)}\right), \qquad (32\text{-}4\text{-}\ A_{>}^{-})$$

$$\xi^{(5)}\left(A_{>}^{-}\right)=\frac{1}{Z_{34}+Z_{5}}\left(\frac{\beta^{(2)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(2)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{2}\left(\frac{Z_{34}}{Z_5}+1\right)^{3}}+\frac{\beta^{(3)}(A)\zeta^{(2)}\left(A_{>}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^{3}\left(\frac{Z_{34}}{Z_5}+1\right)^{2}}\right), \qquad (32\text{-}5\text{-}\ A_{>}^{-})$$

$$\xi^{(6)}\left(A_{>}^{-}\right)=\frac{\beta^{(3)}(A)\zeta^{(3)}\left(A_{>}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(3)}\left(A_{>}^{-}\right)}{(Z_{34}+Z_5)\left(1+\frac{Z_5}{Z_{34}}\right)^3\left(\frac{Z_{34}}{Z_5}+1\right)^3}, \quad (32\text{-}6\text{-}A_{>}^{-})$$

$$\xi^{(0)}\left(A_{\le}^{-}\right)=\frac{\beta^{(0)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{Z_{34}+Z_5}, \quad (32\text{-}0\text{-}A_{\le}^{-})$$

$$\xi^{(1)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}+Z_5}\left(\frac{\beta^{(0)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{\frac{Z_{34}}{Z_5}+1}+\frac{\beta^{(1)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)}{1+\frac{Z_5}{Z_{34}}}\right), \quad (32\text{-}1\text{-}A_{\le}^{-})$$

$$\xi^{(2)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}+Z_5}\left(\frac{\beta^{(0)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^2}+\frac{\beta^{(1)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)\left(\frac{Z_{34}}{Z_5}+1\right)}+\frac{\beta^{(2)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^2}\right), \quad (32\text{-}2\text{-}A_{\le}^{-})$$

$$\xi^{(3)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}+Z_5}\left(\frac{\beta^{(0)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(0)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^3}+\frac{\beta^{(1)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^2\left(1+\frac{Z_5}{Z_{34}}\right)}+\frac{\beta^{(2)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)\left(1+\frac{Z_5}{Z_{34}}\right)^2}+\frac{\beta^{(3)}(A)\zeta^{(0)}\left(A_{\le}^{-}\right)+\gamma^{(0)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)}{\left(1+\frac{Z_5}{Z_{34}}\right)^3}\right), \quad (32\text{-}3\text{-}A_{\le}^{-})$$

$$\xi^{(4)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}+Z_5}\left(\frac{\beta^{(1)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(1)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^3\left(1+\frac{Z_5}{Z_{34}}\right)}+\frac{\beta^{(2)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^2\left(1+\frac{Z_5}{Z_{34}}\right)^2}+\frac{\beta^{(3)}(A)\zeta^{(1)}\left(A_{\le}^{-}\right)+\gamma^{(1)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)\left(1+\frac{Z_5}{Z_{34}}\right)^3}\right), \quad (32\text{-}4\text{-}A_{\le}^{-})$$

$$\xi^{(5)}\left(A_{\le}^{-}\right)=\frac{1}{Z_{34}+Z_5}\left(\frac{\beta^{(2)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(2)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^3\left(1+\frac{Z_5}{Z_{34}}\right)^2}+\frac{\beta^{(3)}(A)\zeta^{(2)}\left(A_{\le}^{-}\right)+\gamma^{(2)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)}{\left(\frac{Z_{34}}{Z_5}+1\right)^2\left(1+\frac{Z_5}{Z_{34}}\right)^3}\right), \quad (32\text{-}5\text{-}A_{\le}^{-})$$

$$\xi^{(6)}\left(A_{\le}^{-}\right)=\frac{\beta^{(3)}(A)\zeta^{(3)}\left(A_{\le}^{-}\right)+\gamma^{(3)}(A)\varepsilon^{(3)}\left(A_{\le}^{-}\right)}{(Z_{34}+Z_5)\left(\frac{Z_{34}}{Z_5}+1\right)^3\left(1+\frac{Z_5}{Z_{34}}\right)^3}. \quad (32\text{-}6\text{-}A_{\le}^{-})$$

Instead of Conclusions

Further development

In the paper, the initial stage of the semiclassical construction of the interaction potential between two boron atoms is described.

Making intermediate conclusions, it can be noted that the desired potential function can be expressed as a linear combination.

$$u\left(Z_{12},Z_{34},Z_5;a\right)=\sum_{n=0}^{n=6}\sum_{\pm}C_n^{(\pm)}(Z_{12},Z_{34},Z_5;a)I_n^{(\pm)}(Z_{12},Z_{34},Z_5;a), \quad (33)$$

of exponential integrals

$$I_n^{(\pm)}(Z_{12},Z_{34},Z_5;a)=\int_{c_0(Z_{12},Z_{34},Z_5)a}^{c_\infty(Z_{12},Z_{34},Z_5)a}dx\,x^n\exp(\pm x), \quad (34)$$

where n is an integer from 0 to 6, $C_n^{(\pm)}(Z_{12}, Z_{34}, Z_5; a)$ are the coefficients of linear expansion, and $c_0(Z_{12}, Z_{34}, Z_5)$ and $c_\infty(Z_{12}, Z_{34}, Z_5)$ are the proportionality coefficients depending on the effective charge numbers of the electronic orbitals in the B atom. Since these integrals can be found in elementary functions, the semiclassical B–B interatomic potential function $u = u(a)$ will be found in an analytical form, allowing in this way *ab initio* determination of key ground state parameters of the diboron B_2 molecule, such as the equilibrium bond length, the dissociation energy and its correction due to the relative vibrations of the atoms.

Corresponding stage finalizing the construction of the semiclassical B–B potential will be given in the next paper.

Thus, it can be concluded that the proposed semiclassical theoretical approach is capable of providing the *ab initio* boron–boron interatomic potential function in an analytical form that is very useful for studying the ground state parameters of all boron-rich bound atomic systems: molecules, clusters, nanostructures, crystals, amorphous materials, and liquids.

References

1. Chkhartishvili L. Quasi-Classical Theory of Substance Ground State. Tbilisi: Publishing House "Technical University". in Russian. 2004;258.
2. Chkhartishvili L, Berberashvili T. Intra-atomic electric field radial potentials in step-like presentation. J Electromagn Anal Appl. 2010;2(4): 205-243. https://doi.org/10.4236/jemaa.2010.24029
3. Chkhartishvili L, Berberashvili T. Again on effective electrical charge of atomic nuclei. Nano Studies 2013;8:267-272.
4. Chkhartishvili L, Lezhava D, Tsagareishvili O. Quasi-classical determination of electronic energies and vibration frequencies in boron compounds. J Solid State Chem. 2000;154(1):148-152. https://doi.org/10.1006/jssc.2000.8826
5. Chkhartishvili L. On quasi-classical estimations of boron nanotubes' ground-state parameters. J Phys Conf Ser. 2009;176:012013. https://doi.org/10.1088/1742-6596/176/1/012013
6. Chkhartishvili L, Murusidze I, Darchiashvili M, Tsagareishvili O, Gabunia D. Metal impurities in crystallographic voids of beta-rhombohedral boron lattice: Binding energies and electron levels. Solid State Sci. 2012;14(11/12):1673-1682. https://doi.org/10.1016/j.solidstatesciences.2012.06.009
7. Sartinska L, Chkhartishvili L, Voynich E, Eren T, Frolov G, Altay E, Murusidze I, Tsagareishvili O, Gabunia D, Maisuradze N. Effect of concentrated light on morphology and vibrational properties of boron and tantalum mixtures. Heliyon. 2018 Mar 26;4(3):e00585. doi: 10.1016/j.heliyon.2018.e00585. PMID: 29862348; PMCID: PMC5968138.
8. Chkhartishvili L, Murusidze I, Becker R. Electronic structure of boron flat holeless sheet. Condensed Matter 2019;4 (1): 28. https://doi.org/10.3390/condmat4010028
9. Chkhartishvili L. How to calculate condensed matter electronic structure based on a multi-electron atom semi-classical model. Condensed Matter. 2021;6(4):46. https://doi.org/10.3390/condmat6040046
10. Chkhartishvili L. Relative Stability of Boron Planar Clusters in Diatomic Molecular Model. Molecules. 2022 Feb 22;27(5):1469. doi: 10.3390/molecules27051469. PMID: 35268570; PMCID: PMC8911741.
11. Chkhartishvili, L. Construction of semiclassical interatomic B–B pair potential to characterize all-boron nanomaterials. Character Appl Nanomater. 2023; 6 (1): 1852. https://doi.org/10.24294/can.v6i1.1852
12. Al-Raeei M. A formula of Tietz potential parameters and applying for scandium iodine, nitrogen iodine, rubidium hydride, nitrogen, and carbon monoxide molecules. Canadian J Phys. 2023;101(4):151-202. https://doi.org/10.1139/cjp-2022-0250
13. Abu-Shady M, Khokha EM. A precise estimation for vibrational energies of diatomic molecules using the improved Rosen-Morse potential. Sci Rep. 2023 Jul 18;13(1):11578. doi: 10.1038/s41598-023-37888-2. PMID: 37463934; PMCID: PMC10354199.
14. Kang D, Fan Q, Fan Zh, Li H, Fu J. Extended improved multiparameter exponential-type potential energy function for diatomic molecules. Int J Quant Chem. 2024; 124 (8): e27373. https://doi.org/10.1002/qua.27373
15. Pirkola P, Horbatsch M. Calculation of DC Stark Resonances for the Ammonia Molecule. Molecules. 2024 Mar 29;29(7):543. doi: 10.3390/molecules29071543. PMID: 38611822; PMCID: PMC11013917.
16. Liu L, Wei Z, Chen Q, Shen C, Shen T, Tian X, Li SD. Benchmarking boron cluster calculations: Establishing reliable geometrical and energetic references for B_n (n = 1-4). J Comput Chem. 2024 Jan 30;45(3):159-169. doi: 10.1002/jcc.27226. Epub 2023 Sep 12. PMID: 37698288.
17. Poluektov YuM. Diatomic model of a quantum crystal. Low Temp Phys. 2008;34(4/5):368-376. https://doi.org/10.1063/1.2911644
18. De Virgiliis A, Meyra A, Ciach A. Lattice Model Results for Pattern Formation in a Mixture with Competing Interactions. Molecules. 2024 Mar 28;29(7):1512. doi: 10.3390/molecules29071512. PMID: 38611792; PMCID: PMC11013164.
19. Durandurdu M. Liquid boron and amorphous boron: An ab initio molecular dynamics study. J Non-Cryst Solids. 2015; 417/418:10-14. https://dx.doi.org/10.1016/j.jnoncrysol.2015.03.004
20. Jalolov FN, Podryabinkin EV, Oganov AR, Shapeev AV, Kvashnin AG. Mechanical properties of single and polycrystalline solids from machine learning. Adv Theory Simul. 2024;7(5):2301171. https://doi.org/10.1002/adts.202301171

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