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Enhanced Quantum Wave function for Mathematical Modeling of Hydrogen and Helium Ionization Energies: Engineering Applications to Plasma Particle Formation

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ABSTRACT

Ionization energy is a key threshold parameter in plasma modeling because it governs the onset of electron-impact ionization that contributes to particle generation and discharge sustainability. This study formulates an enhanced variational trial wavefunction to estimate the ground-state energies of hydrogen (H) and helium (He), then derives the corresponding ionization energies. The total energy functional is obtained from the expectation value of the non-relativistic Hamiltonian under the Born–Oppenheimer approximation and is minimized with respect to the wavefunction parameter(s). The model yields an ionization energy of 13.6 eV for hydrogen agreement with the standard reference within rounding precision, while the helium ionization energy is predicted at approximately 32 eV, indicating a noticeable deviation from the experimental value due to the simplified treatment of electron-electron interaction and the limited flexibility of the trial wavefunction. The results are summarized in a compact comparison model with reference, and the implications for plasma engineering are discussed by positioning ionization energy as the threshold input for ionization rate calculations and source terms in corona/plasma discharge models. These findings highlight the usefulness of variational wavefunction approaches for rapid parameter estimation, while also clarifying the physical limitations that must be addressed for higher-accuracy multi-electron systems.

1. Introduction

elium atoms serving as foundational models in both mathematical models and computational studies. The hydrogen atom, which has only one electron, is noteworthy for producing perfect solutions to the Schrödinger equation, which provides important insight into quantum behavior. In contrast, the helium atom, which has two electrons, causes electron-electron repulsion, making the Schrödinger equation analytically unsolvable. As a result, approximation approaches become necessary for determining its ground-state properties with appropriate precision. Among these strategies, the variational approach is commonly used due to its conceptual simplicity and computational practicality. Based on the variational principle, this method asserts that the expectation value of the Hamiltonian, calculated using any trial wavefunction, serves as an upper bound to the system's true ground-state energy.

The method is particularly advantageous when no closed-form solutions exist, offering both educational clarity and technical robustness [1], [2]. Over the decades, numerous studies have enhanced the variational method to improve energy approximations for the helium atom. Firme [1] pioneered its application in basic helium models, while Reed [2] proposed a refined $(1s)^2$ model that balanced simplicity with improved accuracy. Drake [3] applied high-precision

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techniques with sophisticated trial functions to establish accurate eigenvalue predictions. Matrix-based simplifications by Pingak et al. [4] and the analytical approaches of Nesbet and Watson [5] further demonstrated the method's versatility. Comparative analyses by Chen [6] evaluated the relative strengths of different approximation strategies, while Godunov [7] investigated ionization and excitation phenomena in energetic collisions. Korobov [8] provided benchmark nonrelativistic ionization energies for helium, enabling validation of approximate models. Wikner and Das [9] expanded the method's relevance to dipole polarizabilities, and Hakim et al. [10] explored quantum computing applications through the Variational Quantum Eigensolver (VQE) on hydrogen and helium atoms. More recently, Doma et al. [11] applied variational Monte Carlo and Lagrange mesh techniques to model helium behavior under plasma confinement, highlighting the method's relevance in extreme physical conditions. Plasma, in this case, is described as an ionized plasma made up of freely moving charged and neutral particles. It is quasi-neutral and has distinct collective features; nonetheless, plasma generation is unusual under normal atmospheric conditions due to the equilibrium state of most gases. As highlighted by Rauscher, Perucca, and Buyle [12], the ionization potential E_i refers to the energy necessary to ionize an atom, which is normally around 10 eV. This number is especially important for understanding the creation of corona plasma, where energetic ionization occurs. Although the literature has made significant progress in replicating helium's atomic characteristics, many of these studies require expensive computer resources, advanced trial wavefunctions, or a solid understanding of quantum mechanics. The result provides a challenge for those looking for a strategy that is both accessible and accurate for science or engineering applications.

This paper intends to close this gap by demonstrating a straightforward, computationally efficient, and pedagogically accessible approach for estimating the ionization energies of hydrogen and helium atoms in plasma generator using the variational principle. The proposed approach achieves a balance between accuracy and simplicity, and it is implemented in MATLAB®, making it appropriate for academic study and preliminary plasma modeling. Furthermore, the results are analyzed in terms of corona plasma particle production, emphasizing the broader physical implications of accurate atomic energy modeling.

2. Method

In this study, we used the variational quantum method (Rayleigh–Ritz variational principle) to compute the ground-state energy and then the ionization energy of hydrogen and helium as input parameters for plasma/corona discharge modeling. All calculations were implemented in MATLAB® v7.12.0 (R2011a) using numerical integration to evaluate expectation values and numerical optimization to find the energy minimum. The electronic Schrödinger equation was treated in the non-relativistic form under the Born–Oppenheimer approximation (fixed nucleus), and atomic units($\hbar = \mu = e = 4\pi\varepsilon_0 = 1$) were adopted for computational simplicity. The core procedure is: (1) choose a parametric trial wavefunction $\psi_T(\cdot;\alpha)$, (2) compute the energy functional $E(\alpha) = \langle\psi_T \mid H \mid \psi_T\rangle/\langle\psi_T \mid \psi_T\rangle$, and (3) minimize $E(\alpha)$with respect to $\alpha$to obtain the best variational estimate of the ground-state energy. For hydrogen (one electron), the Hamiltonian contains only the kinetic term and the electron nucleus Coulomb attraction, and the optimized minimum energy directly yields the hydrogen ionization energy relative to the ionized limit. For helium (two electrons), the Hamiltonian also includes the electron–electron repulsion term; we used a normalized two-electron trial function (normalization evaluated with the gamma function) and optimized the variational parameter ςnumerically in MATLAB. The helium ionization energy was obtained from the energy difference between neutral helium and the singly ionized state within the same framework. Finally, numerical convergence was checked by tightening integration/optimizer tolerances and confirming that the minimized energy and optimal parameter values remain stable; the helium result is interpreted as an approximate estimate because the trial function has limited flexibility and does not fully capture electron–electron correlation.

3. Result and Discussion

This study presented a comprehensive derivation of the ground-state energies, ionization energies, and wavefunctions for hydrogen and helium atoms, employing the variational method to approximate solutions to the Schrödinger equation. All calculations were executed using MATLAB®v.7.12.0 (R2011a). For the hydrogen atom, a single-electron system with nuclear charge Z = 1, the Schrödinger equation was formulated under the Born-Oppenheimer approximation, assuming a stationary nucleus. The Hamiltonian, expressed in SI units as shown in Eq. (1.a), included kinetic and potential energy terms:

$$\widehat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_o r} \tag{1.a}$$

$$\widehat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\varepsilon_o r} \tag{1.b}$$

where μ is the reduced mass, $\hbar$ is the reduced Planck constant, e is the electron charge, ε_o is the vacuum permittivity, and r is the electron-nucleus distance. For Helium: Two electrons orbiting a nucleus with charge Z = 2, including electron-electron repulsion. The Hamiltonian was

$$\widehat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2\mu}{\nabla_1}^2 - \frac{\hbar^2}{2\mu}{\nabla_2}^2 - \frac{Ze^2}{4\pi\varepsilon_o r_1} - \frac{Ze^2}{4\pi\varepsilon_o r_2} + \frac{e^2}{4\pi\varepsilon_o r_{12}} \tag{2}$$

where $r_1$and r_2 are the distances of electrons 1 and 2 from the nucleus, and r_{12} is the electron-electron distance. The reduced mass μ for a two-body system (electron and nucleus) is $\mu = \frac{m_e m_n}{m_e + m_n}$, where m_e is the electron mass and m_n is the

nuclear mass. Hydrogen and Helium mass are 9.104 and 9.099 $\times 10^{-31}$kg. For simplicity, the hydrogen atom consists of one proton and one electron. The Hamiltonian in atomic units ($\hbar = \mu = e = 4\pi\varepsilon_o = 1$) was simplified as:

$$\widehat{H} = -\frac{1}{2}\nabla^2 - \frac{1}{r} \quad (3)$$

The exact ground-state wavefunction for hydrogen, corresponding to the 1s orbital with Bohr radius $a = 1$, was:

$$\psi(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} = \frac{1}{\sqrt{\pi}} e^{-r} \quad (4)$$

This yielded a ground-state energy of -0.5 Hartree ($E_0 = -13.6$). To apply the variational method, a trial wavefunction was introduced:

$$\psi(r) = {\xi_1}^2 e^{-\varsigma r} \quad (5)$$

Normalization was achieved by ensuring $\int \varphi^* \varphi \, dV = 1$, leading to:

$$\int \varphi^* \varphi \, dV = 1 \quad (6)$$

$$4\pi \int \varphi^* \varphi \, r^2 dr = 1 \quad (7)$$

$$\int_{r=0}^{\infty} \left({\xi_1}^2\right)^2 e^{-2\varsigma r} \, r^2 dr = \frac{1}{4\pi} \quad (8)$$

Using the gamma function integral, the normalization constant was derived as: (9)

$$\int_{r=0}^{\infty} r^n e^{-\alpha r^m} \, dr = \frac{1}{\frac{n+1}{m}} \Gamma\left(\frac{n+1}{m}\right)$$

$$\xi_1{}^4 \int_{r=0}^{\infty} r^2 e^{-2\varsigma r} \, dr \overset{m\ \alpha}{=} \frac{1}{4\pi} \quad (10)$$

$$\xi_1{}^4 \frac{1}{\left(2\varsigma\right)^{\left(\frac{2+1}{1}\right)}} \Gamma\left(\frac{2+1}{1}\right) = \xi_1{}^4 \frac{1}{2^3\varsigma^3} 2 = \frac{1}{4\pi} \quad (11)$$

$$\xi_1{}^2 = \frac{\varsigma^{\frac{3}{2}}}{\sqrt{\pi}} = C \quad (12.a)$$

$$\xi_1 = \left(\frac{\varsigma^3}{\pi}\right)^{1/4} = \sqrt{C} \quad (12.b)$$

The normalized trial wavefunction became:

$$\psi(r) = \left(\frac{\varsigma^3}{\pi}\right)^{1/4} e^{-\varsigma r} = C e^{-\varsigma r} \quad (13.a)$$

The energy expectation value, $E[\varsigma] = \langle \psi(r) | \widehat{H} | \psi(r) \rangle$, was computed as:

The normalized trial wavefunction became:

$$\psi(r) = \left(\frac{\varsigma^3}{\pi}\right)^{1/4} e^{-\varsigma r} = C e^{-\varsigma r} \quad (13.b)$$

The energy expectation value, $E[\varsigma] = \langle \psi(r) | \widehat{H} | \psi(r) \rangle$, was computed as:

$$E[\varsigma] = \langle \psi(r) | \widehat{H} | \psi(r) \rangle = \left\langle \psi(r) \middle| -\frac{1}{2}\nabla^2 - \frac{1}{r} \middle| \psi(r) \right\rangle =$$

$$\frac{1}{2} \langle \psi(r) | -\nabla^2 | \psi(r) \rangle - \left\langle \psi(r) \middle| \frac{1}{r} \middle| \psi(r) \right\rangle =$$

$$\frac{1}{2} \int -\psi(r) \nabla^2 \psi(r) dV - \int \psi(r) \frac{1}{r} \psi(r) dV \quad (14)$$

The kinetic energy term was evaluated using:

$$\nabla . \left(\psi(r) \nabla \psi(r)\right) = \nabla \psi(r) . \nabla \psi(r) + \psi(r) \nabla^2 \psi(r) \quad (15)$$

$$\nabla . \left(\psi(r) \nabla \psi(r)\right) - \nabla \psi(r) . \nabla \psi(r) = \psi(r) \nabla^2 \psi(r) \quad (16)$$

$$-\left(\nabla \psi(r)\right)^2 = \psi(r) \nabla^2 \psi(r) \quad (17)$$

$$\left(\nabla \psi(r)\right)^2 = -\psi(r) \nabla^2 \psi(r) \quad (18)$$

yielding:

$$E(\varsigma) = \frac{4\pi}{2} \int \left(\frac{d}{dr} \psi(r)\right)^2 r^2 dr - 4\pi \int \frac{1}{r} \psi(r)^2 r^2 dr =$$

$$\frac{4\pi}{2} \int \left(\frac{d}{dr} \psi(r)\right)^2 r^2 dr - 4\varsigma^3 \int r e^{-2\varsigma r} dr =$$

$$\frac{1}{2} \int \left(\varsigma^2 \frac{\varsigma^3}{\pi} e^{-2\varsigma r}\right) r^2 dr - \varsigma = \frac{\varsigma^2}{2} - \varsigma \quad (19)$$

Minimization with respect to ς , resulting in:

$$\frac{dE}{d\varsigma} = 0 \quad (20)$$

$$\varsigma - 1 = 0 \quad (21)$$

$$\varsigma = 1 \quad (22)$$

$$E(\varsigma) = \frac{\varsigma^2}{2} - \varsigma = \frac{1}{2} - 1 = -\frac{1}{2} \text{ Hartree} \quad (23)$$

The ionization energy, defined as the energy required to remove an electron, was:

$$E_i = 0 - \left(-\frac{1}{2}\right) = \frac{1}{2} = 13.6\ eV \quad (24)$$

E_i value result precisely matched the experimental ionization energy [10], validated by photoionization experiments where photons with energy $\geq 13.6\ eV$ ionize hydrogen gas, confirming the accuracy of the Bohr model. For the helium atom (In atomic units), with two electrons and nuclear charge Z = 2, the Hamiltonian incorporated electron-electron repulsion:

$$\widehat{H} = -\frac{1}{2}{\nabla_1}^2 - \frac{2}{r_1} - \frac{1}{2}{\nabla_2}^2 - \frac{2}{r_2} + \frac{1}{r_{12}} = -\frac{1}{2}{\nabla_1}^2 - \frac{1}{2}{\nabla_2}^2 - \frac{2}{r_1} -$$

$$\frac{2}{r_2} + \frac{1}{r_{12}} \quad (25)$$

$$\widehat{H} == -\frac{1}{2}{\nabla_1}^2 - \frac{1}{2}{\nabla_2}^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{\sqrt{{r_1}^2 + {r_2}^2 - 2r_1 r_2 cos(\Delta\theta)}} \quad (26)$$

A trial wavefunction was constructed as a product of single-electron wavefunctions:

$$\psi(r) = \phi(r_1)\phi(r_2), \qquad \phi(r) = \frac{\varsigma^{\frac{3}{2}}}{\sqrt{\pi}} e^{-\varsigma r} \quad (27.a)$$

$$\psi(r) = \phi(r_1)\phi(r_2) = \frac{\varsigma^3}{\pi} e^{-\varsigma(r_1 + r_1)} \quad (27.b)$$

The energy expectation value was:

$$E[\varsigma] = \langle\psi(r)|\hat{H}|\psi(r)\rangle$$
$$= \left\langle\psi(r)\left|-\frac{1}{2}\nabla_1{}^2 - \frac{1}{2}\nabla_2{}^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{\sqrt{r_1{}^2 + r_2{}^2 - 2r_1r_2cos(\Delta\theta)}}\right|\psi(r)\right\rangle$$
$$= \left\langle\psi(r)\left|-\nabla^2 - 2\frac{2}{r} + \frac{1}{\sqrt{r_1{}^2 + r_2{}^2 - 2r_1r_2cos(\Delta\theta)}}\right|\psi(r)\right\rangle$$
$$= \varsigma^2 - 4\varsigma + \left\langle\psi(r)\left|\frac{1}{\sqrt{r_1{}^2 + r_2{}^2 - 2r_1r_2cos(\Delta\theta)}}\right|\psi(r)\right\rangle \quad (28)$$

The electron-electron repulsion term was approximated as: $\left\langle\psi(r)\left|\frac{1}{\sqrt{r_1{}^2+r_2{}^2-2r_1r_2cos(\Delta\theta)}}\right|\psi(r)\right\rangle =$
$\int \frac{1}{\sqrt{r_1{}^2+r_2{}^2-2r_1r_2cos(\Delta\theta)}}\left(\phi(r_1)\phi(r_2)\right)^2 dV_1dV_2$ (29)

This was compared to the literature value [10] of −2.9 Hartree = -78.3 ≈ $-80\,eV$. For the He^+ ion (Z = 2), the Hamiltonian was: Thus, the total energy was:

$$E[\varsigma] = \varsigma^2 - 4\varsigma + \int \frac{4\pi^2}{\sqrt{r_1{}^2+r_2{}^2-2r_1r_2cos(\Delta\theta)}}\left(\frac{\varsigma^3}{\pi}e^{-(r_1+r_2)\varsigma}\right)^2 \ldots (r_1{}^2sin(\theta_1)dr_1d\theta_1)(r_2{}^2sin(\theta_2)dr_2d\theta_2) \quad (30)$$

$$E[\varsigma] = \varsigma^2 - 4\varsigma + \frac{\varsigma^6}{\pi^2}\int \frac{4\pi^2}{\sqrt{r_1{}^2+r_2{}^2-2r_1r_2cos(\Delta\theta)}}e^{-2(r_1)\varsigma}e^{-2(r_2)\varsigma} \ldots (r_1{}^2sin(\theta_1)dr_1d\theta_1)(r_2{}^2sin(\theta_2)dr_2d\theta_2) \quad (31)$$

Solve for $sin(\theta_2)dr_2d\theta_2$ and $\theta_1 - \theta_2 \approx \Delta\theta = \theta$ we found

$$E[\varsigma] = \varsigma^2 - 4\varsigma + 8\varsigma^6\left[\int_0^\pi \frac{\sin(\theta_1)}{\sqrt{r_1{}^2 + r_2{}^2 - 2r_1r_2cos(\theta)}}d\theta_1 \iint_0^\infty r_1{}^2r_2{}^2\, e^{-2(r_1)\varsigma}e^{-2(r_2)\varsigma}dr_1dr_2\right] \quad (32)$$
$$E[\varsigma] = \varsigma^2 - 4\varsigma + 8\varsigma^6\left[\frac{2}{r_2}\iint_0^\infty r_1{}^2r_2{}^2\, e^{-2(r_1)\varsigma}e^{-2(r_2)\varsigma}dr_1dr_2\right]$$
$$= \varsigma^2 - 4\varsigma + 16\varsigma^6\left(\iint_0^\infty r_1{}^2r_2\, e^{-2(r_1)\varsigma}e^{-2(r_2)\varsigma}dr_1dr_2\right)$$
$$\approx \varsigma^2 - 4\varsigma + 16\varsigma^6\left(\int_0^\infty r_1{}^2e^{-2(r_1)\varsigma}dr_1\int_{r_1}^\infty r_2e^{-2(r_2)\varsigma}\,dr_2\right)$$
$$= \varsigma^2 - 4\varsigma + \frac{5}{16}\varsigma = \varsigma^2 - 3.6\varsigma \quad (33)$$

Minimizing $E[\varsigma]$ gave:
$$\frac{dE}{d\varsigma} = 0 \quad (34)$$
$$2\varsigma - 3.6 = 0$$
$$\varsigma = 1.8$$

$$E[\varsigma] = \varsigma^2 - 3\varsigma = -3.2 \text{ Hartree} = -84 \approx -80\,eV \quad (35)$$

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_o r} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{2e^2}{4\pi\varepsilon_o r} \quad (36)$$

Using a similar trial wavefunction, the energy was:

$$E(\varsigma) = \frac{\varsigma^2}{2} - 2\varsigma = 2 - 4 = -2 \text{ hartree} = -2 \times 27eV = 54 \text{ eV} \quad (37)$$

$$E_i = E(\varsigma)_{He^+} - E(\varsigma)_{He} = 2 - (-3.2) \text{ hartree} \approx 32 \text{ eV} \quad (38)$$

This was compared to the literature value [10] of −2.9 Hartree = -78.3 ≈ $-80\,eV$.

For the He^+ ion (Z = 2), the Hamiltonian was:

$$E(\varsigma) = \frac{4\pi}{2}\int\left(\frac{d}{dr}\psi(r)\right)^2 r^2dr - 4\pi\int\frac{2}{r}\psi(r)^2r^2dr =$$
$$\frac{4\pi}{2}\int\left(\frac{d}{dr}\psi(r)\right)^2 r^2dr - 8\varsigma^3\int re^{-2\varsigma r}dr =$$
$$\frac{1}{2}\int\left(\varsigma^2\frac{\varsigma^3}{\pi}e^{-2\varsigma r}\right)r^2dr - 2\varsigma = \frac{\varsigma^2}{2} - 2\varsigma \quad (39)$$
$$\frac{dE}{d\varsigma} = 0 \quad (40)$$
$$\varsigma - 2 = \quad (41)$$
$$\varsigma = 2 \quad (42)$$
$$E(\varsigma) = \frac{\varsigma^2}{2} - 2\varsigma = 2 - 4 = -2 \text{ hartree} = -2 \times 27eV = 54 \text{ eV} \quad (43)$$
$$E_i = E(\varsigma)_{He^+} - E(\varsigma)_{He} = 2 - (-3.2) \text{ hartree} \approx 32 \text{ eV} \quad (44)$$

For $He^+ \rightarrow He^{2+} + e^-$, the ionization energy was 54 eV.

The ionization energy for $He \rightarrow He^+ + e^-$ was calculated as 32 eV. The ionization energy for $He \rightarrow He^+ + e^-$ was calculated as 32 eV, deviating from the experimental 24.6 eV [4], [10] due to simplified electron correlation treatment. The variational method accurately approximated the ground-state and ionization energies, using hydrogen's exact solution as the reference state. The helium model, yet less accurate, confirmed the method's application to multi-electron systems. Moreover, the results are consistent with the observations of Rauscher, Perucca, and Buyle [12], who defined the ionization potential V_i as the energy required to ionize an atom, generally on the order of 10 eV. This energy range is particularly significant in plasma physics, especially in understanding corona plasma formation, where high-energy ionization processes dominate. In such environments, atoms like hydrogen and helium must possess ionization energies exceeding 10 eV to transition into a plasma state, a requirement that closely aligns with the values predicted through this computational approach. In summary, the comparative analysis supports the conclusion that the enhanced variational method not only serves as a valid tool for approximating atomic ionization energies but also offers valuable insights for the study of high-energy particle formation in plasma systems

4. Conclusion

Our study applied the variational method to determine the ionization energies of hydrogen and helium atoms in plasma generator, using a modified trial wavefunction. Computations, performed in MATLAB® v.7.12.0 (R2011a), incorporated reduced mass, Planck's constant, and vacuum permittivity within the Schrödinger equation framework. For hydrogen, a

single-electron system, the exact solution yielded a ground-state energy of -0.5 Hartree, corresponding to an ionization energy of 13.6 eV, precisely matching experimental photoionization data. This concordance validated the computational approach for single-electron systems. For helium, accounting for electron-electron repulsion, a trial wavefunction with an optimized variational parameter produced a ground-state energy of -3.2 Hartree. The ionization energy for $He \rightarrow He^{+} + e^{-}$ was calculated as 32 eV, deviating from the experimental 24.6 eV due to simplified electron correlation treatment. Despite this, the model provided a reasonable approximation for a multi-electron system. Future study could improve precision by including multi-parameter trial wavefunctions, especially for complicated multi-electron systems, expanding the method's utility in atomic physics research.

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6. References

[1] C. L. Firme, "Helium Atom, Variational Method and Perturbation Theory," *Quantum Mechanics*, pp. 426–445, Mar. 2022, doi: 10.1201/9781003050582-21.

[2] B. Reed, "Improved (1s)2 variational model for helium," *Open Physics*, vol. 3, no. 1, pp. 1–7, Mar. 2005, doi: 10.2478/bf02476500.

[3] G. W. F. Drake, "New variational techniques and high precision eigenvalues for helium," *AIP Conference Proceedings*, vol. 189, pp. 146–164, 1989, doi: 10.1063/1.38425.

[4] R. K. Pingak, R. Kolmate, and B. Bernandus, "A Simple Matrix Approach to Determination of the Helium Atom Energies," *Jurnal Penelitian Fisika dan Aplikasinya (JPFA)*, vol. 9, no. 1, p. 10, Jun. 2019, doi: 10.26740/jpfa.v9n1.p10-21.

[5] R. K. Nesbet and R. E. Watson, "Approximate Wave Functions for the Ground State of Helium," *Physical Review*, vol. 110, no. 5, pp. 1073–1076, Jun. 1958, doi: 10.1103/physrev 110.1073.

[6] J. Chen, "Approximate Methods for Calculating Ground-State Energy in Helium Atom," *Highlights in Science, Engineering and Technology*, vol. 141, pp. 59–65, May 2025, doi: 10.54097/y8y88h27.

[7] L. Godunov, "Excitation-ionization of helium in high energy collisions," *AIP Conference Proceedings*, vol. 680, pp. 32–35, 2003, doi: 10.1063/1.1619658.

[8] V. I. Korobov, "Nonrelativistic ionization energy for the helium ground state*," Physical Review A*, vol. 66, no. 2, Aug. 2002, doi: 10.1103/physreva 66.024501.

[9] E. G. Wikner and T. P. Das, "Variational Calculations of Dipole Polarizabilities of Helium-Like Ions," *Physical Review*, vol. 113, no. 6, pp. 1696–1696, Mar. 1959, doi: 10.1103/physrev 113.1696.4.

[10] D. F. Hakim, T. B. Prayitno, and Y. P. Sarwono, "Application of Variational Quantum Eigensolver for Ground State Energies Calculation in Hydrogen and Helium Atomic Sequences," *Spektra: Jurnal Fisika dan Aplikasinya*, vol. 9, no. 3, pp. 155–166, Dec. 2024, doi: 10.21009/spektra 093.03.

[11] S. B. Doma, M. A. Salem, and K. D. Sen, "Plasma Confined Ground and Excited State Helium Atom: A Comparison Theorem Study Using Variational Monte Carlo and Lagrange Mesh Method," *Computation*, vol. 9, no. 12, p. 138, Dec. 2021, doi: 10.3390/computation9120138.

[12] H. Rausher, M. Perucca, and G. Buyle, "Plasma Technology for Hyperfunctional Surfaces", *Wiley-VCH: Weinheim*, 2010.