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Energy and density distribution of a finite number of interacting electrons in quantum dots

Kostrobij P. P., Polovyi V. Ye., Trynoha M. T., Pits O. Y.

Lviv Polytechnic National University,
12 S. Bandera Str., 79013, Lviv, Ukraine

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The paper considers a model of a two-dimensional interacting electron gas confined in an asymmetric oscillator potential well. It is investigated the energy of the system's ground state and electron density using restricted Boltzmann machine.

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1. Introduction

Description of interacting multi-electron systems (with the number of electrons $N \approx 10 - 100$) by solving the Schrödinger equation is a very complex mathematical modeling problem and is in fact NP-hard.

The recent development of quantum computating and machine learning [1–4] gives us a possibility to find energy and electron density for systems with a finite number of electrons without applying Monte–Carlo methods [5] by getting back to the usage of variational methods in quantum mechanics [6].

Since, in general, the variational wave function can have an arbitrary functional form, it is natural to use neural networks to solve a variational problem. As an example, we can provide so-called Boltzmann Machines [2, 4]. In work [7], such an approach was applied to describing a system of a finite number of interacting fermions that models a symmetric quantum dot.

However when developing a model of quantum dots the symmetry of the quantum dot should obviously be taken into account. In this work considered the simplest model of an asymmetric quantum dot – the electron in a potential well that can be described by an asymmetric oscillator. Modeling is conducted for the total energy and electrons density distribution using a restricted Boltzmann machine. The influence of the asymmetry of the quantum well on the calculated characteristics is analyzed.

2. Model Hamiltonian

Let us consider a two-dimensional electronic system in an asymmetric oscillatory potential well. Hamiltonian $\widehat{H}$ that will allow us to model the characteristics of a such system we present in the following form

$$H = -\frac{\hbar}{2m}\sum_{i=1}^{N}\Delta_i + \sum_{i=1}^{N}V(x_i) + \frac{1}{2}\sum_{i\neq j}^{N}\frac{e^2}{|\boldsymbol{r_i}-\boldsymbol{r_j}|}, \tag{1}$$

here

$$\Delta_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} \tag{2}$$

is the Laplace operator, and

$$V(x_i) = \frac{1}{2}m(\omega_1^2 x_i^2 + \omega_2^2 y_i^2)$$

is a potential that models an asymmetric hole; $\boldsymbol{r_i} = (x_i, y_i)$ is a radius vector that describes the position of the electron $(x_i, y_i) \in \mathbb{R}^2$, N is a number of electrons, e is an electron charge, and m is its mass. The last term in Eq. (1) describes the electron-electron interaction.

It is convenient to switch to the so-called atomic system of units [6] in what unit of measurement of coordinates (x_i, y_i) is the Bohr radius

$$a_0 = \frac{\hbar^2}{me^2},$$

and put

$$\hbar = m = e = 1,$$

in such a system of units;

$$H = \frac{1}{2}\sum_{i=1}^{N}\left(-\nabla_i^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \sum_{j\neq i}\frac{1}{r_{ij}}\right),$$

where $r_{ij} = |\boldsymbol{r_i} - \boldsymbol{r_j}|$.

Let us introduce the ellipticity parameter

$$\mu = \left(\frac{\omega_2}{\omega_1}\right)^2, \tag{3}$$

Then we can rewrite Eq. (2) as

$$H = \frac{1}{2}\sum_{i=1}^{N}\left(-\nabla_i^2 + \omega_1^2 (x_i^2 + \mu y_i^2) + \sum_{j\neq i}\frac{1}{r_{ij}}\right). \tag{4}$$

We will use model Hamiltonian (4) to evaluate energies of the ground state

$$E_0 \leqslant \langle\psi|\widehat{H}|\psi\rangle, \tag{5}$$

where H is defined by Eq. (4) and $|\psi\rangle$ is a trial wave function of the variational principle.

Following [7], we formulate several different ansatzes for the wave function $|\psi\rangle$.

The first

$$|\psi\rangle_{\text{Slater}-\text{Jastrow}}(R,\alpha,\beta) = g(R,\beta)\cdot|\psi\rangle_{\text{ref}}, \tag{6}$$

where

$$g(R,\beta) = \exp\left(\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right), \tag{7}$$

the Padé–Jastrow factor models correlations between electrons, where β is a variational parameter,

$$a_{ij} = \begin{cases} 1/3, & \sigma_i = \sigma_j, \\ 1, & \sigma_i \neq \sigma_j, \end{cases}$$

$$|\psi\rangle_{\text{ref}} = e^{-\omega_1(x^2+\sqrt{\mu}y^2)} H_m\big(\sqrt{\omega_1}x\big)\, H_n\big(\sqrt{\omega_2}y\big), \tag{8}$$

is an ansatz based on eigenfunctions of harmonic oscillator [6], $R = |r_i - r_j|$, σ_i is a spin of i-th electron.

The second and third ansatz are set respectively as

$$|\psi\rangle_{\text{RBM}}(R,\alpha,\beta,\omega) = P(R;\alpha,\beta,\omega)\cdot|\Phi\rangle_{\text{Slater}}, \tag{9}$$

$$|\psi\rangle_{\text{RBM+PJ}}(R,\alpha,\beta,\omega) = P(R;\alpha,\beta,\omega)\cdot g(R,\beta)\cdot|\Phi\rangle_{\text{Slater}}. \tag{10}$$

In the two last expressions

$$|\Phi\rangle_{\text{Slater}} = \det\left[\left\{H_m\big(\sqrt{\omega_1}x_i\big)\, H_n\big(\sqrt{\omega_2}y_i\big)\,\xi_k(\sigma_i)\right\}\right] \tag{11}$$

is a Slater determinant [2]

$$P(R;\alpha,\beta,\omega) = \exp\left(-\sum_{i=1}^{2N}\frac{(x_i-a_i)^2}{2\sigma_i^2}\right)\prod_{j=1}^{H}\left(1+\exp\left(b_j+\sum_{i=1}^{2N}\frac{x_i w_{ij}}{\sigma_i^2}\right)\right) \tag{12}$$

is a separated inputs distribution of a restricted Boltzmann machine [1].

According to the variational principle, the total energy of the considered system (4)

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{13}$$

where $\langle\ldots\rangle$ is a dot product in a Hilbert space and ψ is a wave function of the chosen ansatz (6)–(10).

3. Modeling algorithm

Applying parallel computing is crucial for increasing computational efficiency in solving multi-particle quantum systems. However, simply increasing the available computing resources is not always enough. You should also think about developing algorithms that will minimize the number of floating-point operations, minimize the number of caching errors, and minimize communication between parallel processes. As the basis for solving this problem, we adopt the algorithm proposed in [7].

As noted in [7], one of the most computationally expensive parts of the software implementation is finding the kinetic energy in the Schrödinger equation. The calculation process includes, among other elements, finding the Laplacian of the wave function. To increase efficiency, we rewrite the Laplacian as follows:

$$\frac{\nabla_i^2 \psi_T}{\psi_T} = \nabla_i^2 \ln \psi_T + (\nabla_i \ln \psi_T)^2. \tag{14}$$

This way of writing the expression for the Laplacian provides two important advantages. First, the logarithm provides greater numerical stability to the trial wave function, due to its exponential form. In general, this method is often used in various computational problems, including for many other ansatzes that are formulated for the trial wave function [7]. Second, this form allows us to separate the different elements of the wave function by writing the trial wave function as the product $\psi_T = \prod_j \psi_j$. The kinetic energy for each particle can then be written as the sum of the corresponding Laplacians and gradients

$$T = \sum_i \frac{\hbar^2}{2m} \nabla_i, \tag{15}$$

$$\frac{\nabla_i^2 \psi_T}{\psi_T} = \sum_j \nabla_i^2 \ln \psi_j + \left(\sum_j \nabla_i \ln \psi_j^2 \right)^2. \tag{16}$$

The next step will be to optimize the calculation of the Slater determinant,

$$\Psi(X) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_1, \sigma_1) & \psi_2(r_1, \sigma_1) & \dots & \psi_N(r_1, \sigma_1) \\ \psi_1(r_2, \sigma_2) & \psi_2(r_2, \sigma_2) & \dots & \psi_N(r_2, \sigma_2) \\ \dots & \dots & \dots & \dots \\ \psi_1(r_N, \sigma_N) & \psi_2(r_N, \sigma_N) & \dots & \psi_N(r_N, \sigma_N) \end{vmatrix}. \tag{17}$$

Here $X = \{x_1, x_2, \dots, x_N\} = \{\{r_1, \sigma_1\}, \{r_2, \sigma_2\}, \dots, \{r_N, \sigma_N\}\}$.

In the paper [7] it is noted that the direct computation of the Slater determinant is proportional to $O(n^3)$. It is obvious that for large values of n computational complexity will be quite significant, so it is worth looking for methods that will help to reduce the dimensionality for efficient calculation of the determinant.

One approach is to split the Slater determinant into so-called "spin-up" and "spin-down" [6] parts, without affecting the expected energy value in any way:

$$\psi_{\text{RBM}} = \det\left[\{\phi_{nm}(r_\uparrow)\, \xi(\sigma_\uparrow)\}\right] \times \det\left[\{\phi_{nm}(r_\downarrow)\, \xi(\sigma_\downarrow)\}\right]. \tag{18}$$

This reduces the dimension of the determinant.

Finding a general solution requires a matrix inversion procedure, which is quite computationally expensive. Therefore, as in [7], to reduce the computational cost, an approach is proposed in which particles are moved one by one during the configuration selection process. This means that the elements of either one row or one column of the Slater determinant will change. In turn, this approach leads to a simple relationship between the old and new inverse matrices:

$$d_{kj}^{-1} = \begin{cases} \frac{1}{R_i} d_{kj}^{-1}, & j = i, \\ d_{kj}^{-1} - \frac{S_{ij}}{R_i} d_{ki}^{-1}, & j \neq i. \end{cases} \tag{19}$$

Here R_i is the ratio between the new and old determinants, and S_{ij} is the cross product between the columns in the new rows and the old matrix. As a result, finding a new inverse Slater matrix requires

only a few operations if the previous inverse matrix is known. In (19)

$$R_i = \sum_{j=1}^{n} d_{ij} d_{ji}^{-1}, \qquad S_{ij} = \sum_{j=1}^{n} d_{il} d_{lj}^{-1}. \tag{20}$$

Using these expressions, the Slater determinant matrix inversion procedure is performed only once per simulation.

Finally, the gradient and Laplacian of the logarithm of the determinant relative to the i-th particle are given by the expressions

$$\nabla_i \ln \det = \sum_j \nabla_i d_{ji} d_{ij}^{-1}, \qquad \nabla_i^2 \ln \det = \sum_j \nabla_i^2 d_{ji} d_{ij}^{-1}.$$

In these equations, d_{ji} is the element in the j-th row and i-th column of the matrix, and d_{ij}^{-1} is the corresponding element of the inverse matrix.

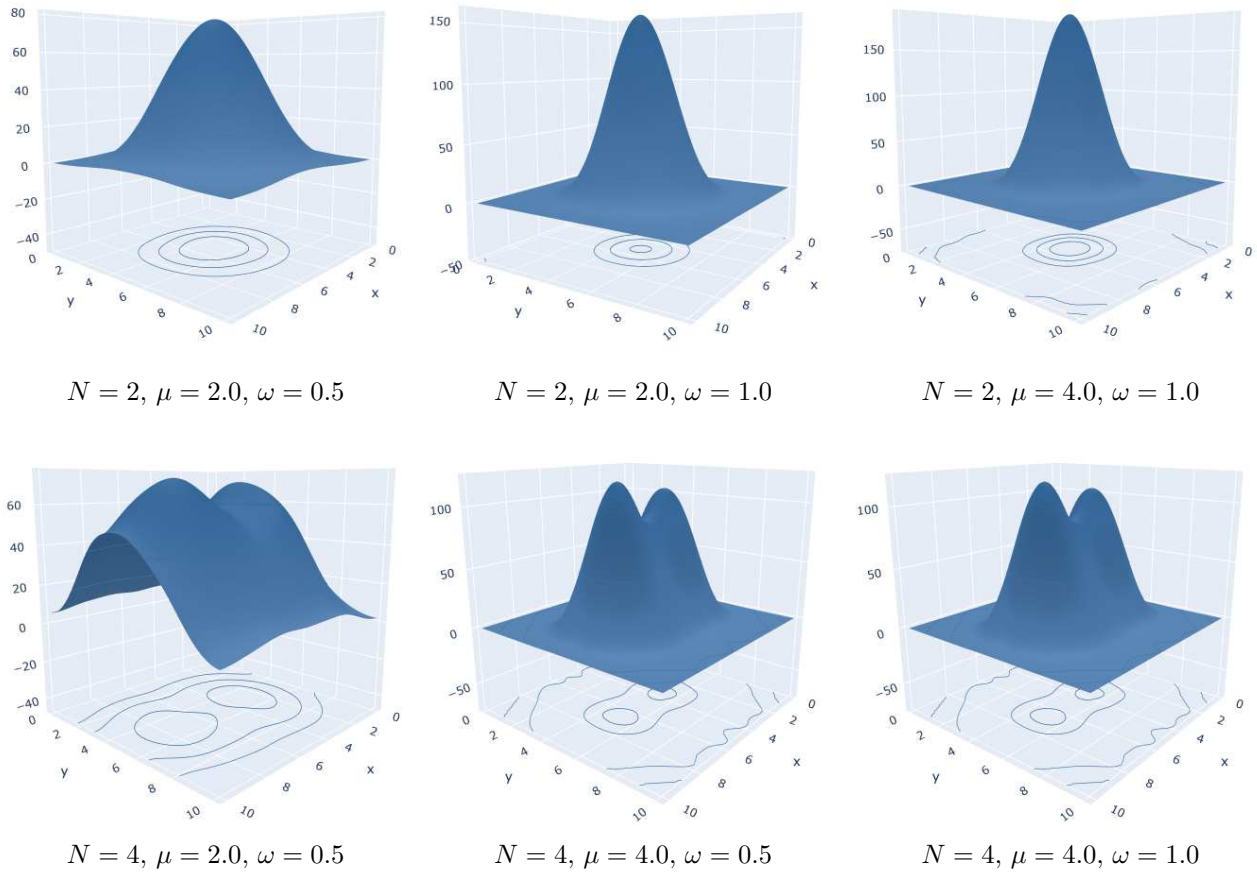
Table 1. In the column μ [7] denotes a row of results from the work [7].

N	ω	μ	RBM	RBM+PJ	Slater-Jastrow
2	0.1	[7]	0.46774	0.44098	0.44129
		1	0.47061	0.44107	0.44249
		2	0.52464	0.50128	0.52162
		4	0.62098	0.61654	0.62239
	0.5	[7]	1.72343	1.65963	1.65974
		1	1.75839	1.65938	1.65949
		2	2.03667	1.94501	1.95664
		4	2.22787	1.99085	2.10934
	1	[7]	3.07891	2.99958	2.99936
		1	3.05688	2.9993	3.018405
		2	3.70162	3.55287	3.56096
		4	4.20132	4.12645	4.34816
6	0.1	[7]	3.69711	3.57000	3.56951
		1	3.70702	3.64006	3.65316
		2	4.20246	4.06737	4.18436
		4	4.97731	4.78665	5.13467
	0.5	[7]	12.26400	11.80494	11.81042
		1	12.39571	11.80637	11.93453
		2	14.09163	13.64388	13.76409
		4	15.91770	15.46373	16.03382
	1	[7]	20.56356	20.17731	20.19182
		1	20.49953	20.18462	20.36222
		2	24.12246	23.42870	23.75789
		4	26.07410	25.25064	27.69342
20	0.1	[7]	30.79068	30.14422	30.04032
		1	30.72012	30.49311	30.91774
		2	36.21925	35.44858	35.65152
		4	39.19712	39.16432	39.73922
	0.5	[7]	96.35655	94.10111	94.04339
		1	96.51876	94.92191	94.17097
		2	109.32720	107.59112	109.76361
		4	120.45402	120.21697	120.95605
	1	[7]	159.42833	156.10411	155.89004
		1	158.69821	156.82013	157.21111
		2	179.84105	178.28382	171.82520
		4	193.39353	192.99321	196.35619

4. Simulation results

Let us analyse the results obtained in the process of calculating the energy of various multi-particle quantum systems (Table 1). As expected, with the parameter value $\mu = 1$, the results are almost identical to those of the work by [7]. The small error can be attributed to the inaccuracy of computer calculations, different outcomes when training the network, and limited computing power. From the results of calculations for $\mu = 2$ and $\mu = 4$) we can see that as the value of the parameter μ increases the energy value increases. Such results is to be expected, because with an increase in μ, the asymmetry of the quantum dot increases, which in turn leads to a weakening of the electron repulsion in the direction of the major axis of the ellipse. Considering the computational time for different ansatzes, we can say that the least expensive in this regard is the RBM ansatz (9). It is because it does not take into account the Padé-Jastrow factor. And the ansatzes (6) and (10) require significantly more time to calculate. As for other patterns and trends in the results, they are mostly similar to the ones presented in [7].

Also, calculations were performed to find profiles of single-particle electron density for different sets of parameters $N = \{2, 4, 6, 12\}$, $\omega = \{0.1, 0.5, 1.0\}$, $\mu = \{1, 2, 4\}$. The calculation results are presented in Figures 1, 2.

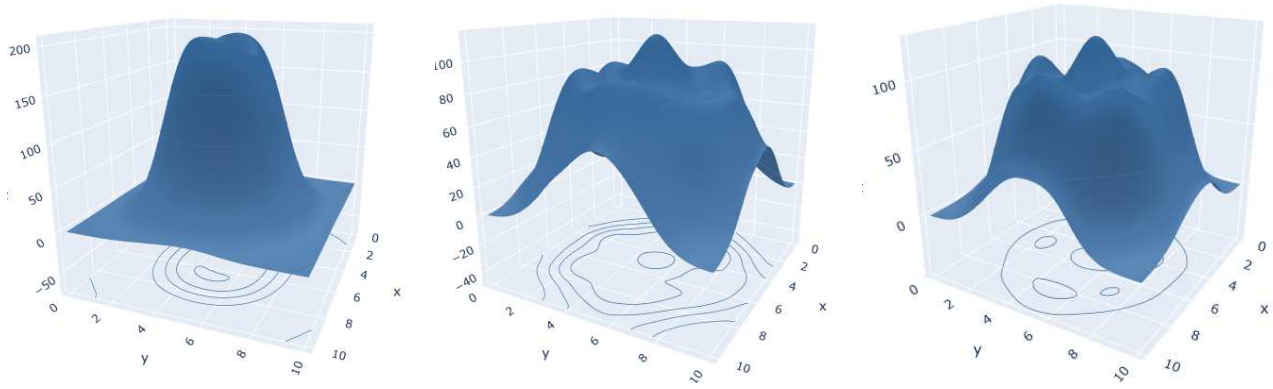


$N = 2$, $\mu = 2.0$, $\omega = 0.5$ | $N = 2$, $\mu = 2.0$, $\omega = 1.0$ | $N = 2$, $\mu = 4.0$, $\omega = 1.0$

$N = 4$, $\mu = 2.0$, $\omega = 0.5$ | $N = 4$, $\mu = 4.0$, $\omega = 0.5$ | $N = 4$, $\mu = 4.0$, $\omega = 1.0$

Fig. 1. One-body electron density profiles $\rho(x, y)$ for $N = 2, 4$, $\mu = 2, 4$ and $\omega = 0.5, 1.0$.

The results show that for high-frequency quantum dots $\omega = 0.5$ with an ellipticity parameter greater than 1 ($\mu = 2$, $\mu = 4$), potential asymmetry significantly affects electron density. However, when the frequency is increased to $\omega = 1.0$ for the same values of μ, the effect of ellipticity decreases, which can be explained by the fact that the increase in ω leads to an increase in the energy of particles that move freely in the field of the asymmetric oscillatory well.



$N = 6$, $\mu = 4.0$, $\omega = 1.0$ $N = 12$, $\mu = 2.0$, $\omega = 1.0$ $N = 12$, $\mu = 4.0$, $\omega = 1.0$

Fig. 2. One-body electron density profiles $\rho(x, y)$ for $N = 6$, 12, $\mu = 2$, 4 and $\omega = 0.5$, 1.0.

5. Conclusions

The paper considers the use of artificial neural networks for modeling two-dimensional multi-particle quantum systems. We considered methods and techniques for modeling the energy of such systems in an oscillatory field.

We investigated the possibility of using a neural network as a means of calculating part of the trial wave function for two-dimensional Coulomb systems in an asymmetric oscillatory field. This approach allows us to study quantum systems for which conventional methods of constructing wave functions require significant understanding and physical intuition. For simulation we considered three ansatzes, two of which are based on the discrete distribution of the restricted Boltzmann machine.

The results were obtained using the variational method with different trial wave functions. To take into account the asymmetry of the system, an ellipticity parameter μ was introduced, which specifies the relationship between the corresponding oscillator frequencies. As a result, we investigated the behavior of electrons in an asymmetric wavepoint model, more closely resembles experimental conditions.

[1] Godfellow I., Bengio Y., Courville A. Deep Learning. The MIT Press, Cambridge, Massachusetts (2016).

[2] Carleo G., Troyer M. Solving the quantum many-body problem with artificial neural networks. Science. **355**, 602 (2016).

[3] Carrasquilla J., Torlai G. Neural networks in quantum many-body physics: a hands-on tutorial. Preprint ArXiv:2101.11099 (2021).

[4] Carleo G., Cirac I., Cranmer K., Daudet L., Schuld M., Tishby N., Vogt-Maranto L., Zdeborová L. Machine learning and the physical sciences. Review of Modern Physics. **91**, 045002 (2019).

[5] Carleo B., Lester W., Reynolds P. Monte Carlo Methods in Ab Initio Quantum Chemistry. World Scientific, Singapore (1994).

[6] Vakarchuk I. O. Quantum Mechanics. Ivan Franko National University of Lviv; 4th edition (2012).

[7] Nordhagen E. M., Kim J. M., Fore B., Lovato A., Hjorth-Jensen M. Efficient solutions of fermionic systems using artificial neural networks. Frontiers in Physics. **11**, 1061580 (2023).

Енергія та розподіл густини скінченної кількості взаємодіючих електронів у квантових точках

Костробій П. П., Польовий В. Є., Тринога М. Т., Піц О. Й.

Національний університет "Львівська політехніка",
вул. С. Бандери, 12, 79013, Львів, Україна

У роботі розглянуто модель двовимірного взаємодіючого електронного газу, що знаходиться в асиметричній осциляторній ямі. Досліджено енергію основного стану системи та розподіл густини електронів, використовуючи обмежену машину Больцмана.

Ключові слова: *обмежена машина Больцмана; квантові точки; багатоелектронна система.*