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Simulation of quantum systems by the tomography Monte Carlo method

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***Abstract*. A new method of statistical simulation of quantum systems is presented which is based on the generation of data by the Monte Carlo method and their purposeful tomography with the energy minimisation. The numerical solution of the problem is based on the optimisation of the target functional providing a compromise between the maximisation of the statistical likelihood function and the energy minimisation. The method does not involve complicated and ill-posed multidimensional computational procedures and can be used to calculate the wave functions and energies of the ground and excited stationary sates of complex quantum systems. The applications of the method are illustrated.**

Keywords: *statistical simulation of quantum systems, Monte Carlo method, statistical likelihood function.*

1. Introduction

The study of quantum systems is important for solving modern applied problems of physics, chemistry, micro and nanoelectronics, biotechnology and other scientific fields. Because only few quantum-mechanical problems can be solved exactly, the methods of numerical mathematical simulation become increasingly urgent. The fundamental breakthrough in the field of information technologies, which can be achieved in the near future, is also related to the development of principles of quantum calculations [1 – 3]. However, the realisation of the concept of a quantum computer itself requires time-consuming calculations for developing the physical principles of functioning and interaction of the basic elements of quantum information – qubits.

The numerical methods of studying the Schrödinger equation can be divided into regular (deterministic) and statistical methods. In the case of multidimensional problems, the deterministic methods run into serious calculation problems. For example, if we wish to specify a regular grid to study a system consisting of 10 particles, even in the absence of a spin the problem is described in the configuration space of dimensionality 30. If we specify the grid of only 10 points for each of the variables, then 10^{30} nodes should be specified in the entire configuration space. We see that the complexity of simulations increases exponentially with the number of particles in the system. It is clear that such a huge amount of data cannot be recorded in and processed with the help of modern materials.

In our opinion, statistical simulation methods can provide a substantial progress in the investigation of multidimensional quantum-mechanical problems. Moreover, the application of these methods is justified due to the fundamental statistical nature of quantum phenomena themselves. It should be taken into account that the statistical behaviour of quantum systems principally differ from classical random processes (such as diffusion). The difference is that the statistical simulation of quantum systems should be performed taking into account the known Bohr principle of complementarity. According to this principle, to perform the complete statistical description of a quantum state, it is necessary to use data from different unitarily coupled representations. For example, data from the coordinate space should be supplemented with data from the momentum space [4, 5].

Within the framework of the statistical approach, a quantum state can be described by two methods: either by using the state vector (ψ functions) or specifying samplings from mutually complementary distributions. If the sizes of mutually complementary samplings are large, both these methods are almost equivalent. In particular, the ψ function can be approximately reconstructed from samplings (by using quantum tomography).

The energy of a quantum state, which we wish to minimise, can be most simply calculated from mutually complementary samplings. In this case, the coordinate sampling is used to calculate the potential energy, and the momentum sampling is used to calculate the kinetic energy. Note that, the problem of minimisation in the classical problem is reduced to the trivial rolling down of all points to the potential well bottom in the coordinate space and to the stopping of all points in the momentum space. In quantum mechanics, according to the uncertainty relation, such a scenario is impossible. According to the complementarity principle, the coordinate and momentum distributions should reflect the same object, namely, the complex ψ function, while the coordinate and momentum wave functions should be related by the Fourier transform.

The manipulation by data in the coordinate and momentum spaces should be performed keeping in mind that a single state vector should correspond to mutually complementary data. This requirement is provided by

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quantum tomography. The so-called root approach was successfully used in experimental studies on the statistical reconstruction of polarisation quantum states of three- and four-level optical quantum systems [6–9]. It was shown by mathematical simulations that statistical methods can be also used to reconstruct and control the state vector in multidimensional Hilbert spaces (for example, when the number of basis states amounts to many hundreds or thousands) [4, 5, 10].

The main goal of mathematical simulations within the framework of the proposed approach is the calculation of the vectors of stationary quantum states by using statistical evolution in the direction of decreasing energy. The method is based on the optimisation of the target functional formed by the factors taken with the opposite signs, which take into account the statistical logarithmic likelihood function and energy. The iterative numerical procedure is performed to define more accurately step-by-step the quantum state vector until the system reaches the minimum energy with a high accuracy. Note that the reconstruction of excited stationary states is achieved by the elementary refinement of the algorithm and does not lead to any complications compared to the determination of the ground state. In this case, it is necessary to work simply in the space of vectors which are the orthogonal complement to the reconstructed stationary state vectors.

This approach has, in our opinion, a substantial advantage over the known method of statistical simulation of quantum systems – the so-called diffusion quantum Monte Carlo method [11, 12]. The traditional quantum Monte Carlo method is based on the representation of the Schrödinger equation in the form of the diffusion equation for the imaginary time. This method ignores the phase of a wave function and, hence, the presence of mutually complementary distributions. Therefore, the diffusion Monte Carlo method can be mainly used to estimate the ground-state energy.

The proposed method of statistical tomography selection of quantum states offers an advantage over the traditional variation method [11, 12]. The main disadvantage of the latter is that, as a rule, it relies on a successful choice of the trial function with one–two unknown free parameters, which are selected from the energy minimisation conditions. If the ψ function has many parameters (tens, hundreds, thousands), the calculation procedure becomes an ill-posed problem of linear algebra. In addition, it is necessary to calculate an astronomical number of integrals. Note that the method proposed in this paper does not require the explicit calculations of integrals. The calculation problem related to the solution of the root likelihood equation is well-posed even if the state vector contains hundreds and thousands parameters, while the possibilities of the method itself are restricted in principle only by the resources of available computers.

2. Computational aspects of the method

Figure 1 illustrates schematically the procedure of statistical tomography simulations.

A quantum state is described by the state vector in the s-dimensional Hilbert space $c = (c_0, c_1, \ldots, c_{s-1})$. The state vector is obtained due to the quantum tomography procedure of optimising the target functional. The optimal value of the target functional corresponds to the compromise

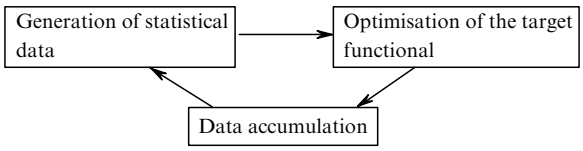

Figure 1. Scheme of the tomography simulation of quantum states.

between the maximisation of the statistical likelihood and energy minimisation. Statistical data are generated by the Monte Carlo method by using the Metropolis algorithm. The state vector is defined more accurately step-by-step by calculating the first principal component of the density matrix corresponding to the accumulated data.

Consider the main elements of the algorithm in more detail. Let us assume that it is necessary to provide the generation of points from a distribution with the probability density $p(x)$. The Metropolis algorithm [13–15] is based on the random walk of points with distribution tending asymptotically to the specified distribution $p(x)$. Practically, the asymptotic distribution can be obtained in the case of the optimal choice of random walk parameters after a few (three–five) iterations. In our case, simulation becomes even simpler because the evolution of distributions occurs continuously and, as follows from calculations, one–two iterations are sufficient.

The random walk algorithm is as follows. Let x_{old} be the position (coordinate) of a point at the given step of the iteration process, and x_{new} be its possible new (trial) position at the next step. The new possible coordinate can be calculated from the expression $x_{\text{new}} = x_{\text{old}} + dg$, where g is a random number uniformly distributed in the interval $[-0.5, 0.5]$ and d is the value specified by the user, which is usually equal to three–seven standard deviations.

The essence of the method is that the new position of the point can be accepted or not, depending on the value generated by a pseudorandom-number generator. For this purpose, the ratio f of the new probability density to the old one is calculated:

$$f = \frac{p(x_{\text{new}})}{p(x_{\text{old}})}. \tag{1}$$

Let us assume that this ratio proved to be greater than a random number γ uniformly distributed in the interval $[0, 1]$, i.e. $f > \gamma$; then, the new value of the coordinate is accepted, otherwise it is rejected, and the point remains in the old place. Due to the action of the algorithm, the point always jumps to a new place, if this is certainly advantageous (i.e. if the probability density at the trial point is higher). If, however, the probability density at a new point is lower, the jump is possible as well, but only with some probability, which is the higher, the smaller difference in the probability densities. It is assumed that the required distribution is established most rapidly (optimally), if 30 % – 50 % points move during one iteration, and the value of the parameter d is usually chosen according to this condition.

The maximum likelihood for the state vector is estimated, taking into account the restriction on the vector norm and energy, by optimising the variational functional of the form [16]

$$S = \ln L - \lambda_1(c_i c_i^* - 1) - \lambda_2 H_{ij} c_j c_i^*, \tag{2}$$

where H_{ij} are the matrix elements of the Hamiltonian; $\lambda_{1,2}$ are the Lagrange factors. Hereafter, summations is performed over repeating indices.

The logarithmic likelihood $\ln L$, taking into account statistical data in mutually complimentary coordinate and momentum spaces, is specified by the expression

$$\ln L = \sum_{k=1}^{n} \ln\left(c_i c_j^* \varphi_i(x_k)\varphi_j^*(x_k)\right) + \sum_{l=1}^{m} \ln\left(c_i c_j^* \tilde{\varphi}_i(p_l)\tilde{\varphi}_j^*(p_l)\right), \tag{3}$$

where $\tilde{\varphi}_i(p)$ is the Fourier transform of the function $\varphi_i(x)$. The term containing the Lagrange factor λ_1 takes into account the normalisation of the state vector.

The choice of the factor $\lambda_2 > 0$ determines the relative contribution of the energy term to the target functional. The maximisation of the value of S is a compromise between an increase in the logarithmic likelihood $\ln L$ and a decrease in the average energy $\bar{E} = H_{ij} c_j c_i^*$. For large values of λ_2, the energy term dominates, in accordance with the variational Monte Carlo method. Small values of λ_2 correspond to the solution of the problem based on the specified fixed data sampling.

The average energy $\bar{E}$ was estimated in particular calculations, which are considered below, from the sample average energy, i.e. the sum of the average potential energy, which can be measured in the coordinate space, and the average kinetic energy, which can be measured in the momentum space.

The equation following from the stability condition for the target functional represented above corresponds to the combination of the statistical maximum likelihood principle with the variational principle of quantum mechanics:

$$(R_{ij} - \lambda_2 H_{ij}) c_j = \lambda_1 c_i. \tag{4}$$

Here, the matrix R is determined by the expression

$$R_{ij} = \sum_{k=1}^{n} \frac{\varphi_i^*(x_k)\varphi_j(x_k)}{P(x_k)} + \sum_{l=1}^{m} \frac{\tilde{\varphi}_i^*(p_l)\tilde{\varphi}_j(p_l)}{\tilde{P}(p_l)}, \tag{5}$$

and the densities $P(x_k)$ and $\tilde{P}(p_l)$ correspond to the mutually complementary data in the coordinate and momentum spaces, respectively, corresponding to the same state vector c. It is assumed that n and m measurements were performed in the coordinate and momentum spaces, respectively.

Similarly, the matrix elements of the Hamiltonian can be estimated by the Monte Carlo method as

$$H_{ij} = \frac{1}{n}\sum_{k=1}^{n} \frac{\varphi_i^*(x_k) V(x_k) \varphi_j(x_k)}{P(x_k)} + \frac{1}{m}\sum_{l=1}^{m} \frac{\tilde{\varphi}_i^*(p_l) T(p_l) \tilde{\varphi}_j(p_l)}{P(p_l)}. \tag{6}$$

Here, T and V are the kinetic and potential energies of the system in the momentum and coordinate spaces, respectively.

By multiplying both sides of Eqn (4) by c_i^* and performing summation over i, we obtain the relation between the Lagrange parameters:

$$(n+m) = \lambda_1 + \lambda_2 \bar{E}. \tag{7}$$

The described algorithm analyses a fraction of statistical data containing, as a rule, a few hundreds or thousand points. The state vector is successively refined by using the accumulated density matrix [16]. Thus, if c_0 is the state vector at a step, corresponding to the sample size n_0, and c is the vector corresponding to the sample size n, the combined not normalised density matrix will be described by the expression

$$\rho = n_0 c_0 c_0^+ + n c c^+. \tag{8}$$

It can be shown in this case that the refined state vector should be estimated as the first principal component of the combined density matrix [16, 17].

Note that the considered method can be used for calculating numerically both the ground and excited states. In the latter case, the algorithm should be supplemented by a simple condition according to which the required state vector should be orthogonal to all the stationary states found earlier.

3. Applications of the method

The first illustrative example is the consideration of the stationary states of motion in the Peschl–Teller potential well. The corresponding potential is described by the expression [18, 19]

$$U(x) = -\frac{U_0}{\cosh^2(x/a)} = -\frac{\hbar^2}{2m_0 a^2}\frac{\lambda(\lambda-1)}{\cosh^2(x/a)}. \tag{9}$$

Here, m_0 is the particle mass; the dimensionless parameter λ characterises the potential well depth; and a is the spatial scale.

This problem can be solved exactly. We restrict our consideration to the discrete-spectrum states, i.e. the bound states corresponding to the negative or zero energy. The corresponding energy levels are described by the expression

$$E_n = -\frac{\hbar^2}{2m_0 a^2}(\lambda - 1 - n)^2, \tag{10}$$

where $n = 0, 1, \ldots, n_{\max}$, the condition $n_{\max} \leqslant (\lambda - 1)$ corresponding to the bound states.

The wave functions (not normalised) of the stationary states expressed in terms of the hypergeometric function can be written in the form

$$\psi_n(x) = \frac{1}{\cosh^{(\lambda-1-n)}(x/a)} \times F\left\{-n, 2\lambda - 1 - n, \lambda - n, \frac{1}{2}[1 - \tanh(x/a)]\right\}, \tag{11}$$

where $-\infty < x < \infty$. These function can be also expressed in terms of Gegenbauer polynomials, which are a particular form of the Jacobi polynomials

$$\psi_n(x) = \frac{1}{\cosh^{(\lambda-1-n)}(x/a)}\, C_n^{(\lambda-n-1/2)}[\tanh(x/a)]. \tag{12}$$

Figure 2 illustrates the agreement of numerical simulations with exact solutions. The shape of the potential well (for $\lambda = 7$), the energy levels of the stationary states (Fig. 2a), and the wave functions for the three first states (Figs 2b–d) are shown. The data are presented in the dimensionless system of units, in which Planck's constant $\hbar$, the particle mass m_0, and the potential spatial scale parameter a are equal to unity. The functions of a harmonic oscillator were used as basis functions in expansions in numerical calculations. The first 40 stationary energy states of the harmonic oscillator were used and a few hundreds of thousands of random points were generated. One can see that the results of statistical tomography simulation well agree with exact solutions. Note that, to increase the accuracy by an order of magnitude, the calculation time should be increased approximately by two orders of magnitude.

Another example concerns the study of a two-electron helium-like atomic system. Consider a negative hydrogen ion. The corresponding bond state of two electrons and a proton is quite 'friable'. The energy of the system (the experimental value is $E \approx -0.5277$ au [20]) is only slightly lower than the level -0.5 au at which the system can spontaneously decompose into a hydrogen atom and an electron. The negative hydrogen ion was first considered in classical papers of Bethe, Hylleraas, and Chandrasekhar [21–23] and papers of other authors.

Here we consider some aspects that are most interesting from the point of view of quantum informatics. Due to the above-mentioned 'friability' of the quantum state of the negative hydrogen ion, its treatment is considerably more complicated than that of the helium atom. In particular, the entanglement effects in the quantum state play a very important role. The negative hydrogen ion has no excited stationary states, while the ground state proves to be stable only to the entanglement effect due to which the wave function of the system of two electrons proves to be inseparable. Because of the entanglement, the self-consistent field Hartree–Fock approximation is insufficient for explaining the existence of a stable negative hydrogen ion.

The system under study has the zero spin. The two-electron wave function of the system can be written as a product of the coordinate and spin functions:

$$|\psi\rangle = \psi(\boldsymbol{r}_1, \boldsymbol{r}_2) \otimes \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \tag{13}$$

where the coordinate wave function should be symmetric with respect to the permutation of particles because the spin function is antisymmetric.

The hydrogen-like functions can be used as convenient basis functions in the study of atomic systems. In this case, the one-particle wave function in the coordinate space is described by the expression

$$\psi(\boldsymbol{r}) = \frac{\varphi_l(r)}{r}\, Y_{lm}(\theta, \varphi), \tag{14}$$

where r, θ, and φ are spherical coordinates; $Y_{lm}(\theta, \varphi)$ are spherical functions; l and m are the orbital and magnetic quantum numbers. The same wave functions in the momentum representation has the form

$$\tilde{\psi}(\boldsymbol{k}) = \frac{\tilde{\varphi}_l(k)}{k}\, Y_{lm}(\Theta, \Phi), \tag{15}$$

where k, Θ, and Φ are spherical coordinates in the momentum space.

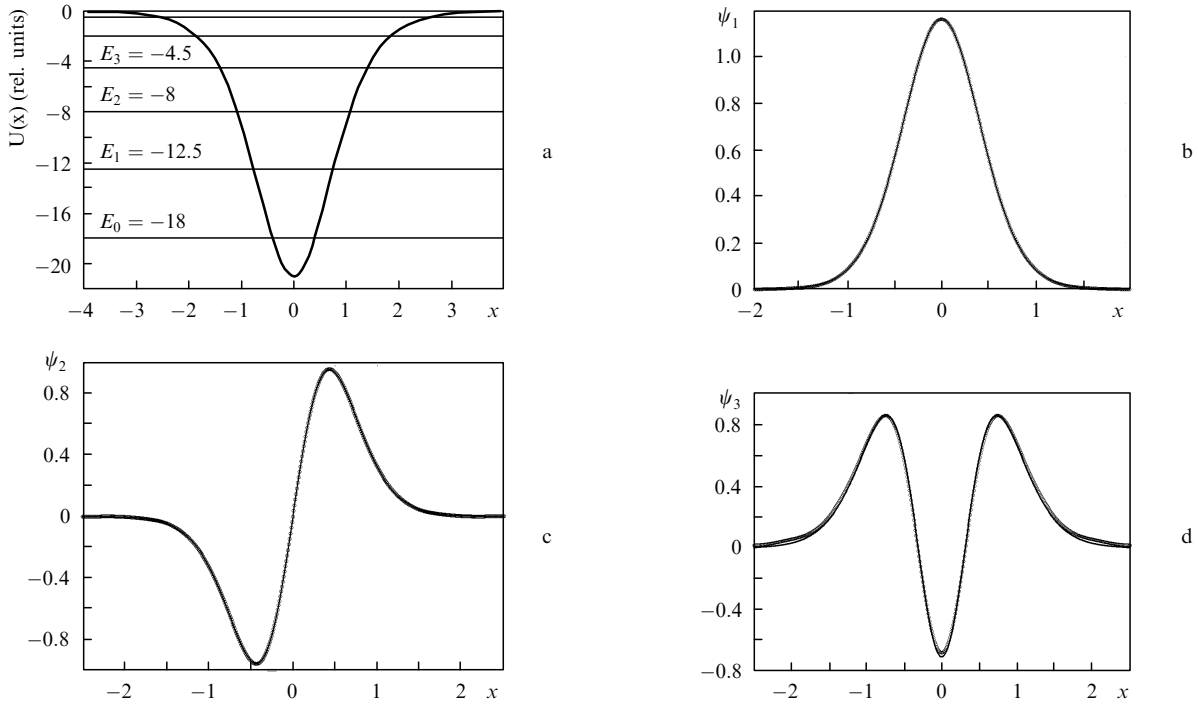

Figure 2. Simulations of stationary quantum states in the Peschl–Teller potential: the shape of the potential well (for $\lambda = 7$) and the energy levels of stationary states (a); the ground state ($F = 0.999993$, $E = -17.995$ au) (b); the first excited state ($F = 0.999992$, $E = -12.497$ au) (c); and the second excited state ($F = 0.998$, $E = -7.997$ au) (d).

The coordinate and momentum wave functions are related by the Hankel transformation [19]

$$\tilde{\varphi}_l(k) = \left(\frac{2}{\pi}\right)^{1/2} \mathrm{i}^{-l} \int_0^\infty \varphi_l(r) j_l(kr) \mathrm{d}r, \tag{16}$$

$$\varphi_l(r) = \left(\frac{2}{\pi}\right)^{1/2} \mathrm{i}^{l} \int_0^\infty \tilde{\varphi}_l(k) j_l(kr) \mathrm{d}k, \tag{17}$$

in which spherical Bessel functions entering integrands are defined as

$$j_l(kr) = \left(\frac{\pi kr}{2}\right)^{1/2} J_{l+1/2}(kr), \tag{18}$$

and the radial parts of the wave function are normalised by the condition

$$\int_0^\infty |\varphi_l(r)|^2 \mathrm{d}r = \int_0^\infty |\tilde{\varphi}_l(k)|^2 \mathrm{d}k = 1. \tag{19}$$

Note that, to calculate the Hankel transformation with hydrogen-like functions, it is only necessary to calculate finite sums and integrate the expressions containing the products of the power and exponential functions.

The basis was restricted in numerical calculations to the ten two-electron functions representing the product of one-electron centrally symmetric hydrogen-like functions ($l = 0$, $n = 1, 2, 3, 4$). The energy of the system was calculated to be $E = -0.5273 \pm 0.0008$ au, which coincides within the error with the experimental value presented above.

To describe the entanglement of a quantum state visually, we represent the wave function of a two-particle state in the form of the Schmidt decomposition [24, 25], in which, as follows from numerical calculations, only the two first modes make a substantial contribution. In this approximation, the radial two-particle wave function has the form

$$\psi(r_1, r_2) = \sqrt{\lambda_1}\psi_1(r_1)\psi_1(r_2) - \sqrt{\lambda_2}\psi_2(r_1)\psi_2(r_2). \tag{20}$$

Similarly to (19), we will normalise this wave function by the condition

$$\int_0^\infty \int_0^\infty |\psi(r_1, r_2)|^2 \mathrm{d}r_1 \mathrm{d}r_2 = 1. \tag{21}$$

The calculation shows that $\lambda_1 \approx 0.88$ and $\lambda_2 \approx 0.12$, and the total contribution of the third and higher modes does not exceed 0.5 %. The modes found in this way are shown in Fig. 3a. Note that the Schmidt modes are mutually orthogonal: $\langle\psi_2|\psi_1\rangle = 0$.

Let us explain the physical meaning of the Schmidt modes. As the degree of closeness of the states $|\psi\rangle$ and $|\chi\rangle$, we will use the square of the modulus of their scalar product (fidelity) $F = |\langle\chi|\psi\rangle|^2$; it is obvious that $0 \leqslant F \leqslant 1$. Among all the separable states specified by the product $\chi(r_1)\chi(r_2)$, the state defined by the first Schmidt mode, for which the parameter F takes the maximum possible value, proves to be the closest to the two-particle state $\psi(r_1, r_2)$. This means that, by using the method of self-consistent Hartree – Fock field corresponding to the separable approximation, the quantum state can be described with accuracy no better than $\lambda_1 \approx 0.88$, which is not sufficient for explaining the stability of the negative hydrogen ion.

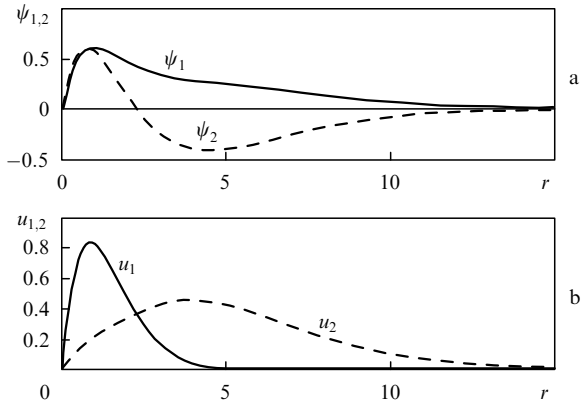

Figure 3. Schmidt modes (a) and orbitals (b) for the negative hydrogen ion.

Among all the two-mode approximations, the wave function specified by the two first Schmidt modes proves to be the closest to the true function. We can easily pass from the Schmidt representation to another visual representation of the entangled quantum state for the negative hydrogen ion

$$\psi(r_1, r_2) = N(u_1(r_1)u_2(r_2) + u_2(r_1)u_1(r_2)), \tag{22}$$

where $N = (\sqrt{\lambda_1} + \sqrt{\lambda_2})/2$ is the normalisation factor. Expression (22) can be called the two-orbital approximation for wave functions. The orbitals and Schmidt modes are related by the transformation

$$u_1(r) = \cos(\alpha)\psi_1(r) + \sin(\alpha)\psi_2(r), \tag{23}$$

$$u_2(r) = \cos(\alpha)\psi_1(r) - \sin(\alpha)\psi_2(r), \tag{24}$$

where the angle α is chosen so that the expansion has form (22) and does not contain the terms proportional to $u_1(r_1)u_1(r_2)$ and $u_2(r_1)u_2(r_2)$. This requirement leads to the condition

$$\alpha = \arctan\left(\frac{\lambda_2}{\lambda_1}\right)^{1/4}, \tag{25}$$

from which it follows that $\alpha \sim 30^\circ$. The obtained orbitals (Fig. 3b), unlike the Schmidt modes, are not orthogonal and

$$\langle u_2|u_1\rangle = \frac{\sqrt{\lambda_1} - \sqrt{\lambda_2}}{\sqrt{\lambda_1} + \sqrt{\lambda_2}}. \tag{26}$$

The two-orbital approximation can be visually interpreted as follows: each of the electrons, attempting to occupy the orbital closest to a proton, 'ejects' another electron into a more distant and more 'blurred' orbital (see Fig. 3b).

4. Conclusions

Let us summarise briefly the main results of the paper.

(i) A new method of the statistical simulation of quantum system has been proposed. The method is based on the generation of mutually complimentary data in the coordinate and momentum spaces and their purposeful tomography with the energy minimisation. Statistical

data were generated by using the Metropolis algorithm. The iteration procedure of the estimate of the state vector was based on the solution of the root likelihood equation and the calculation of the first principal component of the density matrix corresponding to the accumulated data. The method does not involve complicated and ill-posed multidimensional computational procedures and can be used to calculate the wave functions and energies of the ground and excited stationary states of quantum systems.

(ii) The examples of application of the proposed method and algorithm to a quantum system with the Peschl – Teller potential and to the two-electron state describing the negative hydrogen ion have been presented. The results of numerical calculations are in good agreement with analytic solutions and experimental data.

(iii) Based on the Schmidt expansion, the entanglement of the quantum state has been analysed for the negative hydrogen ion. It has been shown that the bound state of two electrons and a proton cannot be interpreted in the self-consistent field Hartree – Fock approximation and is described by the two-orbital model proposed in the paper. The Schmidt modes and quantum orbitals have been calculated numerically for this problem.

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