Bethe logarithm for the helium atom

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The Bethe logarithm is a contribution to the leading order radiative corrections for the atomic or molecular system, which comes mainly from the nonrelativistic energy region for the exchange photons and is defined in terms of the nonrelativistic quantum mechanics [1]. The numerical computation of this quantity for systems more complicated than the hydrogen atom was one of the most challenging problems in atomic physics for a very long time [2–7].

Recently, a new efficient method for calculation of a logarithm of the mean excitation energy (Bethe logarithm) has been suggested in Ref. [8]. It was based on a direct matrix diagonalization of the Hamiltonian with the dipole matrix elements expressed in the “acceleration” gauge. A key point of the approach is that the basis set is extended to include a wide range of distance scales.

The aim of this work is to perform an independent calculation based on these ideas but with a different basis set, in order to show the universality of the basic ideas of Ref. [8] and high efficiency of the exponential variational expansion as applied to this problem.

I. VARIATIONAL APPROXIMATION FOR INITIAL AND INTERMEDIATE STATES

In this work we restrict ourselves to the case of the helium atom with infinite nuclear mass, ^4He. Coordinates of two electrons are \( r_1 \) and \( r_2 \), respectively, and the distance between electrons is denoted by \( r \).

The wave functions both for initial bound states and for the second-order perturbation solutions (or intermediate states) are taken in the form,

\[
\Psi_{\lambda}(l_1, l_2) = \sum_{i=1}^{\infty} (U_i \text{Re}[e^{-\alpha_i r - \beta_i r^2 - \gamma_i r^3}] + W_i \text{Im}[e^{-\alpha_i r - \beta_i r^2 - \gamma_i r^3}]) Y_{lm}^{\lambda}(r_1, r_2),
\]

where \( Y_{lm}^{\lambda}(r_1, r_2) \) are the solid bipolar harmonics as defined in Ref. [10], and \( L \) is a total orbital angular momentum of a state. Complex parameters \( \alpha_i, \beta_i, \) and \( \gamma_i \) are generated in a quasi-random manner [9]:

\[
\alpha_i = \left[ \frac{1}{2} i(i + 1) \sqrt{p_{i\lambda}((A_2 - A_1) + A_{i\lambda})} + i \left[ \frac{1}{2} i(i + 1) \sqrt{q_{i\lambda}((A_2 - A_1') + A_{i\lambda}')}, \right. \right.
\]

[2] \( \lfloor x \rfloor \) designates the fractional part of \( x \), \( p_i \) and \( q_i \) are some prime numbers, \( [A_1, A_2] \) and \( [A_1', A_2'] \) are real variational intervals which need to be optimized. Parameters \( \beta_i \) and \( \gamma_i \) are obtained in a similar way. For the case of singlet states the wave function is to be symmetrized and antisymmetrized for the triplet states.

The variational wave functions for the initial \( S \) and \( P \) states of the helium atom are constructed with the use of three basis sets (layers), for which the variational parameters are searched independently. These basis sets are chosen in a way to achieve the better approximation for different regions of the wave function [9]. The final results for the nonrelativistic energies of the \( S \) and \( P \) states of the helium atom are presented in Table I. The variational wave functions that provide these results have been then used in calculations of the Bethe logarithm.

For the intermediate states the two basis sets with the variational parameters within the same range as for the initial states have been used. Beyond that a set of states with exponentially growing exponents has been included, a particular form of these states is discussed in the following section.

To make the calculations numerically stable against the round-off errors an extended sextuple precision arithmetics (about 48 decimal digits) has been used.

II. CALCULATION OF THE BETHE LOGARITHM

The Bethe logarithm for a general atomic or molecular system is defined as follows [11,12]:

TABLE I. The nonrelativistic energies for the \(^S\) and \(^P\) states of the \(^4\)He atom. Results are exact up to the last shown digit.

| State | Basis (N) | \( E_{nr} \) |
|-------|-----------|-------------|
| \(^1S\) | 1400 | -2.903 724 377 034 119 596 |
| \(^2S\) | 1500 | -2.145 974 046 054 417 38 |
| \(^2P\) | 1200 | -2.175 229 378 236 791 305 73 |
| \(^1P\) | 1200 | -2.123 843 086 498 101 2 |
| \(^2P\) | 1500 | -2.133 164 190 779 283 2 |

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\[\beta(n,L) = \frac{N}{D} = \frac{\langle J(\mathbf{H} - E_0)\ln[(\mathbf{H} - E_0)/R]\rangle}{\langle J(J,H,J)\rangle/2} = \sum_n \frac{J_{0n}(E_n - E_0)\ln[(E_n - E_0)/R]J_{n0}}{J_{00}(E_n - E_0)J_{n0}}, \]
\[\text{(3)}\]

where \(J = \sum e_z p_z/m_0\) is an operator of electric current density of an atom or molecule, and \(A = [H, J]\) is a dipole matrix element in the “acceleration” gauge. In the latter form denominator can be expressed as a solution of the second-order perturbation equation:
\[\langle E_0 - H\rangle \Psi_1 = A \Psi_0, \]
\[\text{(4)}\]

where \(A\) is a sum of terms of type \(r_i/r_j^3\) and thus a singular operator. The denominator is itself then expressed as \(D = \langle \Psi_0|A|\Psi_1\rangle\). In case of the helium atom with an infinite nucleus mass this operator reads
\[A = Z \left(\frac{r_1}{r_1} + \frac{r_2}{r_2}\right). \]
\[\text{(5)}\]

Before proceeding further we have to make two remarks. First, since the denominator has the form of the second-order perturbation, \(D_{\text{var}}\) obeys a variational principle or in other words is bounded from above. This is used to optimize the variational parameters for the intermediate states. Thus in our strategy we try to get a numerical value of \(D_{\text{var}}\) as close to
\[D_{\text{exact}} = 2\pi Z \langle \Psi_0|\Delta(r_1) + \Delta(r_2)|\Psi_0\rangle\]
as possible. If \(D_{\text{var}} \rightarrow D_{\text{exact}}\), then the variational solution converges to \(\Psi_1\) of Eq. (4).

Next, the exact solution of Eq. (4) is singular at \(r_i \rightarrow 0\) and in order to get good convergence rate it is required to augment a basis set (1) for the intermediate states by a series of states of the type
\[\Psi^{(k)}_g(l_1,l_2:L') = \gamma^{(l_1,l_2)}(\mathbf{r}_1,\mathbf{r}_2) \sum_{i=1}^{N_i} r_i^{-1}(U_i, \text{Re}[e^{-g^2\alpha_i r_i -\beta r_i^2 -\gamma r_i}] + W_i \text{Im}[e^{-g^2\alpha_i r_i -\beta r_i^2 -\gamma r_i}]) \pm (r_1 \leftrightarrow r_2), \]
\[\text{(6)}\]

where \(g \approx 10\) is a scaling parameter. And the complete trial wave function is made up as follows:
\[\Psi_1 = \Psi_1^{(a)} + \Psi_1^{(b)} + \sum_{k=1}^{K} \Psi_1^{(g)}, \]
\[\text{(7)}\]

where \(\Psi_1^{(a)}\) and \(\Psi_1^{(b)}\) are the trial functions of the type (1) of length \(N_a\) and \(N_b\), respectively, with optimal parameters taken independently. In present calculations randomly generated exponents \(\alpha\) and \(\beta\) are taken real. For \(\Psi_1\), a parameter \(g\) is defined as \(g = A_2/A_1\) from the variational interval \([A_1,A_2]\) for \(\Psi^{(i)}_g\). And thus \(\alpha\) takes values within an interval \([gA_1,A_2]\) for \(k=2\), etc. Other intervals: \([B_1,B_2]\), \([C_1,C_2]\), and \([C_1',C_2']\), are kept intact when \(k \geq 2\). So the whole set is defined by the variational parameters for the \(\Psi^{(i)}_g\), which are varied to get the best value for \(D_{\text{var}}\).

With this amendment of the basis set one can expect that the numerical convergence of the numerator \(N\) will be of the similar rate as for the denominator, since for large \(E\) (or large \(g^2\)) the logarithmic factor slowly varies with \(E\) and can be approximately replaced by a constant.

### III. RESULTS AND DISCUSSION

It causes no difficulty to make up the intermediate states, when the Bethe logarithm for an \(S\) state of the helium atom is evaluated. In this case a set of angular states is restricted to the \(P\) state only. The following distribution of intermediate states between different terms in expansion (7) has been used in the calculation of \(\beta(1S)\): \(N_a = 450\), \(N_b = 450\), \(N^{(1)} = 160\), \(N^{(2)} = 130\), \(N^{(3)} = 90\), \(N^{(4)} = 80\), \(N^{(5)} = 70\), \(N^{(6)} = 60\), \(N^{(7)} = 50\), \(N^{(8)} = 40\), \(N^{(9)} = 30\), \(N^{(10)} = 20\).

The total length of the basis is \(N = 1800\). Convergence of the numerical calculations with respect to a number of intermediate states for the \(1S\) and \(2S\) states is shown in Table II.

It is more complicated to construct the intermediate states in a general case of nonzero total orbital angular momentum \(L\). One has to sum over the states with \(L' = L + \pm 1\) of a spatial parity \(\pi = -(-1)^L\). For \(L' = L + 1\) one has an expansion over angular states of electrons
\[\Psi_1(L+1) = \sum_{l_1+l_2=L+1} \Psi_1(l_1,l_2;L+1). \]
\[\text{(8)}\]

For \(L' = L - 1\)\n\[\Psi_1(L) = \sum_{l_1+l_2=L-1} \Psi_1(l_1,l_2;L-1). \]
\[\text{(9)}\]

And thus the angular part in the latter case is described by the function \(\gamma_{L,M}^{(g)}\) with \(l_1 + l_2 = L + 2\).

The final results of this work are presented in Table III.

### TABLE II. Convergence of the Bethe logarithm for the 11S and 21S states.

| Number of states (N) | \(\beta(1S)\) | \(\beta(2S)\) |
|----------------------|---------------|---------------|
| 1000                 | 4.3701602260  | 4.3664127181  |
| 1200                 | 4.3701602228  | 4.3664127242  |
| 1400                 | 4.3701602221  | 4.3664127257  |
| 1600                 | 4.3701602220  | 4.3664127259  |
| 1800                 | 4.3701602220  | 4.3664127259  |

### TABLE III. The Bethe logarithm for the S and P states of the helium atom.

| State | This work | Drake, Goldman |
|-------|-----------|----------------|
| \(\beta(1S)\) | 4.3701602220(1) | 4.370160218(3) |
| \(\beta(2S)\) | 4.3664127259(1) | 4.36641272(7) |
| \(\beta(2P)\) | 4.369985356(1) | 4.36998520(2) |
| \(\beta(2P)\) | 4.369985356(1) | 4.36998520(2) |
They are compared with the best published results obtained in Ref. [8]. An excellent agreement demonstrates the power of the method. And thus we may conclude that the problem of the numerical evaluation of the Bethe logarithm for the two electron atoms is now satisfactorily solved. A progress in evaluating the mean excitation energy for the ground state of the helium atom is shown in Table IV.

To be unbiased we have to say a few words about deficiencies of the method. First, a singularity of the dipole operator $A$ presents substantial difficulty in numerical evaluation of matrix elements using analytical expressions for integrals related to this operator. That is especially important for a case of large $L$, when evaluation of the matrix elements become very time consuming and numerically unstable. And we have found that it is practically impossible to apply this approach to calculate the Bethe logarithm for the metastable states of the antiprotonic helium [13], where $L \approx 35$.

The other disappointing result was discovered when we tried to evaluate the Bethe logarithm $b_{s0,0}$ for the ground state of the $H_2^+$ molecular ion. The best result achieved by the method of this work was less accurate than the corresponding result evaluated by the modification of the Schwartz approach studied in Ref. [7].

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|                | Present work and previous results. |
|----------------|------------------------------------|
| P. K. Kabir, E. E. Salpeter (1953) | 4.39(20) |
| C. Schwartz (1961)                      | 4.370(4) |
| J. Baker et al. (1993)                   | 4.37012 |
| A. K. Bhatia, R. J. Drachman (1998)     | 4.367   |
| V. I. Korobov, S. V. Korobov (1999)     | 4.370 158(1) |
| J. Baker et al. (1999)                   | 4.370 159(2) |
| G. W. F. Drake, S. P. Goldman, (1999)   | 4.370 160 218(3) |
| this work                                 | 4.370 160 2220(1) |

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[1] H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Plenum, New York, 1977).
[2] P. K. Kabir and E. E. Salpeter, Phys. Rev. 108, 1256 (1957).
[3] C. Schwartz, Phys. Rev. 123, 1700 (1961).
[4] J. D. Baker, R. C. Forrey, J. D. Morgan III, R. N. Hill, M. Jerzierska, and J. Schertzer, Bull. Am. Phys. Soc. 38, 1127 (1993).
[5] A. K. Bhatia and R. J. Drachman, Phys. Rev. A 57, 4301 (1998).
[6] J. D. Baker, R. C. Forrey, M. Jerzierska, and J. D. Morgan III (unpublished).
[7] V. I. Korobov and S. V. Korobov, Phys. Rev. A 59, 3394 (1999).
[8] G. W. F. Drake and S. P. Goldman, Can. J. Phys. 77, 835 (1999).
[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, J. Phys. B 31, 3547 (1998).
[12] A. Yelkhovsky, Phys. Rev. A 64, 062104 (2001).
[13] V. I. Korobov, Phys. Rev. A 67, 062501 (2003).