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Article

Modeling the Properties of Magnetostrictive Elements Using Quantum Emulators

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Abstract: The article discusses mathematical and numerical methods for modeling magnetostrictive multielectronic systems based on a combination of quantum and classical methods. The algorithm development suitable for the investigation of magnetostrictive phenomena at the micro level using the classical-quantum method implemented on a modern classical computer is justified. The algorithms and structure of the software package are given. The adequacy of the quantum-classical method is verified by comparing the calculated results of the properties of known magnetostrictive materials with the real properties of magnetostrictive alloys.

Keywords: quantum-classical numerical methods; investigation of magnetostrictive phenomena at the micro level

1. Introduction

When modeling magnetostrictive phenomena at the micro level, the problem of solving the Schrodinger equation (SE) arises. Currently, many numerical methods for solving it are known [1–10]. Depending on the type of computer designed for their implementation, all these methods can be divided into classical and quantum. Classical methods are designed to be implemented on classical computers and are based on the classical approach to the numerical solution of differential equations. They allow you to effectively solve a wide range of tasks in an acceptable time and with high enough accuracy. However, in many cases, for example, when modeling polyatomic systems, the use of such an approach leads either to an excessively large error or to an exponentially increasing solution time, unacceptable with the modern power of classical computers [11–19]. In scientific papers [20–27], modifications of classical methods are proposed that can significantly increase accuracy and reduce calculation time, but still this problem remains relevant.

Another fundamentally new and actively developing way of numerically solving the SE is the use of quantum methods [11,12,28–31]. Such methods are based on algorithms designed to be performed by quantum computers, which, as is known [23,32–36], are more effective for solving such problems. The main problem with the use of quantum computing is the insufficient level of modern technological development in this direction: the lack of available fully functional quantum computers, and the small number of known effective quantum algorithms and scientific works in this direction. However, existing quantum computer emulators make it possible to develop and test new quantum numerical methods for solving particular problems of modeling polyatomic systems and to substantiate the theoretical possibility of using these methods in the general case in the future, when full-fledged quantum computers appear [37–41].

It is also possible to apply a combined approach to modeling quantum systems using quantum-classical methods using the resources of conventional computers and quantum emulators. The algorithms of quantum-classical numerical methods (QCNM) are designed



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to be executed on a classical computer in a software environment equipped with a classical computing module and a module for emulating quantum computing, with the possibility of exchanging data between them (Figure 1).

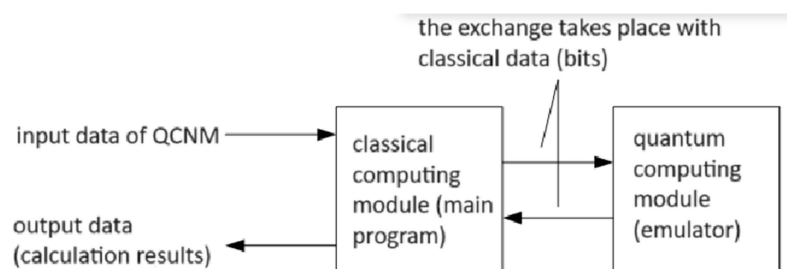


Figure 1. Simplified structure of the software package for the implementation of the QCNM.

This method of modeling will make it possible to use the most useful properties of quantum algorithms to speed up the work and increase the efficiency of classical ones.

The main task considered in this article is the development of a QCNM algorithm suitable for the investigation of magnetostrictive phenomena by their mathematical modeling at the micro level using a classical computer. At the same time, it should be borne in mind that the capabilities of a classical computer for the implementation of quantum computing emulators are currently severely limited by the amount of quantum memory, which is a maximum of about 400 qubits (when using cloud technologies).

The proposed QCNM algorithm is implemented as part of a software package (Figure 1), and with its help, a study of magnetostrictive phenomena in *Ni-Mn-Ga* Geisler alloys has been carried out [42–47].

2. Materials and Methods

Atoms with N electrons differ from the hydrogen atom and hydrogen-like systems. Firstly, the Hamiltonian takes into account the contributions to the kinetic and potential energy of all N electrons, and a summand describing the interelectronic interaction arises in the potential energy. Secondly, the wave function must obey the Pauli principle—it must be antisymmetric when rearranging the coordinates of any pair of electrons.

This leads to the fact that the solution of the Schrodinger equation for multielectronic atoms becomes much more complicated. It cannot be obtained analytically and requires approximate numerical solution methods [13,20,48,49].

However, the properties of multielectronic systems can be described qualitatively quite simply if we take advantage of the fact that certain relations related to the angular momentum must be fulfilled for the atom.

1. Each state of the atom must have a certain value of the total angular momentum.
2. The total moment of all electrons in an atom must obey the rules of quantization and spatial quantization.
3. Since the spin of electrons is also the moment of momentum, it should also contribute to the total moment of the atom.
4. The moments and spins of individual electrons should be combined so that the total moment remains an observable quantity and obeys the postulates and equations of quantum mechanics.

The total moment is associated with the moments of individual electrons, but since the moment of each electron is ambiguously oriented in space (spatial quantization does not allow you to uniquely define all projections of the vector), the total moment, according to the superposition principle, can become a combination of any possible orientations of the vectors of individual moments. These principles were used in the modeling of multielectronic Geisler alloys of the *Ni-Mn-Ga* type.

Consider the Schrodinger time equation:

$$\hat{H}\Psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\bar{r}, t) \right)\Psi(\bar{r}, t) = j\hbar\frac{\partial\Psi(\bar{r}, t)}{\partial t}, \tag{1}$$

where \hat{H} —the Hamiltonian; $\Psi(\bar{r}, t)$, $U(\bar{r}, t)$ —the wave function and potential energy of a particle located at a point in space with coordinates (x, y, z) and a radius-vector $\bar{r} = x\bar{i} + y\bar{j} + z\bar{k}$ at a time t ; $\nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ —the Laplace operator; m —particle mass; and \hbar —reduced Planck constant.

The solution of Equation (1) on a quantum computer can be performed by the Zalka–Wiesner method [15], which is applicable, including for polyatomic systems. The general scheme of the numerical solution of the SE by this method is as follows:

1. Write down the formally exact solution of the SE (1) Ψ in the form of a vector $|\psi(t)\rangle$:

$$|\psi(t)\rangle = e^{-j\hat{H}t}|\psi(0)\rangle. \tag{2}$$

2. Set the initial state $|\psi(0)\rangle$, the time point t_f , or whichever is required to determine the solution and discretization step Δt , such that $i\Delta t = t_f$, for some integer i . To accept $|\psi_0\rangle = |\psi(0)\rangle$, $i = 0$.
3. Construct a quantum circuit of $U_{\Delta t}$ in the form:

$$U_{\Delta t} = \text{IQFT}\exp\left(-\frac{j}{\hbar}\frac{p^2}{2m}\Delta t\right)\text{QFT}\exp\left(-\frac{j}{\hbar}V(\bar{r})\Delta t\right), \tag{3}$$

where $V(\bar{r})$ —potential energy of a quantum particle system, and QFT, IQFT—forward and reverse quantum Fourier transform.

4. The beginning of the iterative process.
5. At one iteration step, the value $|\psi_{i+1}\rangle = U_{\Delta t}|\psi_i\rangle$ is calculated, and the counter i is incremented by one.
6. The iterative process stops when the condition $i\Delta t \geq t_f$ is met. The result is returned to $|\psi(t_f)\rangle = |\psi_i\rangle$.

This algorithm is performed on a quantum computer in polynomial time, is the most versatile, and is suitable for modeling a wide range of quantum systems, including magnetostrictive phenomena. The result is obtained with an error, the value of which can be obtained from the estimate:

$$\left| \langle \psi(t_f) | e^{-j\hat{H}t_f} | \psi(0) \rangle \right|^2 \geq 1 - \varepsilon. \tag{4}$$

The Zalka–Wesner method without modifications can be implemented on a classical computer using the software package in Figure 1, but it is suitable only for modeling a quantum system with a small number of particles. To increase its efficiency, it is proposed to use the QCNM based on the Trotter–Suzuki transformation [24,50–52], which can be expressed by the following recursive formulas:

$$\left(\prod_{i=1}^m e^{-jH_i t/2n} \prod_{i=m}^1 e^{-jH_i t/2n} \right)^n = e^{-jHt} + O\left(\frac{m^3 t^3}{n^2}\right) = U_2(t), \tag{5}$$

$$U_{2k}(t) = [U_{2k-2}(s_k t)]^2 U_{2k-2}([1 - 4s_k]t) [U_{2k-2}(s_k t)]^2 = e^{-jHt} + O\left(\frac{(mt)^{2k+1}}{n^2}\right), s_k = \left(4 - 4^{1/(2k-1)}\right)^{-1}.$$

The use of this transformation makes it possible to increase the accuracy of the approximation using the same computing resources. The effectiveness of the Trotter–Suzuki method can be clearly and simplistically demonstrated using the illustration in Figure 2. If we conditionally assume that the quantum algorithm must move from state 1 to state 2, and the lengths of the sides of the triangle A , B , and $U_{2k}(t)$ —the total amount of computing re-

sources needed for this transition, then the shortest path is $U_{2k}(t)$, which is a Trotter–Suzuki transform of order $2k$.

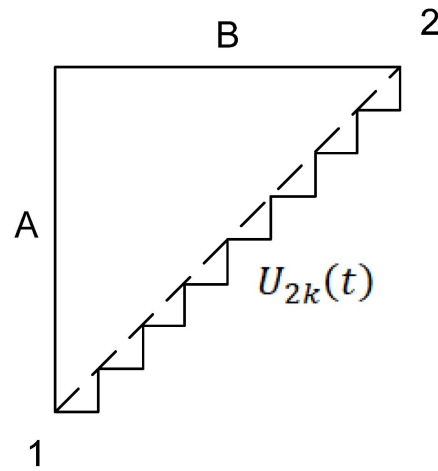


Figure 2. The principle of operation of the Trotter–Suzuki transformation.

An important point in the implementation of the proposed QCNM is the use of the quantum Fourier transform (QFT). The peculiarity of QFT in comparison with the usual Fourier transform is that it does not speed up the transformation itself, but makes it possible to more efficiently search for initial approximations for the eigenvalues of unitary operators, which are needed for other numerical methods.

In an orthonormal basis $|0\rangle, \dots |N - 1\rangle$ Q QFT is a linear operator acting as follows [14]:

$$|x\rangle \rightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{-2\pi j k x / N} |k\rangle. \tag{6}$$

Or if you accept $N = 2^n$, where n —an integer, and represent the state $|x\rangle$ as a binary number $x = x_1 x_2 \dots x_n$, (6), then you can rewrite it in a more convenient form for practical purposes:

$$\frac{|x\rangle = |x_1 x_2 \dots x_n\rangle \rightarrow (|0\rangle + e^{-2\pi j 0 \cdot x_n} |1\rangle) (|0\rangle + e^{-2\pi j 0 \cdot x_{n-1}} |1\rangle) \dots (|0\rangle + e^{-2\pi j 0 \cdot x_1} |1\rangle)}{2^{n/2}}, \tag{7}$$

where the notation of type $0.x_1 x_2 \dots x_n$ denotes a binary fraction $\frac{x_1}{2} + \frac{x_2}{4} + \dots + \frac{x_n}{2^n}$.

Representation (7) allows to construct a simple quantum scheme for calculating QFT based on quantum gates of Hadamard H and controlled phase shifts $R_k = R_\phi$ at $\phi = \pi 2^{1-k}$, shown in Figure 3.

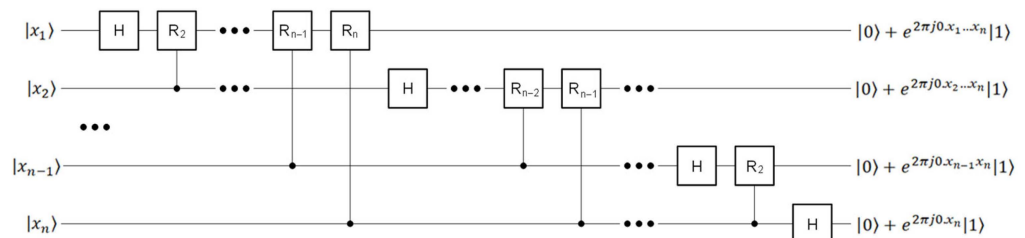


Figure 3. A quantum scheme for calculating the QFT.

Thus, to conduct studies of magnetostrictive phenomena at the microlevel, the proposed QCNM was used, based on the modified Zalka–Wesner method, which can be implemented on a classical computer due to quantum simulation of the Trotter–Suzuki transformation and QFT.

The implementation of the software package for conducting research in accordance with the proposed algorithm was performed in the MS Visual Studio environment using the C#—programming languages for the classical computing module and Q#—for the quantum emulator module (see Figure 1). The scheme of the algorithm of the classical computing module is shown in Figure 4.

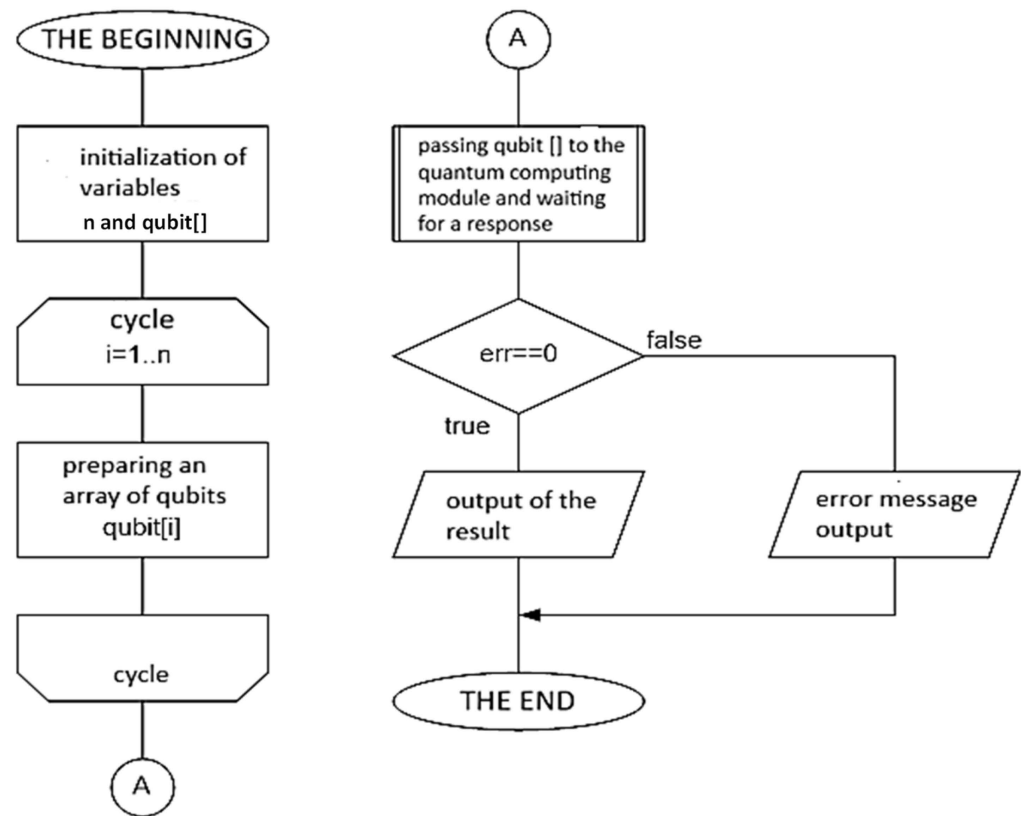


Figure 4. The scheme of the algorithm of the classical computing module.

The classical computing module is the main module of the program, and its task is to manage the QCNM, namely, to prepare the initial data, transfer them to the quantum emulator module and process the results obtained. At the initial stage of the module algorithm, an array of qubits [i] of length n is initialized, which is necessary for modeling the quantum system under consideration. Next, the elements of this array are prepared, depending on the type of Hamiltonian \hat{H} of SE (1), and transferred to the quantum computing module for simulation on a quantum emulator. After receiving a response from this, in the absence of an error flag, output data are generated based on the obtained simulation results.

The scheme of the algorithm of the quantum computing module is shown in Figure 5.

At the initial stage, this module converts the resulting qubit array into the corresponding Hamiltonian matrix and simulates its quantum evolution using the proposed modified Zalka–Wiesner method. At the same time, to emulate quantum operations, it is possible to use built-in Q# language operations, such as *Exp*—to calculate the matrix exponent, *DcomposedIntoTimeStepsCA*—to perform a single step in the evolution of the Hamiltonian, etc. [12,53,54]. The main part of the quantum module algorithm is the iterative process of calling the Trotter–Suzuki transformation procedure, in accordance with expression (5). In this case, the QFT algorithm is used, based on formulas (6) and (7), implemented according to the scheme in Figure 3. Upon completion of the iterative process, an array of “result” is formed containing the numerical data of the simulation and the variable “err”, equal to 1 in case of errors in the operation of the module and 0 in their absence. These data are passed back to the classical computing module for processing.

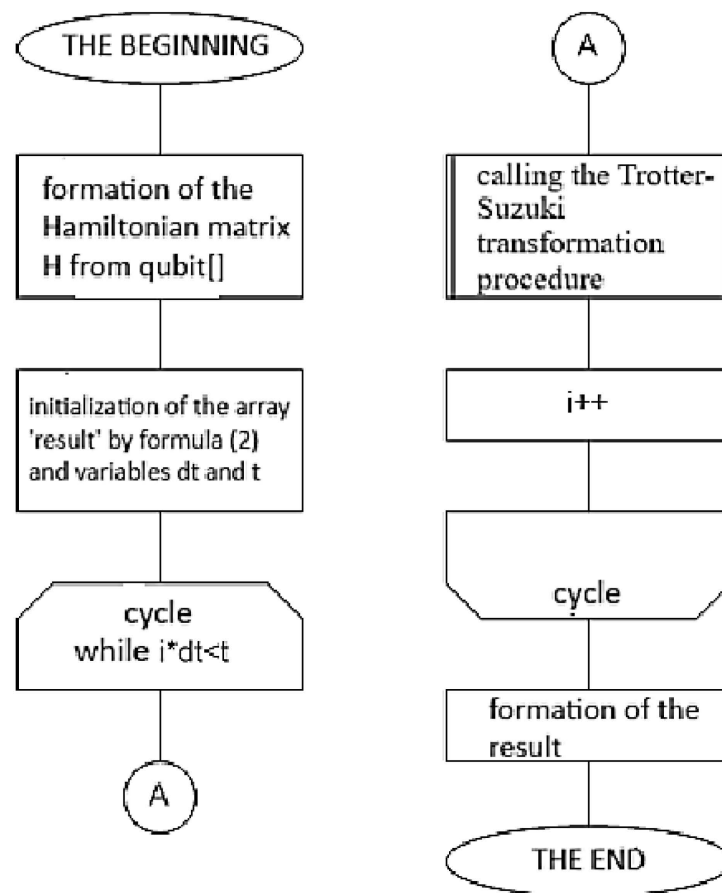


Figure 5. The scheme of the algorithm of the quantum computing module.

3. Results

Using the developed software package implementing the algorithm of the proposed QCNM, we conducted a study of a magnetostrictive Geisler alloy of the *Ni-Mn-Ga* type, the crystal lattice structure of which is shown in Figure 6. In the case when the atom of matter in question contains electrons, it is necessary to take into account the influence of each of them on the total kinetic and potential energy, as well as the interelectronic interaction between them. The Hamiltonian of the SE (1) for such an alloy, as is known [42,53–57], can be written in the Born–Oppenheimer approximation as:

$$\hat{H} = \sum_{i=1}^N \left[-\frac{\hbar^2}{2m_i} \left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right) - k \frac{Ze^2}{|\bar{r}_i|} + k \sum_{\substack{j=1 \\ (j>i)}}^{i-1} \frac{e^2}{|\bar{r}_i - \bar{r}_j|} \right], \quad (8)$$

where m_i —the mass of the i -particle, \hbar —the reduced Planck constant, Z —the total charge of the atom, e —the charge of the electron, k —the proportionality coefficient in Coulomb’s law, and \bar{r}_i —the radius-vectors of electrons.

As a result of modeling the microparticle system described by the Hamiltonian (8) using the QCNM algorithm on a classical computer, numerical data of its energy characteristics were obtained. When studying magnetostrictive phenomena, the values of possible magnetostrictive deformations of a material, depending on its structure, temperature, the presence of an external magnetic field, etc., are of the greatest interest. Based on the numerical data obtained, using a well-known technique, given for example in [42], graphs of some of these dependencies were constructed. Figure 7 shows graphs of the dependence of magnetostrictive deformations e_i on the modulus of elasticity a (Figure 7a) and temperature t (Figure 7b) when the alloy is in magnetic fields of different intensity.

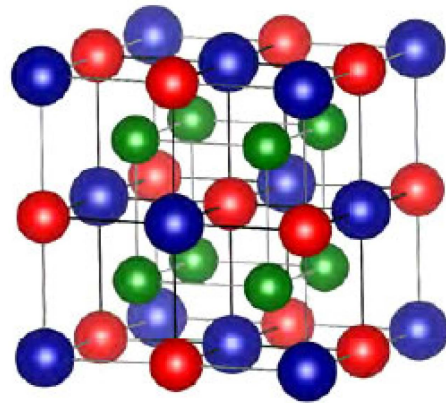


Figure 6. The crystal lattice cell of the *Ni-Mn-Ga* alloy [42].

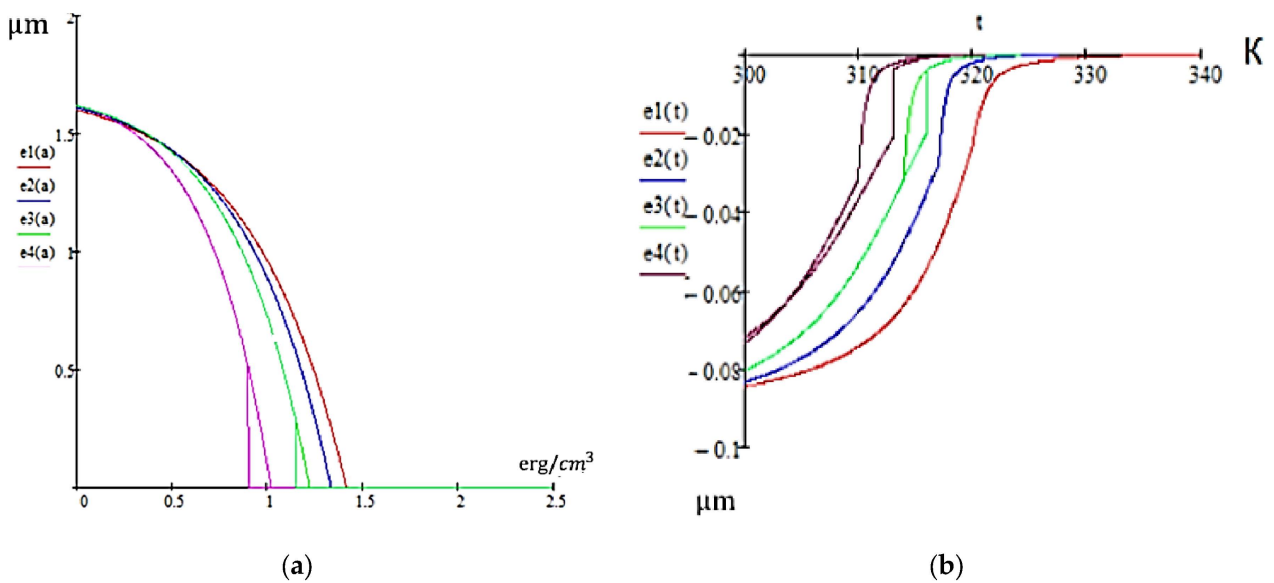


Figure 7. Dependency graphs of magnetostrictive deformations of *Ni-Mn-Ga* alloy at constant magnetic fields of 5, 14, 25, and 30 T. (a) graphs of the dependence of magnetostrictive deformations on the modulus of elasticity; (b) graphs of the dependence of magnetostrictive deformations on temperature.

The temperature and elastic dependences of deformations at constant magnetic fields of 5, 14, 25, and 30 T, shown in Figure 7, show that the hysteresis width decreases with increasing value of the external field, and in a field with an induction value of more than 25 T, the hysteresis disappears. A comparison of the graphs in Figure 7 with the known results of modeling *Ni-Mn-Ga* alloys and experimental data of similar characteristics shown in Figure 8 shows deviations of no more than 5% when modeling the dependence of deformation on the modulus of elasticity and no more than 7% when constructing its dependence on temperature, at the boundary points of the hysteresis loop or at the inflection points of graphs, in its absence. This indicates the correctness of the QCNM algorithm in the investigation of magnetostrictive phenomena.

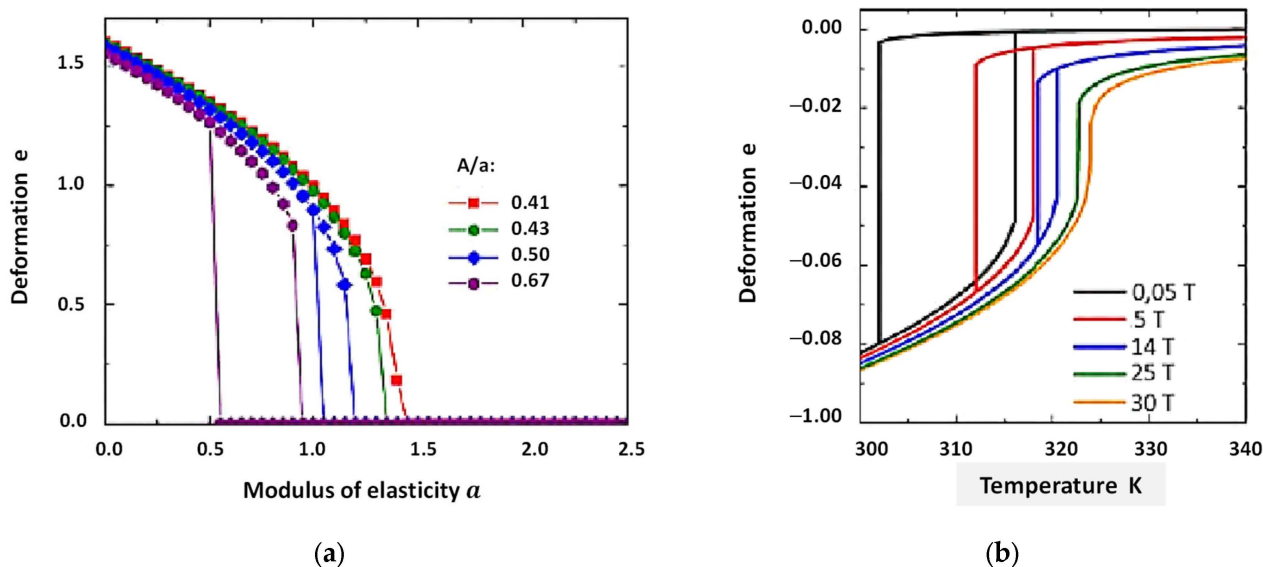


Figure 8. Experimental characteristics of magnetostrictive deformations of *Ni-Mn-Ga* alloy [42–47]. (a) graphs of the dependence of magnetostrictive deformations on the modulus of elasticity; (b) graphs of the dependence of magnetostrictive deformations on temperature.

4. Conclusions

Within the framework of the study, the development of a QCNM algorithm was carried out, suitable for modeling polyatomic systems, including magnetostrictive phenomena, at the micro level, suitable for modeling the magnetostrictive properties [58–61]. The approach used to solve the problem is the most effective because it allows one to combine the capabilities of modern numerical methods, complementing them with the advantages of quantum methods.

The proposed QCNM algorithm is based on a modification of the Zalka–Wesner method for solving the Schrodinger equation by using the Trotter–Suzuki transform and the quantum Fourier transform implemented on a quantum emulator.

During the research of magnetostrictive phenomena in *Ni-Mn-Ga* Geisler alloys using the developed software package, similar results were obtained to the known experimental ones, which confirms the correctness of the algorithm of the proposed QCNM.

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Data Availability Statement: The raw data cannot be shared at this time as the data also form part of an ongoing study.

Conflicts of Interest: The authors declare no conflict of interest.

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