Calculation of the nonrelativistic Bethe logarithm in the velocity gauge

V. I. Korobov
Joint Institute for Nuclear Research, 141980 Dubna, Russia
(Received 8 March 2012; published 20 April 2012)

We consider a general procedure to evaluate the Bethe logarithm for a general few-body atomic or molecular system. As benchmarks we use calculations for the ground states of a helium atom and a H$_2^+$ molecular ion. The obtained values are $\beta_{\text{He}} = 4.37016022306(2)$ for the helium atom and $\beta_{\text{H}_2^+} = 3.012230335(1)$ for the H$_2^+$ molecular ion. Both results substantially improve the best-known values for these quantities.

DOI: 10.1103/PhysRevA.85.042514  PACS number(s): 31.30.jf, 31.15.xt

I. INTRODUCTION

It is known that in the leading-order radiative contribution to the binding energy of atomic or molecular systems the most complicated quantity for numerical evaluation is the Bethe logarithm [1]. One of the most accurate results for the helium ground state was obtained by Schwartz [2] in 1961 and it remained the best one for over 30 years. In 1999, Drake and Goldman [3] suggested another way to evaluate the Bethe logarithm, $\beta(n, L)$, for a helium atom, which is based on another representation of $\beta(n, L)$ in terms of the acceleration gauge dipole operators and a full diagonalization of the Hamiltonian. This method works well for two- and three-electron helium- and lithium-like atoms [4] but attempts to apply it to other systems like H$_2^+$ molecular ions have not been very successful. The other disadvantage of the method is a necessity to add some extra terms to a basis set, which looks like $1/r$ times the regular solution.

The major aim of the present work is to present a universal method, which uses the definition of the Bethe logarithm in terms of dipole operators in the velocity gauge and still is as efficient as the Goldman-Drake method [3] in the case of hydrogen- and helium-like atoms. In fact, we have tried to carefully reanalyze the ideas of Ref. [2] and to present them in a more explicit and general form. The numerical results are confined to three-body systems while the theoretical expressions are valid for a general few-body case.

The paper is organized as follows. In Sec. II we consider a derivation of the leading-order radiative corrections that allows us to define the Bethe logarithm for a general few-body Coulomb system as an integral over photon energy $k$. Next the asymptotic behavior of the core integrand, $J(k) = \langle J(E_0 - H - k) \rangle$, and its first order perturbation wave function, $\psi_1(k)$, are derived; the leading-order terms are obtained as expectation values of some operators. A variational property of the integral over $k$ is discussed. It allows us to work out an efficient numerical scheme to calculate the Bethe logarithm using optimal parameters, which are variationally chosen.

In Sec. III the numerical method, which is the main goal of our studies, is describe in detail. And finally, the results of the Bethe logarithm calculation for the hydrogen, helium, and H$_2^+$ molecular ion ground states are presented and compared with other available results. We use atomic units ($\hbar = \varepsilon = m_p = 1$) throughout unless something else is explicitly stated.

II. THEORETICAL OVERVIEW

A. Radiative correction: Low-energy contribution

Let us first consider a case of a hydrogen-like atom. The $\alpha(Za)^2 E_m$ order low-energy contribution, which results from the nonrelativistic QED diagram [see Fig. 1(a)], may be written as

$$E_L = \frac{\alpha^3}{4\pi^2 m^2} \int |k| < \Lambda \frac{d^3 k}{k} \left( g^{ij} - \frac{k^i k^j}{k^2} \right) \times \langle \psi_0 | \rho \left( \frac{1}{E_0 - H - k} \right) p^j | \psi_0 \rangle - \delta m \langle \psi_0 | \psi_0 \rangle, \quad (1)$$

where the last term is the “mass renormalization” contribution. Averaging the integrand over angular variables one gets

$$E_L = \frac{2 \alpha^3}{3 \pi m^2} \int_0^\Lambda kd k \left( \frac{1}{E_0 - H - k} \right) - \delta m \langle \psi_0 | \psi_0 \rangle. \quad (2)$$

The integrand may be rewritten using the following operator identity,

$$(E_0 - H - k)^{-1} = -1/k - \frac{1}{k^2} (E_0 - H) + \frac{1}{k^2} \frac{(E_0 - H)^2}{E_0 - H - k},$$

which results in

$$E_L = \frac{2 \alpha^3}{3 \pi m^2} \left[ -(\langle p^2 \rangle \Lambda + \langle p[H, p] \rangle \ln \Lambda \right. \right.$$

$$\left. \left. + \int \frac{dk}{k} \left( \frac{(E_0 - H)^2}{E_0 - H - k} p \right) \right] - \delta m \langle \psi_0 | \psi_0 \rangle. \quad (3)$$

As was shown by Bethe in 1947 [5], the linearly divergent term should be associated with the mass renormalization of an electron and should be subtracted with the last term in expression (3). Thus, the remaining part may be split into a finite nonlogarithmic contribution,

$$E_L^{(0)} = \frac{2 \alpha^3}{3 \pi m^2} \int_0^E kd k \left( \frac{1}{E_0 - H - k} + \frac{1}{k} \right) p \right)$$

$$+ \frac{2 \alpha^3}{3 \pi m^2} \int_{E_0}^{\infty} kd k \left( \frac{1}{E_0 - H - k} \right) p \right), \quad (4a)$$
and a divergent part,

$$E^{(1)}_L = \frac{2e^3}{3\pi m^2} \left( \int_{E_h}^{\Lambda} \frac{dk}{k} \right) \langle p|H,p] = \frac{e^3}{3\pi} \ln \frac{\Lambda}{E_h} 4\pi Z(r),$$

(4b)

which results in the appearance of the logarithmic term; the cutoff parameter is later canceled out by the logarithmic contribution from the high-energy part. Here $E_h$ is the Hartree energy.

The high-energy part is obtained from the one-loop scattering amplitude for an electron in an external field [6]:

$$M_1 = \frac{\alpha}{2\pi} \left[ 2 \left( \ln \frac{m}{\lambda_{\min}} - 1 \right) - \frac{2\theta}{\tan 2\theta} + \theta \tan \theta + \frac{4}{\tan 2\theta} \int_0^\theta \alpha \tan \alpha \, d\alpha \, a_r\gamma^r + \alpha \frac{2\pi}{m} q_{\mu} a_{\nu} \Sigma_{\mu\nu} \left\{ \frac{2\theta}{\sin 2\theta} + r a_r \gamma^r \right\},$$

(5)

where $\Sigma_{\mu\nu} = (\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})/(2i)$, $r = \ln(\lambda/m) + 9/4 - 2\ln(m/\lambda_{\min})$, and $q^2 = 4m^2 \sin^2 \theta$. Here amplitude is expressed in the natural relativistic units ($c = 1$).

At small $q$, the scattering amplitude may be expanded:

$$M_1 \approx \frac{\alpha}{\pi} \left[ -\frac{1}{8m^2} + \frac{1}{3m^2} \ln \frac{m}{\lambda_{\min}} a_r \gamma^r q^2 + \frac{i}{4m} q_{\mu} a_{\nu} \Sigma_{\mu\nu} \right] + \frac{\alpha}{\pi} \left[ -\frac{11204m^4}{240m^4} + \frac{1016m^2}{50\lambda_{\min}} a_r \gamma^r q^4 + \frac{i}{24m} q_{\mu} a_{\nu} \Sigma_{\mu\nu} q^2 \right].$$

In order to get this expression, $\ln m/\lambda_{\min}$ should be replaced by $[\ln m/(2\lambda) + 5/6]$ [6]. Using the NRQED formalism this renormalization has been derived in Ref. [7].

The leading-order contribution for a static scalar field with renormalization to a new infrared regularization parameter $\lambda$, which is a cutoff of virtual quanta of momentum less than $\lambda$, ($\lambda = \alpha \Lambda$), is expressed as

$$M^{(0)}_1 = -\frac{\alpha}{2\pi} \left[ \frac{q^2}{3m^2} \left( \ln \frac{m}{2\lambda} + \frac{5}{6} - \frac{3}{8} \right) a_0 + \frac{1}{2\pi} \left( -\frac{q^2}{4} + \frac{i\pi}{2} + \frac{\pi}{2} \right) a_0 \right],$$

(6)

In the coordinate space and atomic units the energy displacement due to the respective interaction is expressed in NRQED by

$$\Delta E_H = \frac{\alpha^3}{3\pi m^2} \left[ \ln a^2 + \ln \frac{\Lambda}{E_h} + \ln 2 - \frac{5}{6} \right] \langle \Delta V \rangle - \frac{\alpha^2 m^2}{2\pi} \left( -\frac{r \times p}{r^3} + \frac{\sigma}{2} \right).$$

(7)

Summing up the low-energy contribution (II A) and the high-energy contribution (7), which comes from modification of the interaction of electrons with a static field due to the one-loop self-energy diagram [Fig. 1(a)], one gets

$$\Delta E_{SE} = \frac{\alpha^3}{3\pi m^2} \left[ \ln a^2 + \ln 2 + \beta(n,l) - \frac{5}{6} \right] \langle \Delta V \rangle - \frac{\alpha^3}{2\pi m^2} \left( \frac{r \times p}{r^3} + \frac{\sigma}{2} \right).$$

(8)

where $\beta(n,l)$ is the so-called Bethe logarithm; it accumulates the contribution from Eq. (4a) and is formally defined later in Eq. (11). The cutoff parameter $\Lambda$ cancels out.

When both particles have finite masses one needs to include the retardation. The $\alpha(Za)^2(m/M)E_{ma}$ order low-energy contribution [Fig. 1(b)] may be written as

$$E^{ret}_{L}(a,b) = \frac{\alpha^3}{(4\pi)^2} \int_{k<\Lambda} \frac{dk}{k} \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \langle \phi|p_{h^i} \frac{1}{m_a} \left( E_0 - k - H_0 + \frac{1}{k} \right) p_{h^j} \phi \rangle.$$  

(9)

(9)

(here $m_a$ and $m_b$ are masses of the two particles). The last term in the inner round brackets, $1/k$, corresponds to the retardation interaction as it appears in the Breit-Pauli approximation (and is of order $(Za)^2(m/M)E_{ma}$) and should be subtracted from the initial NRQED expression to avoid double counting. Consideration of the high-energy contribution ($k > \Lambda$), which comes from the same diagram, may be found in Ref. [8].

Summing up the contributions to the Bethe logarithm from Eqs. (4a) and (9) one finds that the dipole operator on the right-hand sides of the angle brackets may be recast as a nonrelativistic electric current density operator,

$$J = \sum_i \frac{z_i}{m_i} \mathbf{P}_i,$$

(10)

as may be expected, since in QED a virtual photon interacts with a current density. For a general many-particle system the above speculations may be repeated directly in order to get the nonlogarithmic part of the low-energy contribution.

FIG. 1. NRQED diagrams for the self-energy and retarded transverse photon at ultralow energies.
In summary, the Bethe logarithm may be defined as follows:
\[ N(L,v) = \int_0^{E_k} dk \left[ \frac{1}{E_0 - H - k} + \frac{1}{k} \right] J \]
and the next iteration would be
\[ \psi_1^{(1)} = -\frac{i}{k} J \psi_0 + \frac{1}{k^2} [H,iJ] \psi_0. \]

The key quantity for our numerical studies is
\[ D(L,v) = \langle J[H,J]\rangle = \frac{\langle [J[J,H,J]]\rangle}{2}. \]

And the Bethe logarithm itself is a ratio of these two quantities:
\[ \beta(L,v) = \frac{N}{D}. \]

B. First-order perturbation wave function, \( \psi_1(\cdot) \), and asymptotic expansion of \( J(k) \) at \( k \to \infty \)

Knowing this function one immediately gets a value for the nonrelativistic Bethe logarithm using Eq. (11).

A general procedure to calculate \( J(k) \) is to solve the equation
\[ (E_0 - H - k)\psi_1 = iJ\psi_0 \]
for different values of \( k \). Since we are interested in the asymptotic behavior of \( J(k) \) for \( k \to \infty \), it is assumed that \( k \) is sufficiently large and as a first approximation one may take
\[ \psi_1^{(0)} = -(i/k)J\psi_0. \]

Any approximate solution for \( \psi_1 \) may be (formally) iteratively improved:
\[ \psi_1^{(n)} = -\frac{i}{k} J \psi_0 + \frac{1}{k}(E_0 - H)\psi_1^{(n-1)}, \]

and the next iteration would be
\[ \psi_1^{(1)} = -\frac{i}{k} J \psi_0 + \frac{1}{k^2} [H,iJ] \psi_0, \]

where
\[ [H,iJ] = \sum_{i>j} z_i z_j \left( \frac{z_j}{m_j} - \frac{z_i}{m_i} \right) r_{ij}, \quad r_{ij} = r_j - r_i. \]

At small \( r_{ij} \), \( \psi_j \) should be smooth. In order to get a proper behavior, one has to consider Eq. (13) for \( r_{ij} \to 0 \) and keep only the important terms
\[ \frac{1}{2m_{rij}} \Delta_{ij} - k)\psi_1(r_{ij},\cdot) = 0, \]

which gives homogeneous solutions of the type
\[ \sim \frac{r_{ij}}{\rho_{ij}} e^{-\mu_{ij} r_{ij}} (1 + \mu_{ij} r_{ij}), \]

with \( \mu_{ij} = \sqrt{2m_{ij}} k \). These solutions, taken for different pairs of particles, may be added to \( \psi_1^{(1)} \) to make the whole wave function smooth. So, we come to an approximation of \( \psi_1 \) for \( k \to \infty \), which is of the required quality for our goals and has the following form:
\[ \psi_1^{(1)} = -\frac{i}{k} J \psi_0(\cdot) + \frac{1}{k^2} \sum_{i>j} z_i z_j \left( \frac{z_j}{m_j} - \frac{z_i}{m_i} \right) r_{ij} \]
\[ \times \left[ 1 - e^{-\mu_{ij} r_{ij}} (1 + \mu_{ij} r_{ij}) \right] \psi_0(\cdot). \]

As is seen from this equation, there is no singular term in the wave function corresponding to a pair of identical particles.

Integrand \( J(k) \) may be evaluated using the variational formalism as a stationary solution of a functional on \( \psi_1 \):
\[ J(k) = -2 \langle \psi_0|J|\psi_1 \rangle - \langle \psi_1(E_0 - H - k)\psi_1 \rangle. \]

To get asymptotic expansion we substitute \( \psi_1^{(1)} \) into this functional. A derivation of the asymptotic expansion for the hydrogen ground state and comparison with known analytical results may be found in Appendix A.

At small \( r_{ij} \) we get
\[ J_{\rho_-} = -\langle \psi_1^{(1)}(E_0 - H - k)\psi_1^{(1)} \rangle_{\rho_-} = -\frac{1}{k^3} \sum_{i>j} z_i^2 z_j^2 \left( \frac{z_i}{m_i} - \frac{z_j}{m_j} \right)^2 \]
\[ \times \left[ \sqrt{2m_{ij} k} + z_i z_j m_{ij} (\ln(m_{ij} k) - \ln 2 + 2\gamma_k + 2\ln \rho) \right] 4\pi \langle \delta(r_{ij}) \rangle + \cdots, \]

where \( \rho_- \) means integration from 0 to \( \rho \). We assume that \( \rho \) satisfies \( 1/\mu_{ij} \ll \rho \ll 1 \).

For regular \( r_{ij} \) we use \( \psi_1^{(1)} \) in the form
\[ \psi_1^{(1)} = -\frac{i}{k} J \psi_0 + \frac{1}{k^2} [H,iJ] \psi_0. \]

Then
\[ -2\langle \psi_0|J|\psi_1^{(1)} \rangle = -\frac{2}{k} \langle J \psi_0 \rangle - \frac{2}{k^2} \langle [iJ,[H,iJ]] \rangle \]

and
\[ -\langle \psi_1^{(1)}(E_0 - H - k)\psi_1^{(1)} \rangle_{\rho_-} = k\langle \psi_1^{(1)}|\psi_1^{(1)} \rangle_{\rho_-} - \langle \psi_1^{(1)}(E_0 - H)\psi_1^{(1)} \rangle_{\rho_-} \]
\[ = \frac{1}{k} \langle J \psi_0 \rangle + \frac{1}{k^2} \langle [iJ,[H,iJ]] \rangle \}
\[ - \frac{1}{k^3} \left[ \langle [H,iJ]^2 \rangle_{\rho_-} - \sum_{i>j} z_i^2 z_j^2 m_{ij} 4\pi \langle \delta(r_{ij}) \rangle \right]. \]
That results in
\[
\hat{J}_{\mu} = -\frac{1}{k} \left( \hat{J}^2 - \frac{1}{k^2} \left[ (i [J, [H, J]]) \right] \right) - \frac{1}{k^3} \left[ \left( [J, [H, J]] \right)_{\rho\nu} - \sum_{i>j} \frac{z_i^2 z_j^2 m_{ij}}{\rho_{ij}} 4\pi \delta(\mathbf{r}_{ij}) \right] + \ldots .
\] (19b)

Now we have to introduce a finite functional, which should replace a divergent expectation value of the 1/r^4 operator:
\[
\mathcal{R} = \lim_{\rho \to 0} \left\{ \frac{1}{4\pi r^4} \left[ \frac{1}{\rho} \delta(\mathbf{r}) \right] + \ln \rho + \gamma_E \right\}(\delta(\mathbf{r}))
\]
where
\[
\langle \phi_1 | \delta(\mathbf{r}) | \phi_2 \rangle = \langle \phi_1 | \nabla \delta(\mathbf{r}) | \phi_2 \rangle = - \langle \delta, \phi_1 | \delta(\mathbf{r}) | \phi_2 \rangle - \langle \phi_1 | \delta(\mathbf{r}) | \partial_1 \phi_2 \rangle.
\]

Then summing up Eqs. (19a) and (19b) one gets
\[
J(k) = -\frac{1}{k} \left( \hat{J}^2 - \frac{1}{k^2} \left[ (i [J, [H, J]]) \right] \right) - \frac{1}{k^3} \sum_{i>j} z_i z_j z_k \left( \frac{z_i}{m_i} - \frac{z_j}{m_j} \right) \left( \frac{z_k}{m_k} - \frac{z_l}{m_l} \right) r_{ij} r_{kl}/r_{ij} r_{kl}^2
\]
\[- \frac{1}{k^3} \sum_{i>j} z_i^2 z_j^2 \left( \frac{z_i}{m_i} - \frac{z_j}{m_j} \right)^2 \left( 4\pi \mathcal{R}_{ij} + \sqrt{2m_{ij}} k + z_i z_j m_{ij} (\ln(m_{ij}) - \ln 2 - 1) \right) \delta(\mathbf{r}_{ij}) \right] + \ldots
\] (21)

For mixed terms, (r_{ij} r_{kl})/(r_{ij} r_{kl})^2, in the case of a three-body calculation with the Hylleraas or exponential basis functions (see Refs. [3,9]) a new type of singular integral is required:
\[
\Gamma_{2,-2,a}(\alpha, \beta, \gamma) = \frac{1}{2} \int r_1 \cdots r_2 \cdots r_2 e^{-\gamma r_1 r_2} dr_1 dr_2.
\]

A derivation of the explicit form for \(\Gamma_{2,-2,0}\) and stable recursions to get integrals for arbitrary n are presented in Appendix B.

C. Variational property

If we consider the quantity
\[
\mathcal{J}_\Lambda = \int_0^\Lambda k dk J(k)
\]
\[
= \sum_n \left| \langle \psi_n | J | \psi_n \rangle \right|^2 \left( \Lambda - (E_0 - E_n) \ln \left| \frac{E_0 - E_n}{E_0 - E_n - \Lambda} \right| \right),
\]
we would find that for the ground state of a system this quantity possesses the variational property, since for the integrand for all k the following inequality is fulfilled:
\[
\mathcal{J}_{\text{exact}}(k) \geq \mathcal{J}_{\text{numerical}}(k).
\]

The same property remains satisfied for other states if integration is performed from some \(k_0 \sim 1\), which lies above the poles related to the states \(E_n < E_0\). It is known from the practical calculations that the low k contribution becomes numerically converged to a high accuracy at a moderate basis length of intermediate states, and thus with a good confidence the variational property (the higher the value of \(\mathcal{J}_\Lambda\), the more accurate solution) still remains in force. That allows us to perform optimization of the variational parameters of the basis set.

III. NUMERICAL RESULTS

A. Numerical scheme

Here we consider the numerical scheme for the three-body Coulomb problem, which is then used in calculations of the Bethe logarithm for the helium and \(H_3^+\) ground states. The wave functions both for the initial bound state and for the first-order perturbation solution (or intermediate state) are taken in the form
\[
\Psi_L(l_1, l_2) = \sum_{i=1}^{\infty} \left( U_i \Re[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r}] + W_i \Im[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r}] \right) Y_{LM}^{\alpha \beta} (\mathbf{r}_1, \mathbf{r}_2),
\] (23)

where \(Y_{LM}^{\alpha \beta} (\mathbf{r}_1, \mathbf{r}_2)\) are the solid bipolar harmonics as defined in Ref. [10] and L is the total orbital angular momentum of a state. Complex parameters \(\alpha_i, \beta_i, \gamma_i\) are generated in a quasirandom manner [9]:
\[
\alpha_i = \left[ -\left[ \frac{1}{2} i (i + 1) \sqrt{\rho} \right] (A_2 - A_1) + A_1 \right]
+ i \left[ \frac{1}{2} i (i + 1) \sqrt{\rho} \right] (A_2' - A_1') + A_1',
\] (24)

TABLE I. Convergence of the Bethe logarithm for the ground state of hydrogen and comparison with results of Drake and Goldman [3].

| N       | \(\beta\)   | \(\beta\)   | N       |
|---------|-------------|-------------|---------|
| 40      | 2.984 128 555 765 49\(\beta\) | 2.984 128 49\(\beta\) | 45      |
| 60      | 2.984 128 555 765 49\(\beta\) | 2.984 128 555 1\(\beta\) | 66      |
| 80      | 2.984 128 555 765 49\(\beta\) | 2.984 128 555 75\(\beta\) | 91      |
| 100     | 2.984 128 555 765 49\(\beta\) | 2.984 128 555 76\(\beta\) | 120     |

Exact \(2.984 \times 10^5 \times 75 697 610 759 777 000 2\)
Bethe logarithm for the ground state of hydrogen for \( \tau \) the initial state with regular values of parameters (26).

\[
\int_{E_0}^{\infty} dk \left( \frac{1}{E_0 - H - k} + \frac{1}{k} \right) \int_{E_n}^{\infty} \frac{dk}{k} \left( \frac{(E_0 - H)^2}{E_0 - H - k} \right)
\]  

(27)

From the thus obtained \( J(k) \) we extrapolate coefficients of asymptotic expansion:

\[
f_{\text{fit}}(k) = \sum_{m=1}^{M} C_{1m} \sqrt{k} + C_{2m} \ln k + C_{3m},
\]

(28)

which are taken in the same form as in the analytic expression for the hydrogen atom [see Appendix A, Eq. (A2)]. A similar asymptotic expansion has been used in Ref. [11]. The leading-order terms of \( J(k) \) are obtained from Eq. (21). That allows us to obtain the high-energy part of the numerator:

\[
\int_{\Lambda}^{\infty} \frac{dk}{k} \left( \frac{(E_0 - H)^2}{E_0 - H - k} \right)
\]

B. Results

As the first example to demonstrate the capabilities of our method we take the ground state of a hydrogen atom. The results of the numerical calculations are summarized in Table I. The basis set used for these calculations is a sum of exponentials with real parameters generated in a quasirandom way; the initial wave function is taken as exact. In Fig. 2 an excerpt of the listing of output with the parameters of the basis set for the case of \( N = 100 \) functions is shown. “Exact” in Table II is the value obtain by Huff’s method [12], which is a series expansion. It is interesting to note that if the Huff series is taken with 100 terms only the result would be of the same accuracy as in our approach for \( N = 100 \). As is seen from Table I the new method demonstrates better accuracy than in Ref. [3], especially for small \( N \), and a good convergence rate. It is worth to noting that variational parameters were roughly optimized for \( N = 80 \) and kept the same for all other cases.

The main results of our studies are presented in Tables II and III. Table II contains the Bethe logarithm calculations for the ground state of helium and Table III contains the Bethe logarithm calculations for the ground state of the \( H_2^+ \) molecular ion. Convergence is analyzed in two dimensions, with respect to the number of basis functions of the initial state and similarly for the basis size of the intermediate state. The major conclusion is that for ultimate precision it is important to check how the studied quantity depends on the accuracy of the initial state. Indeed, it is reasonable to expect that the

| \( N_a \) | 3000 | 3500 | 4000 | \( \infty \) |
|---------|------|------|------|------|
| 4000    | 4.370 160 223 11 | 4.370 160 223 01 | 4.370 160 223 021 |
| 5000    | 4.370 160 223 14 | 4.370 160 223 03 | 4.370 160 223 044 |
| 6000    | 4.370 160 223 04 | 4.370 160 223 058 |
| \( \infty \) | 4.370 160 223 06(2) | 4.370 160 223 08(2) |
fractional error in the Bethe logarithm evaluation would be no better than the square root of the fractional uncertainty in the variational energy of the initial state, like in the behavior of the expectation values of, say, the $\delta$ function or $p^1$ operators.

Comparing our results for the ground state of helium with those of Ref. [13] based on the Goldman-Drake method (see Table IV) we see a discrepancy which requires an explanation. This puzzle was a serious challenge for us, since the study of stability had been achieved. So, we came back to our old calculations, which were based on the Goldman-Drake approach, and it was found that some essential part in the intermediate state wave function had been missed. If we add a new set of “regular” basis functions with exponentials having parameters $\alpha$ and $\beta$ (in front of $r_1$ and $r_2$, respectively) up to 40(!), then the numerical result becomes $\beta = 4.370 \pm 0.00249948$ for the case of the initial $N = 1400$ state used in Ref. [13]. That showed a good coincidence with our “velocity gauge” result for the same initial state, as it might be expected.

For convenience of comparison with other calculations we present here explicitly the asymptotic expansion of $J(k)$ ($k \rightarrow \infty$) for the helium ground state:

$$J(k) + \frac{1}{k} \langle F^1 \rangle = \frac{4\pi}{k^2} \left\{ \frac{Z}{2} - \frac{Z^2}{2k} - \frac{Z^3}{3k} \ln k + 20.00249948 + \frac{80.3063}{k^2} - \frac{70.989}{k} + 136.5 \cdots \right\}. \qquad (29)$$

The numerical coefficient in the first line was calculated using Eq. (21). Coefficients shown in the second line were obtained by a linear least-squares fit using the SVD algorithm [16]. The fitting interval was $k \in [20, 6000]$; the number of data points was 100, which were taken equidistant on the logarithmic scale of $k$; and the number of terms in the asymptotic expansion is 14–18. The results of the fitting procedure are not sensitive to the number of data points.

Similarly, the asymptotic expansion of $J(k)$ for the ground state of a $H_2^+$ molecular ion is

$$J(k) + \frac{1}{k} \langle F^1 \rangle = 2\pi \left[ Z_1 \langle \delta(r_1) \rangle + Z_2 \langle \delta(r_2) \rangle \right] - \left( \frac{1}{m_e} + Z_1 M_1 \right) \left[ Z_1^2 \frac{\sqrt{2} \mu_k}{k} - Z_1 \mu_1 \ln \mu_1 k \right] \frac{4\pi}{k^3} \langle \delta(r_1) \rangle$$

$$- \left( \frac{1}{m_e} + Z_2 M_2 \right) \left[ Z_2^2 \frac{\sqrt{2} \mu_k}{k} - Z_2 \mu_2 \ln \mu_2 k \right] \frac{4\pi}{k^3} \langle \delta(r_2) \rangle$$

$$- 2\pi \left[ Z_1 \langle \delta(r_1) \rangle + Z_2 \langle \delta(r_2) \rangle \right] \left\{ \frac{2.247 \times 10^8}{k^3} + \frac{10.052 \sqrt{k} - 4.4}{k^4} + \frac{2.2}{k^4} \cdots \right\}, \qquad (30)$$

where $\mu = m_e M_1/(m_e + M_1)$ is the reduced mass of a respective proton of mass $M_1$. Since $\langle \delta(r_{12}) \rangle < 10^{-10}$, the term

| $N_b \backslash N_a$ | 3000          | 4000          | 5000          | $\infty$          |
|------------------|---------------|---------------|---------------|-------------------|
| 7000             | 3.012 230 340 7 | 3.012 230 333 4 | 3.012 230 334 1 | 3.012 230 334 1   |
| 8000             | 3.012 230 343 1 | 3.012 230 335 7 | 3.012 230 334 1 | 3.012 230 334 9   |
| 9000             | 3.012 230 344 2 | 3.012 230 336 7 | 3.012 230 334 9 | 3.012 230 335(1)  |

which is related to a nucleus-nucleus part (say, for the HD$^+$ case) may be neglected.

One additional remark on the $H_2^+$ molecular ion is needed. Analyzing our new results for the Bethe logarithm we found that they have a systematic shift compared to the ones of Ref. [17]. This is because the formula for asymptotic expansion used in previous calculations [see Ref. [18], Eq. (12)] does not incorporate reduced masses into the leading terms of the expansion. This shift is almost state independent and ( for both $H_2^+$ [17] and HD$^+$ [18]) is of about 15 in the last two digits indicated in the tables of Refs. [17,18] and should be subtracted. A new systematic calculation of the Bethe logarithm for the hydrogen molecular ions, which should...
provide better accuracy of about 8–9 significant digits, is in progress now.

ACKNOWLEDGMENTS

The author thanks K. Pachucki, V. A. Yerokhin, L. Hilico, and J.-Ph. Karr for helpful discussions. Comments on the manuscript by Z.-X. Zhong are greatly appreciated. The work was supported in part by the Russian Foundation for Basic Research, Grant No. 12-02-00417-a. The author also acknowledges the support of the Chinese Academy of Science (CAS) during his stay at WIPM, the Wuhan Branch of the CAS.

APPENDIX A: ASYMPTOTIC EXPANSION OF J(k): HYDROGEN GROUND STATE

Here the Hamiltonian and the charge current density operator are expressed as

\[ H = -\nabla^2 \frac{Z}{r}, \quad iJ = -\nabla. \]

The following commutations are helpful for our derivation:

\[ [H, \nabla] = -Z \frac{r}{r^3}, \quad [\nabla, [H, \nabla]] = -4\pi Z \langle \delta(r) \rangle. \]

We substitute the wave function \( \psi_1^{(1)}(r) = \frac{1}{k} \nabla \psi_0(r) - \frac{1}{k^2} [H, \nabla][1 - e^{-\mu r}(1 + \mu r)] \psi_0(r) = -\frac{Z}{k} \psi_0(r) + \frac{Z^2 r}{k^2 r^2} [1 - e^{-\mu r}(1 + \mu r)] \psi_0(r), \]

where \( \psi_0 = 2Z^{3/2} e^{-Zr} \) is the ground-state wave function and \( \mu = \sqrt{2k} \), into the variational functional

\[ J(k) = -2 \langle \psi_0 | \nabla | \psi_1 \rangle - \langle \psi_1 (E_0 - H - k) \psi_1 \rangle. \]

For \( r < \rho (\rho \to 0, \text{ and } \mu \rho \gg 0) \), one gets

\[ J_{\rho <} = 4\pi \langle \delta(r) \rangle Z^{-3} \left[ - \frac{Z^5 \sqrt{2k}}{k^3} + \frac{Z^6 (\ln k - \ln 2 + 1)}{k^3} + \frac{2Z^6 (\gamma_E + \ln \rho)}{k^3} \right] \]

For \( r > \rho \), one gets

\[ J_{\rho >} = \frac{1}{k} \langle \nabla^2 \rangle - \frac{1}{k^2} \left( \frac{\langle [\nabla, [H, \nabla]] \rangle}{2} - \frac{1}{k^3} \left[ (\langle H, \nabla \rangle^2 \rangle_{\rho <} - \frac{Z^2}{\rho} \langle \delta(r) \rangle \right] = -\frac{Z^2}{k} + \frac{2Z^4}{k^2} - \frac{8Z^6 [\gamma_E + \ln(2Z\rho)]}{k^3} + \ldots. \]

Summing up, we obtain the leading terms of the asymptotic expansion:

\[ J(k) = \frac{1}{k} \langle \nabla^2 \rangle - \frac{1}{k^2} \left( \frac{\langle [\nabla, [H, \nabla]] \rangle}{2} - \frac{1}{k^3} \left[ (\langle H, \nabla \rangle^2 \rangle_{\rho <} - \frac{Z^2}{\rho} \langle \delta(r) \rangle \right] \right] \]

\[ + \left[ - \frac{Z^5 \sqrt{2k}}{k^3} + \frac{Z^6 (\ln k - \ln 2 + 1)}{k^3} + \frac{2Z^6 (\gamma_E + \ln \rho)}{k^3} \right] Z^{-3} 4\pi \langle \delta(r) \rangle \]

\[ = -\frac{Z^2}{k} + \frac{2Z^4}{k^2} - \frac{4Z^5 \sqrt{2k}}{k^3} + \frac{4Z^6 (\ln k - \ln Z^2)}{k^3} - \frac{4Z^6 (3 \ln 2 - 1)}{k^4} + \ldots, \quad (A1) \]

which is exact up to the free term in the \( 1/k^3 \) order as it may be checked from comparison with the analytical expression known for this case [19] (\( Z = 1 \)):

\[ J(k) = -384 \frac{\tau^5}{(1 + \tau)^4 (2 - \tau)} \, _2F_1(4,2 - \tau,3 - \tau; \xi) \]

\[ = -\frac{1}{k} + \frac{2}{k^2} \left( \frac{4\sqrt{2k}}{k^3} + \frac{4\ln k - 12 \ln 2 + 4}{k^3} + \frac{(21 + 2\tau^2)\sqrt{2k}}{3k^4} - \frac{8 \ln k - 24 \ln 2 + 14 + 2\psi''(2)}{k^4} \right) + \ldots, \quad (A2) \]

where \( \tau = Z/\sqrt{-2(E_0 - k)} \) and \( \xi = [(1 - \tau)/(1 + \tau)]^2. \)
APPENDIX B: $\Gamma_{-2,-2,n}(\alpha,\beta,\gamma)$

In this appendix we show how to evaluate the integral

$$\Gamma_{-2,-2,n}(\alpha,\beta,\gamma) = \frac{1}{2} \int \int r_1^{-2} r_2^{-2} e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}} \, dr_1 dr_2 dr_{12}$$

by means of

$$\Gamma_{-2,-2,n}(\alpha,\beta,\gamma) = \left(-\frac{\partial}{\partial \gamma}\right)^n \Gamma_{-2,-2,0}(\alpha,\beta,\gamma).$$

To do this we have to obtain an analytical expression for $\Gamma_{-2,-2,0}(\alpha,\beta,\gamma)$. Let us consider

$$\Gamma_{-2,-2,0}(\alpha,\beta,\gamma) = \frac{1}{2} \int_0^{\infty} dr_1 e^{-\alpha r_1} \left[ \int_0^{r_1} e^{-\beta r_2} \int_0^{r_1+r_2} e^{-\gamma r_{12}} dr_{12} dr_{12} + \int_0^{r_1} dr_2 e^{-\beta r_2} \int_0^{r_1} e^{-\gamma r_{12}} dr_{12} \right]$$

which is divergent and in order to get some meaningful finite expression one has to introduce some counterterm similar to those in Eq. (B1). So we may choose it in the following form:

$$\int \int \frac{e^{-\alpha \gamma r_{12}}}{r_1^2} \int_0^{r_1} e^{-\beta r_2} dr_2 \int_0^{r_1+r_2} e^{-\gamma r_{12}} dr_{12} + \int_0^{r_1} e^{-\beta r_2} \int_0^{r_1} e^{-\gamma r_{12}} dr_{12}$$

To get some meaningful finite expression one has to introduce some counterterm similar to those in Eq. (B1). So we may choose it in the following form:

$$\frac{1}{2}\int_0^{\infty} dr_1 e^{-\alpha r_1} \left[ \int_0^{r_1} e^{-\beta r_2} dr_2 \int_0^{r_1+r_2} e^{-\gamma r_{12}} dr_{12} + \int_0^{r_1} e^{-\beta r_2} \int_0^{r_1} e^{-\gamma r_{12}} dr_{12} \right]$$

Here we use the notation from Ref. [20]:

$$L_\rho(x,\epsilon) = \int_0^{\infty} e^{-\frac{x t}{\rho}} \frac{dt}{t^{p-1}} \Gamma(1-p, x \epsilon), \quad L_1(x, \epsilon) = \psi(1) - \ln(x\epsilon), \quad L_2(x, \epsilon) = \frac{1}{\epsilon} - x [\psi(2) - \ln(x\epsilon)] - \frac{x^2 \epsilon}{2},$$

$$I_\rho(x, y, \epsilon) = \int_0^{\infty} e^{-\frac{x t}{\rho}} E_1(y t) \frac{dt}{t^{p-1}}, \quad I_1(x, y, \epsilon) = \frac{e^{-x \rho} E_1(y \rho)}{(p-1)\rho^{p-1}} - \frac{x}{p-1} I_{\rho-1}(x, y) - \frac{1}{p-1} L_\rho(x + y, \epsilon),$$

$$I_1(x, y, \epsilon) = \frac{1}{2} \left( \ln \epsilon + \ln y + \gamma_E \right)^2 - \frac{\pi^2}{12} - \frac{1}{2} \ln \frac{y}{x} - \text{dilog} \left( 1 + \frac{y}{x} \right).$$

In expressions above $\psi(n)$ is a digamma function: $\psi(1) = -\gamma_E, \psi(n+1) = \psi(n) + 1/n$.

The integral is divergent and in order to get some meaningful finite expression one has to introduce some counterterm similar to what was done for the functional $R$ in Eq. (20). Still for our purposes it is not needed, since we will be using $\Gamma_{-2,-2,0}$ only for evaluation of finite integrals and, thus, any form of $\Gamma_{-2,-2,0}$, which is self-consistent with other $\Gamma_{lnn}(\alpha,\beta,\gamma)$ via differentiation relations like Eq. (B2), would be sufficient. So we may choose it in the following form:

$$\Gamma_{-2,-2,0}(\alpha,\beta,\gamma) = \left( 3 - 2\gamma_E - \frac{\pi^2}{12} \right) \gamma - (\alpha + \beta) - \frac{\alpha + \gamma}{2} [2 - \gamma_E - \ln(\alpha + \gamma)]^2 - \frac{\beta + \gamma}{2} [2 - \gamma_E - \ln(\beta + \gamma)]^2$$

$$+ (\alpha + \beta) \ln(\alpha + \beta) - (\alpha + \gamma) \ln(\alpha + \gamma) - (\beta + \gamma) \ln(\beta + \gamma) + \frac{(\alpha + \gamma)(\beta + \gamma)}{4\gamma} \ln^2 \left( \frac{\alpha + \gamma}{\beta + \gamma} \right)$$

$$+ \frac{\alpha \beta \pi^2}{12 \gamma} + \frac{(\alpha - \gamma)(\beta + \gamma)}{2\gamma} \text{dilog} \left( \frac{\alpha + \beta}{\alpha + \gamma} \right) + \frac{(\beta - \gamma)(\alpha + \gamma)}{2\gamma} \text{dilog} \left( \frac{\alpha + \beta}{\alpha + \gamma} \right).$$

Evaluation of $\Gamma_{-2,-2,n}$ is straightforward (see Ref. [21] for details) except for two terms, which require additional remarks. We introduce two recursions:

$$A_n = \left(-\frac{\partial}{\partial \gamma}\right)^n \left[ \frac{1}{\gamma} \text{dilog} \left( \frac{\alpha + \beta}{\alpha + \gamma} \right) \right] = \frac{1}{\gamma} [n A_{n-1} + B_n], \quad B_n = \left(-\frac{\partial}{\partial \gamma}\right)^n \left[ \ln^2 \left( \frac{\alpha + \gamma}{\beta + \gamma} \right) \right].$$

and

$$E_n = \left(-\frac{\partial}{\partial \gamma}\right)^n \left[ \frac{1}{\gamma} \ln^2 \left( \frac{\alpha + \gamma}{\beta + \gamma} \right) \right] = \frac{1}{\gamma} [n E_{n-1} + F_n], \quad F_n = \left(-\frac{\partial}{\partial \gamma}\right)^n \left[ \ln^2 \left( \frac{\alpha + \gamma}{\beta + \gamma} \right) \right].$$

At first glance these recursions are not stable when $\gamma$ is small. However, more careful analysis shows that, for example, $A_{n-1}$ and $B_n$ (as well as $E_{n-1}$ and $F_n$) are of the same sign, and no subtraction, which leads to loss of numerical accuracy, occurs.
[1] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1977).

[2] C. Schwartz, *Phys. Rev.* **123**, 1700 (1961).

[3] G. W. F. Drake and S. P. Goldman, *Can. J. Phys.* **77**, 835 (1999).

[4] Z.-C. Yan and G. W. F. Drake, *Phys. Rev. Lett.* **91**, 113004 (2003); Z.-C. Yan, W. Nörtershäuser, and G. W. F. Drake, *ibid.* **100**, 243002 (2008).

[5] H. A. Bethe, *Phys. Rev.* **72**, 339 (1947).

[6] R. P. Feynman, *Phys. Rev.* **76**, 769 (1949).

[7] T. Kinoshita and M. Nio, *Phys. Rev. D* **53**, 4909 (1996).

[8] K. Pachucki, *J. Phys. B* **31**, 3547 (1998).

[9] V. I. Korobov, *Phys. Rev. A* **61**, 064503 (2000).

[10] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific, Singapore, 1988).

[11] K. Pachucki and V. A. Yerokhin, *Phys. Rev. A* **79**, 062516 (2009).

[12] R. W. Huff, *Phys. Rev.* **186**, 1367 (1969).

[13] V. I. Korobov, *Phys. Rev. A* **69**, 054501 (2004).

[14] V. I. Korobov and S. V. Korobov, *Phys. Rev. A* **59**, 3394 (1999).

[15] J. D. Baker, R. C. Forrey, M. Jerzierska, and J. D. Morgan III (unpublished).

[16] C. L. Lawson and R. J. Hanson, *Solving Least Squares Problems* (Prentice-Hall, New Jersey, 1974).

[17] V. I. Korobov, *Phys. Rev. A* **73**, 024502 (2006).

[18] V. I. Korobov, *Phys. Rev. A* **70**, 012505 (2004).

[19] M. Gavrila and A. Costescu, *Phys. Rev. A* **2**, 1752 (1970); K. Pachucki, *Ann. Phys. (NY)* **226**, 1 (1993).

[20] F. E. Harris, A. M. Frolov, and V. H. Smith Jr., *J. Chem. Phys.* **121**, 6323 (2004).

[21] V. I. Korobov, *J. Phys. B* **35**, 1959 (2002).