ISSN: 2997-8440 www.aristonpubs.com/matsci-express https://doi.org/10.69626/mse.2024.0262

RESEARCH ARTICLE

Magnetoexciton in the Ellipsoidal Quantum Dots

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ABSTRACT: This study presents a comprehensive theoretical analysis of exciton states within a strongly prolate GaAs ellipsoidal quantum dot, specifically focusing on the influence of an external magnetic field. Employing the variational method, we have developed an exciton trial wave function based on one-particle wave functions, allowing for precise computation of exciton energy and binding energies. These computations are explored as functions of both the minor semiaxis of the quantum dot and the varying strength of the external magnetic field. Additionally, we have calculated the total magnetization of the quantum dot by deriving the total energy with respect to the magnetic field, offering insights into the magnetic properties of the system. The study further extends to estimating the radiative lifetime of the magnetoexciton, which is analyzed as a function of the small geometrical parameter and the external magnetic field. The findings provide a detailed understanding of the interplay between quantum dot geometry, magnetic field strength, and exciton dynamics, contributing to the broader knowledge of quantum dot behavior in varying electromagnetic environments.

Keywords: Magnetoexciton, Ellipsoidal quantum dot, GaAs, Binding energy, Quantum dot magnetization, Radiative lifetime.

Received: 15 May 2024; Revised: 03 July 2024; Accepted: 19 July 2024; Published Online: 29 July, 2024

1. INTRODUCTION

The field of nanotechnology is marked by its rapid advancements, with semiconductor quantum dots (QDs) standing out as one of the most promising innovations due to their unique and tunable electronic and optical properties. These nanometer-scale semiconductor particles are celebrated for their quantum confinement effects, which result in discrete energy levels similar to those observed in isolated atoms. Such confinement leads to remarkable phenomena, including size-tunable emission spectra, where the color of the emitted light can be precisely controlled by altering the size of the QDs [1- 4]. This tunability has paved the way for their application in a variety of fields, ranging from light-emitting diodes (LEDs) and solar cells to biological imaging and quantum computing.

Among the most compelling features of quantum dots is the formation of excitons—bound states of an electron and a hole that are attracted to each other by the Coulomb force. Excitons are central to the optical and electronic behavior of QDs, influencing processes such as absorption, emission, and charge separation. Given their pivotal role, understanding exciton dynamics within QDs is critical not only for advancing fundamental physics but also for optimizing QDs in practical applications, including photovoltaics, where they contribute to efficient light absorption and conversion, and in quantum computing, where they are explored for information storage and processing [5- 8].

The study of excitons becomes even more intriguing when considering their behavior under external perturbations, such as magnetic fields. When a magnetic field is applied to a quantum dot, it alters the motion of the charged particles within, directly impacting the properties of excitons. This interaction can result in phenomena like Zeeman splitting, where the excitonic energy levels are split into distinct sublevels in the presence of a magnetic field. Such splitting provides deeper insights into the fine structure and dynamics of excitons, revealing intricate details about the interplay between quantum confinement and magnetic influences [9]. Moreover, magnetic fields can be used to control the spin states of excitons, a feature that is particularly valuable in the emerging fields of spintronics and quantum information processing. In these domains, the ability to manipulate spin states opens up possibilities for developing new types of

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memory storage and logic devices that operate at the quantum level [10, 11].

This paper delves into the theoretical investigation of exciton states within strongly prolate ellipsoidal quantum dots (SPEQDs) made of GaAs, under the influence of an external magnetic field. The choice of GaAs is driven by its well-known semiconductor properties, which make it an excellent material for studying quantum effects. The focus on an ellipsoidal quantum dot geometry is particularly significant because this shape allows for the manipulation of energy states using two geometric parameters—the large and small semiaxes. By varying these parameters, it is possible to gain a more comprehensive understanding of how quantum confinement affects exciton behavior in non-spherical QDs [12, 13].

The theoretical framework employed in this study is the variational method, a powerful technique for approximating the behavior of quantum systems. By applying this method, we aim to compute exciton energies and binding energies as functions of both the minor semiaxis of the ellipsoidal QD and the strength of the external magnetic field. Additionally, this study investigates how these energies influence the total magnetization of the quantum dot, calculated by deriving the total energy with respect to the magnetic field. Finally, the radiative lifetime of the magnetoexciton, a critical parameter for understanding the optical properties of QDs, is estimated as a function of the small geometrical parameter and the magnetic field. The findings from this research are expected to contribute significantly to the understanding of quantum dot behavior under magnetic influence, with potential applications in fields ranging from optoelectronics to quantum computing.

2. THEORETICAL DETAILS

To begin our investigation, let's examine the single-particle scenario in the SPEQD subjected to the external magnetic field. Because of the QD's geometric characteristics, the particle moves more rapidly along the radial direction compared to the OZ direction. This situation is similar to the problem analyzed in [14], enabling the use of the adiabatic approximation, but with the roles of the "fast" and "slow" subsystems reversed. The Hamiltonian that characterizes the system in cylindrical coordinates is expressed in [15].

The interaction between the particle and the external magnetic field is important, and it incorporates electron (hole) spin, Bohr magneton, and the effective Lande factor of the electron (hole), the extensive description of the above-mentioned interaction in QDs, made from *GaAs* is discussed and explained in Ref. [14].

The parallel alignment of the magnetic field with the axial direction is guaranteed through calibration $A_\rho = 0,\ A_\varphi = \frac{1}{2}B\rho,\ A_z = 0$, where A is vector potential of the magnetic field. Considering this calibration, the system's Hamiltonian in cylindrical coordinates can be expressed as:

$$\hat{\mathrm{H}} = -\frac{\mathrm{h}^2}{2m^*}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] - i\frac{\mathrm{h}\omega_B}{2}\frac{\partial}{\partial\varphi} + \frac{m^*\omega_B^2}{8}\rho^2 + U_{potential}^{e(h)}\left(\rho,\varphi,Z\right) \tag{1}$$

The latter can be expressed as the dimensionless sum of the Hamiltonians of the "fast" $\hat{H}_1$ and "slow" $\hat{H}_2$ subsystems as follows:

$$\begin{aligned}
\hat{H} &= \hat{H}_1 + \hat{H}_2 + U_{potential}^{e(h)}\left(\rho,\varphi,Z\right) \\
\hat{H}_1 &= -\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right) - i\gamma_B\frac{\partial}{\partial\varphi} + \frac{1}{4}\gamma_B^2 r^2 \\
\hat{H}_2 &= -\frac{\partial^2}{\partial z^2} + U\left(r,\varphi,z\right)
\end{aligned} \tag{2}$$

Here, $\omega_B = \frac{eB}{m^* s}$, $\gamma_B = \frac{\mathrm{h}\omega_B}{2E_R}$, $z = \frac{Z}{a_B}$ and $r = \frac{\rho}{a_B}$. Here a_B is electron effective Bohr radius. Note that to switch to dimensionless quantities, all lengths are presented in effective Bohr radii a_B and all the energies - in effective Rydberg energy E_R.

Moreover, adopting the adiabatic approximation's logic, the particle wave function will be considered in the form:

$$\psi\left(r,\varphi,z\right) = Ce^{im\varphi}R\left(r;z\right)\chi\left(z\right) \tag{3}$$

For a relatively weak magnetic field intensity, at a fixed value of the z coordinate, in the radial direction the particle motion is localized in an "effective" two-dimensional potential well with a width:

$$L\left(z\right) = a\sqrt{1 - \frac{z^2}{c^2}} \tag{4}$$

After some transformations, one can show that the wave function and energy can be determined by the help of the following equations:

$$\begin{aligned}
&\psi_{gr}\left(\rho,\varphi,z\right) = \frac{e^{im\varphi}}{\sqrt{2\pi}}\frac{\sqrt{2}}{L(z)J_{m+1}\left(\alpha_{n+1,m}\right)}J_m\left(\frac{\alpha_{n+1,m}}{L(z)}r\right)\sqrt[4]{\frac{\alpha_{n+1,m}}{ac}}\frac{1}{2^{\frac{N}{2}}\sqrt[4]{\pi}\left(N!\right)^{\frac{1}{2}}}e^{-\frac{\alpha_{n+1,m}}{2ac}z^2}H_N\left(\sqrt{\frac{\alpha_{n+1,m}}{ac}}z\right) \\
&\varepsilon = \alpha_{n_1,n_2} + 2\beta_{n_2}\left(N + \frac{1}{2}\right);\ \alpha_{n1,n2} = 2\gamma_B\left(n_1\frac{|m| + m + 1}{2}\right) + \frac{4n_2}{a^2};\ \beta_{n_2} = \frac{2\sqrt{n_2}}{ac}
\end{aligned} \tag{5}$$

Here $N = 2n_r + |m|$, where n_r and m are the radial and magnetic quantum numbers, respectively. n_1 and n_2 are some quantum numbers, depending on the magnetic field magnitude [14]. $J_m\left(\frac{\alpha_{n+1,m}}{L(z)}r\right)$ is the Bessel function of the first kind of m-th order and $H_N\left(\sqrt{\frac{\alpha_{n+1,m}}{ac}}z\right)$ is the Hermit function.

After obtaining energy spectra and wave function for one-particle problem, lets determine magnetoexciton energy using the variational method. The Hamiltonian describing the biexciton under the influence of an external magnetic field is given by:

$$\hat{H} = \hat{H}_{XX}^{kin} + V_{\text{int}} + U_{conf}$$

$$\hat{H}_X\left(\vec{r}_1, \vec{r}_\alpha\right) = \sum_i \frac{\hat{P}_i^2}{2m_i^*} + \sum_i U_{conf}\left(\vec{\rho}_i, z_i\right) - \left(\frac{1}{\varepsilon\left|\vec{r}_1 - \vec{r}_\alpha\right|}\right) \tag{6}$$

Where, $i = \{1, \alpha\}$, $\vec{r}_1$ and $\vec{r}_\alpha$ are electron's and hole's coordinates, respectively, ε is dielectric constant of the material. As it has already been mentioned before, the confinement potential U_{conf} in the cylindrical coordinates for electrons and holes is taken from [14]. As previously emphasized, the magnetoexciton energy is computed using the variational method. In this approach, the magnetoexciton variational function for the ground level exhibits the following structure [17]:

$$\Psi_X\left(\vec{r}_1, \vec{r}_\alpha\right) = C\psi_{100}\left(\vec{r}_1\right)\psi_{100}\left(\vec{r}_\alpha\right)e^{-\mu\rho_{1\alpha}}, \tag{7}$$

where μ is the variational parameter, which can be revealed as a result of the minimization of the following integral:

$$E_X = \left\langle \Psi_X(\vec{r}_1, \vec{r}_\alpha) \middle| \hat{H}_X \middle| \Psi_X(\vec{r}_1, \vec{r}_\alpha) \right\rangle \tag{8}$$

It is worth to note, that equation (8) incorporates the variational quantum Monte Carlo method, which is elaborated in detail in Ref. [18]. By employing the derived energy dependence on the geometric parameters of the QD and the magnetic field strength, key physical and optical parameters, including the binding energy, can be determined. The magnetoexciton binding energy is defined as follows:

$$E_{bind}(X) = (E_e + E_h) - E(X) \tag{9}$$

where E_e, E_h are the energies of the electron and hole, respectively.

Since this paper focuses on results obtained for *GaAs*, then corresponding material parameters, taken from Ref [14], will be used in the calculations.

Understanding the recombination processes of excitons is crucial, the recombination radiative lifetime of the latter can be estimated via the following formula [19]:

$$\tau(XX) \approx \frac{2\pi\varepsilon_0 m_0 s^3 \hbar^2}{\sqrt{\varepsilon}e^2 E(X) E_P \left|\int_V \Psi_{exc}\left(\vec{r}_e, \vec{r}_h\right) d\vec{r}\right|^2} \tag{10}$$

where m_0 is free electron mass, ε is dielectric constant of the material and E_P is the Kane energy. It is pertinent to mention that the Eq. (10) does not consider the impact of exciton-phonon interaction.

The next task is to measure the total magnetization of the QD system by calculating the derivative of the QD's total energy with respect to the magnetic field [20]:

$$M_X = -\frac{\partial E(X)}{\partial B}. \tag{11}$$

3. RESULTS AND DISCUSSION

The investigation of magnetoexciton properties within strongly prolate ellipsoidal quantum dots (SPEQDs) under the influence of an external magnetic field has yielded several insightful results. The analysis focuses on how the exciton binding energy, magnetization, and radiative lifetime are affected by variations in both the external magnetic field and the small semiaxis of the SPEQD. The results provide a comprehensive understanding of the complex interplay between quantum dot geometry and external magnetic influences, which is critical for optimizing quantum dot-based applications in optoelectronics and quantum information processing.

3.1. Magnetoexciton Binding Energy:

Figure 1(a) illustrates the relationship between magnetoexciton binding energy and the strength of the external magnetic field for different values of the small semiaxis, with the large semiaxis kept constant. The binding energy initially increases with the magnetic field, suggesting that the magnetic field strengthens the Coulomb attraction between the electron and hole, thereby stabilizing the exciton. This trend continues until a critical magnetic field strength is reached, beyond which the binding energy begins to decrease. This decrease may be attributed to the Zeeman effect, where the magnetic field induces a splitting of energy levels, reducing the effective binding energy of the exciton.

The data also reveal that the magnetoexciton binding energy is inversely related to the small semiaxis of the quantum dot. Specifically, the binding energy decreases as the small semiaxis increases, indicating that larger quantum dots with more elongated shapes have weaker Coulomb interactions between the electron and hole. This can be understood in terms of the increased spatial separation between the charge carriers in larger quantum dots, which weakens their mutual attraction.

In Figure 1(b), the dependence of the magnetoexciton binding energy on the small semiaxis for different magnetic field strengths is presented. Here, the binding energy decreases as the small semiaxis increases for all magnetic field values, reinforcing the observation that a larger quantum dot geometry leads to a reduction in binding energy. The influence of the magnetic field is more pronounced for quantum dots with smaller semiaxes, where the spatial confinement is stronger, leading to greater sensitivity to external perturbations.

3.2. Exciton Magnetization:

The behavior of exciton magnetization in response to the external magnetic field and variations in the small semiaxis is depicted in Figure 2. Figure 2(a) shows the magnetization as a function of the external magnetic field for different small semiaxis values. The magnetization decreases as the magnetic field strength increases, which is a counterintuitive result that suggests the magnetoexciton may undergo diamagnetic behavior under certain conditions. This behavior can be linked to the redistribution of electron and hole wavefunctions in the presence of the magnetic field, leading to a decrease in the overall magnetic moment of the system.

Figure 2(b) highlights the dependence of exciton magnetization on the small semiaxis for various magnetic field strengths. As the small semiaxis increases, the magnetization decreases, consistent with the earlier observation that larger quantum dots have lower binding energies and, consequently, weaker magnetic moments. This decrease in magnetization with increasing small semiaxis and magnetic field suggests that quantum dots with more pronounced prolate geometries exhibit less magnetic response, potentially limiting their use in applications that require strong magnetic interactions.

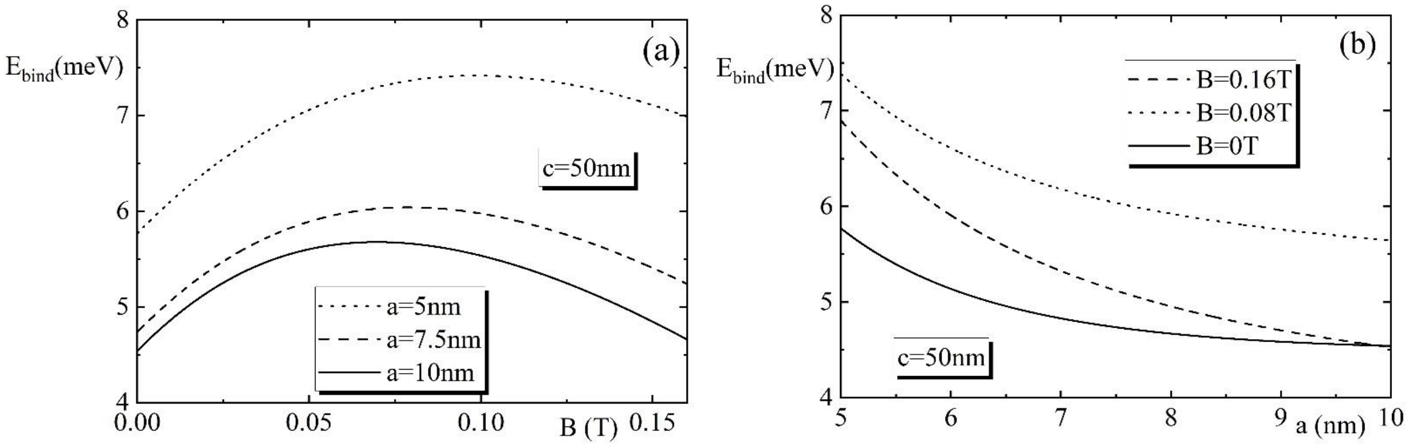

Fig. 1. **(a)** Dependence of the magnetoexciton binding energy on the external magnetic field's magnitude for the different values of the small semiaxis, and **(b)** Dependence of the magnetoexciton binding energy on the small semiaxis for the different values of the external magnetic field.

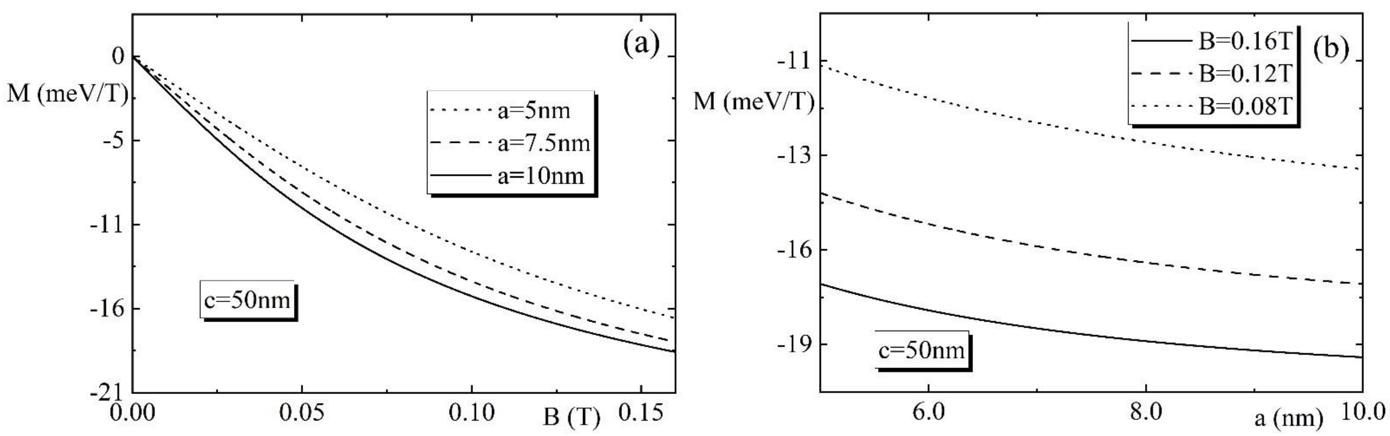

Fig. 2. **(a)** Dependence of the exciton magnetization on the external magnetic field for the different values of the small semiaxis, and **(b)** Dependence of the exciton magnetization on the small semiaxis for the different values of the magnetic field magnitude.

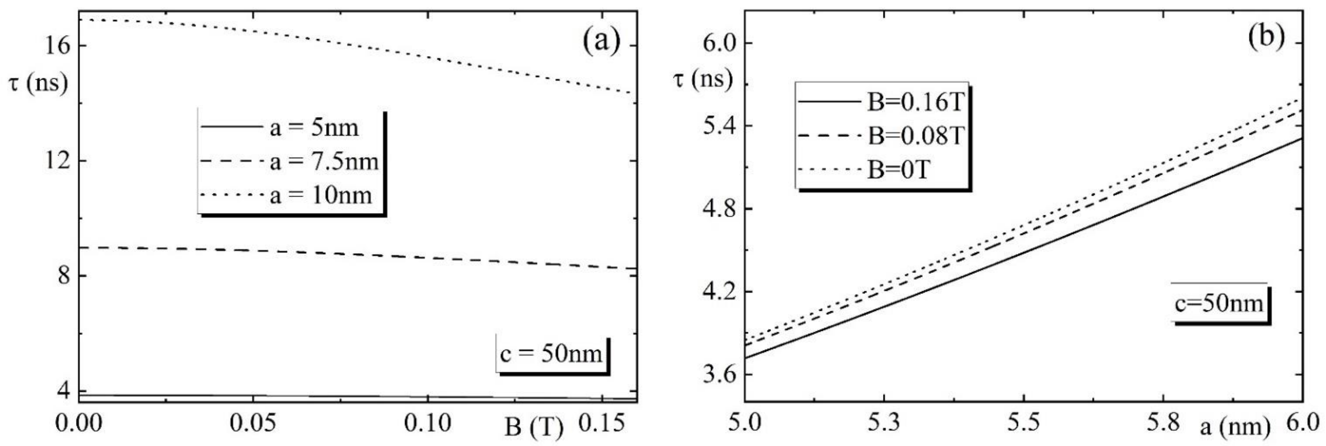

Fig. 3. (a) Dependence of the magnetoexciton radiative lifetime on the external magnetic field's magnitude for the different values of the small semiaxis, and **(b)** Dependence of the magnetoexciton radiative lifetime on the small semiaxis for the different values of the external magnetic field.

3.3. Radiative Lifetime of Magnetoexciton:

The radiative lifetime of magnetoexcitons, a critical parameter for understanding the optical properties of quantum dots, is presented in Figures 3(a) and 3(b). Figure 3(a) demonstrates that the radiative lifetime decreases with increasing magnetic field strength for various small semiaxis values. This trend is attributed to the fact that higher magnetic fields increase the magnetoexciton energy, which is inversely proportional to the radiative lifetime. The higher the energy, the faster the recombination process, leading to shorter lifetimes.

In Figure 3(b), the radiative lifetime is shown as a function of the small semiaxis for different magnetic field strengths. The radiative lifetime increases as the small semiaxis increases, indicating that larger quantum dots, with their lower binding energies, exhibit slower recombination rates. This observation is consistent with the earlier findings on binding energy and magnetization, where larger quantum dots exhibit weaker interactions and, consequently, longer radiative lifetimes.

These results provide a detailed understanding of how the interplay between quantum dot geometry and external magnetic fields influences the fundamental properties of magnetoexcitons. The findings highlight the importance of considering both geometric and magnetic factors when designing quantum dot-based devices, as these factors can significantly impact the performance and functionality of such systems in real-world applications.

4. CONCLUSION

This study presents a theoretical investigation of exciton states within strongly prolate ellipsoidal quantum dots (SPEQDs) under the influence of an external magnetic field, using the variational method. Key findings include the complex relationship between exciton binding energy and magnetic field strength, where the binding energy initially increases with the field but decreases after reaching a critical point. This behavior underscores the significant impact of magnetic fields on excitonic properties, with implications for quantum confinement effects and the Zeeman effect. Additionally, the study highlights the inverse relationship between binding energy and the small semiaxis of the quantum dot, indicating that larger dots exhibit weaker exciton binding. The investigation also reveals that magnetization decreases with both increasing magnetic field strength and the size of the small semiaxis, suggesting a transition towards diamagnetic behavior under certain conditions. This has important implications for the magnetic properties of quantum dot-based devices. Lastly, the radiative lifetime of magnetoexcitons is shown to decrease with increasing magnetic field strength and increase with the size of the small semiaxis, indicating faster recombination processes in smaller or more magnetically influenced quantum dots. Overall, the study provides valuable insights into the interplay between quantum dot geometry and external magnetic fields, offering guidance for the design and optimization of quantum dot-based technologies in optoelectronics, spintronics, and quantum information processing. The findings emphasize the importance of tailoring both geometric and magnetic parameters to achieve desired excitonic behavior in nanoscale devices.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests.

ACKNOWLEDGEMENTS

This work was supported by the RA MESCS Higher Education and Science Committee under No. 23RL-1C005 research project. The article was completed as well as part of funding within the framework of a competition for incentive bonuses to the salaries of young scientists at Russian-Armenian University in 2023.

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