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Nanotube on Ballistic Conduction

Inspection of Remodeling Impacts

Highlights

Errors of the Schrödinger Equation

Movements in Hydrosoluble Protein

Discovering Thoughts, Inventing Future

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Neutron, Proton, Electron are Questionable as the Basis of the Atom as Proton, Neutron, Electron Can be Seen as Reactions with Radium by British Scientists- We Can Return to A Mysterious Cloudy View of the Atom

By James T. Struck
Imaginary Heaven University

Abstract- Neutron discovered by James Chadwick could be questioned as alpha causes particle emission reaction product. Neutrons may not be fundamental but rather a reaction product. Electron discovered by JJ Thompson could be questioned as particles deflect to positive plate are possibly a gas or gravity effect? Proton could be questioned as radium effect with Au or Gold not fundamental.

Keywords: *electron, proton, neutron, radium, fundamental particles.*

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Neutron, Proton, Electron are Questionable as the Basis of the Atom as Proton, Neutron, Electron Can be Seen as Reactions with Radium by British Scientists- We Can Return to A Mysterious Cloudy View of the Atom

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Keywords: electron, proton, neutron, radium, fundamental particles.

I. Introduction

The discovery of fundamental particles neutron, electron and proton was based on reactions with radium by a few British scientists Ernest Rutherford, James Chadwick and JJ Thompson soon after the discovery of radium. One can argue all three fundamental particles are reaction products of radiation with radioactive radium and not really fundamental particles.

II. Methodology

3 Basic fundamental particles proton, electron, neutron are questionable based on the origin or discover of electron, proton and neutron. One could say electron, proton and neutron are reaction products with radium and not fundamental particles. Much like we see light as wave particle reality; we can argue again that the atom also is partly a reaction product with radium and really an electron, proton and neutron. [1]

III. Results and Discussion

We can return to the idea of a somewhat mysterious atom as all three fundamental particles could or may be reaction products with radioactive radium. Radium chemistry and radium physics can be seen as the origin of the electron and proton and neutron not really fundamental particles. Electron, proton, neutron may have been reaction products with radium and not fundamental parts of the atom.

IV. Conclusion

Radium reactions are the basis of the British discovered electron, proton and neutron. James Chadwick threw radium at atoms and got radium reactions. Rutherford threw radium at gold and got radium reactions not fundamental particles. JJ Thompson used a Crookes and possibly learned about the way radium behaves not the fundamental particles. British discoveries of fundamental particles are limited in importance and the whole atom may actually be more of a mysterious atom.

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References Références Referencias

1. References to how the Neutron, Proton, Electron were discovered or accessed from yahoo and google website searches on these fundamental particles origins.

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Inspection of Remodeling Impacts of Domain Movements in Hydrosoluble Protein using Dual Artificial Intelligence Methods

By Katsuhiko Nishiyama

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Abstract- Remodeling impacts of domain movements in protease are of interest in many fields such as medical treatments, food processing, and bio-electronic devices. However, they are yet to be precisely explained. In this study, the remodeling effects in ficin were investigated via a deep neural network, genetic programming, and computer simulations. The replacement (Y113F) in ficin using domain movements exhibited a critical effect on the peptide compatibilities. Specifically, modification of amino acid allows the remodeling of the domain movements, and types of compatible peptides should be modulated by the remodeling. Moreover, the decision tree revealed important factors in peptides and ficin.

Keywords: protein, deep neural networks, genetic programming, molecular dynamics simulations.

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INSPECTIONOFREMODELINGIMPACTSOFDOMAINMOVEMENTSINHYDROSOLUBLEPROTEINUSINGDUALARTIFICIALINTELLIGENCEMETHODS

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Inspection of Remodeling Impacts of Domain Movements in Hydrosoluble Protein using Dual Artificial Intelligence Methods

Katsuhiko Nishiyama

Abstract- Remodeling impacts of domain movements in protease are of interest in many fields such as medical treatments, food processing, and bio-electronic devices. However, they are yet to be precisely explained. In this study, the remodeling effects in ficin were investigated via a deep neural network, genetic programming, and computer simulations. The replacement (Y113F) in ficin using domain movements exhibited a critical effect on the peptide compatibilities. Specifically, modification of amino acid allows the remodeling of the domain movements, and types of compatible peptides should be modulated by the remodeling. Moreover, the decision tree revealed important factors in peptides and ficin.

Keywords: protein, deep neural networks, genetic programming, molecular dynamics simulations.

I. Introduction

Thermally produced movements of proteinous structure are perceived as the dominant factors involved in its biotic performance [1, 2, 3, 4], and their deliberate remodeling might lead to the discovery of an untapped resource. The majority of protein is organized via certain domain parts, and these domains are moving. Remodeling the domain movements would considerably influence molecular interactions between protein and ligand. Such interactions are of interest in many fields such as medical treatments, food processing, and bio-electronic devices [5, 6, 7, 8, 9], and their remodeling would provoke a breakthrough in these fields.

Hydrosoluble protein ficin separates certain peptides bound in sites near its active center, and its characteristics are beneficial to the improvement of transfusion safety, the development of novel antimicrobial therapeutics, and as a method for meat tenderization [10, 11, 12]. The structure of ficin is formed from two domains, and the binding areas of peptides are found in the two domains. Peptide binding is strongly affected by the domain movements, and therefore, remodeling the domain movements should affect the separation properties.

The two domains of ficin are joined by the β strand, which acts as a hinge. Modification of amino acid in the β strand would guide ficin to remodel the domain movements. It is desirable to be able to clearly explain the resulting effects of remodeling on peptide binding in more detail. Considering that ficin is a member of the protease family, reports on protease inhibitors play a large role in perceiving the effects [13, 14, 15, 16, 17]. However, remodeling effects of the domain movements in ficin to peptide bindings have not yet been clearly revealed.

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The purpose of this research was to remodel the domain movements in ficin by modifying its local structure, and to clarify the effects of the remodeling to peptide bindings. Several possible combination patterns are possible for peptide, but the priority order of the search was unclear. The selection of combinations was conducted using deep neural networks (DNN) [18], and factors which enormously influence the peptide bindings were identified via genetic programming (GP) [19]. Characteristic features of various proteins were analyzed by molecular dynamics (MD) and docking simulations [20, 21, 13, 14, 22]. The moving structures of locally modified ficin were produced by MD simulation, while the binding states of peptides on the structures were assessed by docking simulations.

For the site near the center of the β strand between the two domains of ficin, the amino acid was replaced by another one (Y113F). For the first trial, a similar amino acid (F) was selected for this replacement. In the previous study, the binding properties between the tetrapeptides and ficin were investigated by DNN, GP, MD and docking simulations [23]. Tetrapeptide structures have multiple structures, and they often have weights comparable to the protease inhibitor E64. In this study, the behavior of tetrapeptides on the replaced structure of ficin (ficin_Y113F) was researched using the dual artificial intelligences (AIs) and the simulations.

II. Methods

The selection speed of candidate peptides was better for DNN than for GP, and thus DNN was utilized to select the candidates for this pursuit. The factors that influence the peptide bindings need to be clarified, but they cannot be derived using DNN. Therefore, the factors were extracted using GP.

The potential candidates were selected through the use of a convolutional neural network (CNN) [24]. CNN is a type of DNN, and its structure was constructed using the deep learning library TensorFlow [25]. CNN is actively used in fields of image processing, and is capable of treating a large amount of partially reliable data. Its structure is composed of seven layers, namely, input layer, first convolutional layer, first pooling layer, second convolutional layer, second pooling layer, fully connected layer, and output layer. A tetrapeptide comprises a combination of four amino acids, and the amino acids contain multiple atoms. For each amino acid, each atom was numbered. The numbers were set in the input layer. For more stable binding states between tetrapeptide and sites near active center of ficin_Y113F, the distance between atoms in the peptides and its active center was calculated. The binding characteristics of peptides were classified by the respective numbers of atoms nearer than 4.0 Åto its active center. The classification rule was as follows: NA1$\geqq$3 atoms, 3 atoms>NA2$\geqq$2 atoms, 2 atoms>NA3$\geqq$1 atoms, or 1 atoms>NA4. The successive numbers from 1 to 4 were assigned to NAα (α = 1–4), and were set in the output layer. Further, the first ten tetrapeptides were derived from the DNN for ficin [23], and their binding properties to ficin_Y113F were investigated by the simulations. Thereafter,

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the first training data was created from the investigated results and training data of ficin [23]. Subsequently, the first DNN was constructed from the first training data, and consequently produced the second set of ten tetrapeptides. The properties of the second set of ten tetrapeptides were investigated in a similar manner, and second training data was made from the investigated results and the first training data. Consequently, the second DNN was constructed from the second training data, and subsequently produced the third ten tetrapeptides. Thus, this process was repeated, and various tetrapeptides were produced.

Highly Influencing factors to the peptide bindings were identified via GP. GP is an extended genetic algorithm (GA) technique, and it allows the exploration of the space of computer programs. The hyperparameters of GP were set with reference to a previous study [26], and evolutionary computing iteration was used to optimize the decision tree. The first time, entire areas of the decision tree were target of optimization. Thereafter, for the second and subsequent times, partial areas of the decision tree were randomly selected as optimization targets [27]. During the construction process of the decision tree, its size was expanded to satisfy the training data. Then, one of the successive numbers from 1 to 4 was set in the output of the decision tree, where the successive numbers corresponded to NAα (α = 1–4). For a tetrapeptide, four amino acids were labeled as amiβ, β = 1–4 from the N-terminus to the C-terminus. Each amino acid (amiβ) contained different types of atoms, and the number of each atom was represented by adding the atomic symbol at the end of amiβ. For instance, ami4S represented the number of sulfur atoms in amino acid of the C-terminus. The 20 attributes related to tetrapeptide were represented as amiβC, amiβN, amiβO, amiβS, and amiβAC (β = 1–4) [28]. 113 th amino acid of ficin was represented as ami113fic, and the number of each atom in ami113fic was represented by adding the atomic symbol at the end of ami113fic. The distance between domains of ficin was represented as domainDist, and it was assigned a numerical value of 0 for minimum distance, 1 for average distance, and 2 for maximum distance [23]. Further, 6 attributes related to ficin were represented as ami113ficC, ami113ficN, ami113ficO, ami113ficS, ami113ficAC, and domainDist. 19 operations (Add, Sub, Mul, Div, Fmod, Log, Log10, Sin, Cos, If, Equal, NotEqual, GT, GE, And, Or, Not, Fmod2, and Sqrt) and the 12 constants(a constant integer number CSTγ (γ) (γ = 0–9) and a boolean value TRUE (1), FALSE (0)) were inherited from our previous studies [23, 27, 29, 28]. Furthermore, the construction factors of the decision tree were chosen from the 26 attributes, 19 operations, and 12 constants.

The structures of ficin_Y113F with movements were produced by MD simulation through the use of the packaged software AMBER 12.0 [30]. The initial coordinate data of ficin_Y113F was produced by homology modeling through the use of the software MODELLER [31, 32]. For homology modeling, structural prediction was performed from sequence homology with known structures. The produced structure of ficin_Y113F was solvated with 11,843 TIP3P water molecules [33] inside a rectangular box. For the solvated system, its temperature was gradually increased from 5 to 300 K over

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a period of 140 ps, and subsequently it was retained over a period of 100 ns until the precipitous structural changes vanished. Moreover, the ff03.r1 force field [34] was applied to manage MD simulation, and the hyperparameters were set by referencing the previous study [28]. In addition, the pressure and temperature were set using the Berendsen algorithm [35]. The long-distance electrostatic interactions were calculated using the particle mesh Ewald method [36]. The domain movements in ficin_Y113F were characterized as the distance variation between them for the period after the disappearance of precipitous structural changes. Thereafter, the average and snapshot structures were produced after the disappearance of the precipitous changes. The average structure was defined as $ficin_Y113F_ave$. Moreover, if the distance between the two domains of ficin_Y113F was at a maximum, the structure was defined as $ficin_Y113F_max$. Whereas, if the distance was at a minimum, the structure was defined as $ficin_Y113F_min$. The snapshot structures were made up of $ficin_Y113F_max$ and $ficin_Y113F_min$.

For $ficin_Y113F_ave$, $ficin_Y113F_max$ and $ficin_Y113F_min$, binding affinities of the peptides were evaluated through the use of AutoDock Vina [37]. This simulation software was executed by using the iterated local search global optimizer algorithm [38, 39] and the Broyden–Fletcher–Goldfarb–Shanno method [40], with its scoring function derived by machine learning. These methods contributed significantly to approximately two orders of size speed-up compared to the molecular docking software AutoDock 4 [41, 42, 43]. Further, the coordinate data of the tetrapeptides was built by using the LEaP module in AMBER 12.0 [30]. The exploration space over the surface of ficin_Y113F was restricted to the regions near the active center. The explorations were executed 10 times for each tetrapeptide, and the most stable state was chosen from them. For the most stable state, atoms in the tetrapeptide were counted only if they were found near the active center of ficin_Y113F. However, if there were certain members in the most stable docking state, the counted numbers were averaged.

III. Results

The temperature of the system was maintained at 300 K via MD simulations, and the precipitous structural changes of ficin_Y113F were surveyed at regular time intervals. For the structure of ficin_Y113F, the root-mean-square deviation (RMSD) between successive simulations was calculated to survey the precipitous changes(Figure S1). Consequently, the precipitous structural change was determined from the larger RMSD value, and they disappeared after 98,840 ps. The $ficin_Y113F_ave$ was estimated in the range of 99,901 to 100,000 ps, and the snapshot structures ($ficin_Y113F_max$ and $ficin_Y113F_min$) were derived from this range. Figure 1 shows the average structures of ficin and ficin_Y113F. The positional relation between the active center and the α–helix structure near the active center was changed by the replacement (Y113F). 10 tetrapeptides ((a) of Table S1) were selected as first candidates by using the data regarding ficin [23]. Thereafter, the candidates were docked to sites near active center of $ficin_Y113F_ave$, and the most stable styles were extracted.

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Ficin is member of the family of cysteine protease, and the thiol (SH) group of its Cys25 can efficiently separate peptide. Consequently, the sulfur atom of Cys25 (S-Cys25) was considered as the active center. To discover the talented peptides for ficin_Y113F, the number of the atoms nearer than 4.0 Åto S-Cys25 in the most-stable docking state were estimated. In case of certain most-stable states, the estimated numbers were averaged. These results were represented by NAα ($\alpha = 1$–4), and are listed in Table S2. Within the first ten peptides, one member (Asn–Ser–Lys–Gln) was compatible with the sites near S-Cys25 of ficin_Y113F. Moreover, machine learning of the CNN was executed with the addition of these results, and the next ten candidates ((b) of Table S1) were guided. The characteristics of the ten peptides were estimated by docking simulations (Table S2), and one member (Arg–Ala–Val–Val) was compatible with the sites. This process was repeated eight times, and thereby, the characteristics of 80 peptides were obtained (Table S2), within which 17 members were compatible. The compatible 17 peptides were deposited in ave of Table 1. Simultaneously, 38 members were identified as especially incompatible peptides (Table S3). The docking simulations of the compatible 17 peptides (ave of Table 1) to the sites near S-Cys25 of two snapshot structures ($ficin_Y113F_max$ and $ficin_Y113F_min$) were executed, and the results are presented in Table S4. Within the 17 peptides, nine members (max of Table 1) were compatible to the sites near S-Cys25 of $ficin_Y113F_max$ and six members (min of Table 1) were compatible to those of $ficin_Y113F_min$. Furthermore, the five members (both of Table 1) were compatible to them of both $ficin_Y113F_max$ and $ficin_Y113F_min$.

To determine the important factors related to the peptide bindings, a decision tree was constructed from the results of 17 tetrapeptides to the three states of ficin_Y113F ($ficin_Y113F_min$, $ficin_Y113F_ave$, and $ficin_Y113F_max$)(Table 1)and those of 4 tetrapeptides to the three states of non-modified ficin ($ficin_min$, $ficin_ave$, and $ficin_max$) [23]. The decision tree comprised 45 nodes, and its layout is indicated in Table 2 and Table 3. 11 attributes were included in the decision tree, and these were considered as the important factors. They were one ami1N, one ami1O, one ami1S, two ami2C, one ami3C, two ami3N, one ami113ficO, and two domainDist.
The acronyms were explained in Table S5.

IV. Discussion

The compatibilities of the 100 tetrapeptides to the sites near S-Cys25 of $ficin_Y113F_ave$ were revealed via a DNN, and MD and docking simulations. The 17 compatible peptides were found, and about 47 percent of them were not compatible for $ficin_Y113F_max$, and about 65 percent of them were not compatible for $ficin_Y113F_min$(Table 1). The compatibilities of the tetrapeptides to the sites near S-Cys25 of ficin_Y113F were grossly influenced by their domain movements. The five peptides were found to be compatible for the three states of ficin_Y113F(Table 1). The five peptides were not influenced by the domain movements of ficin_Y113F, and their structures would be an informative guide to drug development.

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For average structure of non-modified ficin ($ficin_ave$), only four peptides were compatible to the sites near S-Cys25 [23]. The replacement (Y113F) in ficin spread the compatible peptides within those of $ficin_ave$. Within the four peptides, only one peptide was compatible for the structure of non-modified ficin when the distance between their domains was at a maximum ($ficin_max$) [23]. In contrast, the replacement (Y113F) spread the compatible peptides within those of $ficin_max$ as well. Further, all the four peptides were not compatible for the structure of non-modified ficin when the distance between their domains was at a minimum ($ficin_min$) [23]. The replacement (Y113F) spread the compatible peptides within those of $ficin_min$ as well as above two structures and had significant influence on the compatibilities between the peptides and ficin with domain movements. Moreover, modification of amino acid in the hinge structure of protease can enable us to remodel the domain movements, while the types of compatible peptides should be regulated by the remodeling. The collaboration of a DNN, and MD and docking simulations can be utilized as a tool in clarification of induced effects by modification of domain movements in protease.

The decision tree was constructed to satisfy the results for the three structures of ficin_Y113F ($ficin_Y113 \quad F_min$, $ficin_Y113Fave$, and $ficin_Y113Fmax$) (Table 1) and also for the three structures of non-modified ficin ($ficin_min$, $ficin_ave$, and $ficin_max$) [23]. The tree was composed of 45 nodes, and the breakdown of its 45 nodes was 11 attributes, 25 operations, and 9 constants (Table 2 and Table 3). The 11 attributes included one ami1N, one ami1O, one ami1S, two ami2C, one ami3C, two ami3N, one ami113ficO, and two domainDist. Carbon atoms in second amino acid from the N-terminus of the peptide, nitrogen atoms in third amino acid from the N-terminus of it, and domain movements of the protein are the important factors governing the peptide compatibility. The three atoms (nitrogen, oxygen, and sulfur) in the N-terminus amino acid of the peptide, carbon atom in third amino acid from the N-terminus of it, and oxygen atom in 113 th amino acid in the protein must also be focused on. The 25 operations included four Add, three Sub, seven Mul, three Div, two Fmod, one Fmod2, three Sqrt, and two Sin. Many of the operations were the four basic arithmetic operations, and the peptide compatibility can be derived from comparatively elementary manner. The number of Sqrt was also relatively large, and numerical value could be be moderately changed. Furthermore, the logical operations were not included, and the derivation of the compatibility could not be expressed in binary form.

V. Conclusions

The remodeling effects of the domain movements in ficin were analyzed by using DNN, GP, MD, and docking simulations. The replacement (Y113F) in ficin had critical effect on the compatibilities between the peptides and ficin with domain movements. Further, modification of specific amino acid in protease can enable remodeling of the domain movements, and types of compatible peptides must be modulated by the remodeling. Moreover, the decision tree revealed that particular atom in particular amino acid in peptide and domain movements of the protease would be of central importance for the

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peptide compatibility. Furthermore, the tree indicated the contribution of oxygen atom in 113 th amino acid in the protease to the compatibility. Thus, the analytical approach consisting of DNN, GP, MD and docking simulations can offer valuable lessons to understand the remodeling effects of the domain movements for some structures of protease, and the other structures should be analyzed for further research.

Acknowledgments

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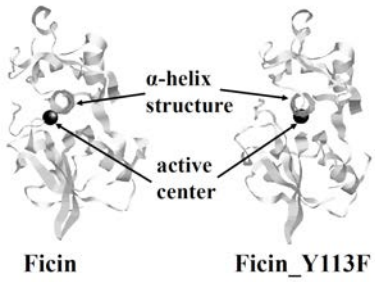


Figure 1: The average structures of ficin and ficin_Y113F.

Table 1: The compatible peptides.

ave	max	min	both
Arg–Ala–Val–Val			
Arg–Asp–Lys–Arg	◯	◯	◯
Arg–Gly–Arg–Gln	◯		
Arg–Gly–Asn–Ile	◯	◯	◯
Arg–Gly–Asn–Leu	◯	◯	◯
Arg–Gly–Asn–Lys	◯	◯	◯
Arg–Gly–Asn–Val	◯	◯	◯
Arg–Gly–Gln–Lys			
Arg–Gly–Pro–Ile	◯		
Arg–Gly–Pro–Leu			
Arg–Gly–Ser–Leu	◯		
Arg–Gly–Thr–Leu			
Arg–Gly–Val–Leu	◯		
Arg–Ser–Leu–Lys			
Asn–Ser–Lys–Gln		◯	
Lys–Gly–Leu–Gln			
Lys–Ser–Ile–Arg			

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Table 2: Layout of first part of decision tree (α:Input, β:Output, γ:Node).

$\gamma 0$	Fmod2[$\alpha 0 = \beta$ of $\gamma 1$][β = Solution]
$\gamma 1$	Fmod[$\alpha 0 = \beta$ of $\gamma 2$][$\alpha 1 = \beta$ of $\gamma 33$][$\beta = \alpha 0$ of $\gamma 0$]
$\gamma 2$	Mul[$\alpha 0 = \beta$ of $\gamma 3$][$\alpha 1 = \beta$ of $\gamma 32$][$\beta = \alpha 0$ of $\gamma 1$]
$\gamma 3$	Fmod[$\alpha 0 = \beta$ of $\gamma 4$][$\alpha 1 = \beta$ of $\gamma 27$][$\beta = \alpha 0$ of $\gamma 2$]
$\gamma 4$	Mul[$\alpha 0 = \beta$ of $\gamma 5$][$\alpha 1 = \beta$ of $\gamma 6$][$\beta = \alpha 0$ of $\gamma 3$]
$\gamma 5$	ami3N[$\beta = \alpha 0$ of $\gamma 4$]
$\gamma 6$	Sub[$\alpha 0 = \beta$ of $\gamma 7$][$\alpha 1 = \beta$ of $\gamma 8$][$\beta = \alpha 1$ of $\gamma 4$]
$\gamma 7$	domainDist[$\beta = \alpha 0$ of $\gamma 6$]
$\gamma 8$	Mul[$\alpha 0 = \beta$ of $\gamma 9$][$\alpha 1 = \beta$ of $\gamma 20$][$\beta = \alpha 1$ of $\gamma 6$]
$\gamma 9$	Add[$\alpha 0 = \beta$ of $\gamma 10$][$\alpha 1 = \beta$ of $\gamma 18$][$\beta = \alpha 0$ of $\gamma 8$]
$\gamma 10$	Mul[$\alpha 0 = \beta$ of $\gamma 11$][$\alpha 1 = \beta$ of $\gamma 17$][$\beta = \alpha 0$ of $\gamma 9$]
$\gamma 11$	Mul[$\alpha 0 = \beta$ of $\gamma 12$][$\alpha 1 = \beta$ of $\gamma 16$][$\beta = \alpha 0$ of $\gamma 10$]
$\gamma 12$	Div[$\alpha 0 = \beta$ of $\gamma 13$][$\alpha 1 = \beta$ of $\gamma 15$][$\beta = \alpha 0$ of $\gamma 11$]
$\gamma 13$	Sin[$\alpha 0 = \beta$ of $\gamma 14$][$\beta = \alpha 0$ of $\gamma 12$]
$\gamma 14$	Cst2[$\beta = \alpha 0$ of $\gamma 13$]
$\gamma 15$	domainDist[$\beta = \alpha 1$ of $\gamma 12$]
$\gamma 16$	ami2C[$\beta = \alpha 1$ of $\gamma 11$]
$\gamma 17$	Cst6[$\beta = \alpha 1$ of $\gamma 10$]
$\gamma 18$	Sqrt[$\alpha 0 = \beta$ of $\gamma 19$][$\beta = \alpha 1$ of $\gamma 9$]
$\gamma 19$	Cst3[$\beta = \alpha 0$ of $\gamma 18$]
$\gamma 20$	Add[$\alpha 0 = \beta$ of $\gamma 21$][$\alpha 1 = \beta$ of $\gamma 25$][$\beta = \alpha 1$ of $\gamma 8$]
$\gamma 21$	Mul[$\alpha 0 = \beta$ of $\gamma 22$][$\alpha 1 = \beta$ of $\gamma 24$][$\beta = \alpha 0$ of $\gamma 20$]
$\gamma 22$	Sqrt[$\alpha 0 = \beta$ of $\gamma 23$][$\beta = \alpha 0$ of $\gamma 21$]

Table 3: Layout of second part of decision tree (α:Input, β:Output, γ:Node).

$\gamma 23$	Cst4[$\beta = \alpha 0$ of $\gamma 22$]
$\gamma 24$	Cst7[$\beta = \alpha 1$ of $\gamma 21$]
$\gamma 25$	Sqrt[$\alpha 0 = \beta$ of $\gamma 26$][$\beta = \alpha 1$ of $\gamma 20$]
$\gamma 26$	Cst5[$\beta = \alpha 0$ of $\gamma 25$]
$\gamma 27$	Sub[$\alpha 0 = \beta$ of $\gamma 28$][$\alpha 1 = \beta$ of $\gamma 31$][$\beta = \alpha 1$ of $\gamma 3$]
$\gamma 28$	Mul[$\alpha 0 = \beta$ of $\gamma 29$][$\alpha 1 = \beta$ of $\gamma 30$][$\beta = \alpha 0$ of $\gamma 27$]
$\gamma 29$	ami1O[$\beta = \alpha 0$ of $\gamma 28$]
$\gamma 30$	ami3C[$\beta = \alpha 1$ of $\gamma 28$]
$\gamma 31$	ami1S[$\beta = \alpha 1$ of $\gamma 27$]
$\gamma 32$	Cst2[$\beta = \alpha 1$ of $\gamma 2$]
$\gamma 33$	Add[$\alpha 0 = \beta$ of $\gamma 34$][$\alpha 1 = \beta$ of $\gamma 35$][$\beta = \alpha 1$ of $\gamma 1$]
$\gamma 34$	Cst6[$\beta = \alpha 0$ of $\gamma 33$]
$\gamma 35$	Div[$\alpha 0 = \beta$ of $\gamma 36$][$\alpha 1 = \beta$ of $\gamma 37$][$\beta = \alpha 1$ of $\gamma 33$]
$\gamma 36$	ami2C[$\beta = \alpha 0$ of $\gamma 35$]
$\gamma 37$	Div[$\alpha 0 = \beta$ of $\gamma 38$][$\alpha 1 = \beta$ of $\gamma 43$][$\beta = \alpha 1$ of $\gamma 35$]
$\gamma 38$	Add[$\alpha 0 = \beta$ of $\gamma 39$][$\alpha 1 = \beta$ of $\gamma 40$][$\beta = \alpha 0$ of $\gamma 37$]
$\gamma 39$	ami3N[$\beta = \alpha 0$ of $\gamma 38$]
$\gamma 40$	Sub[$\alpha 0 = \beta$ of $\gamma 41$][$\alpha 1 = \beta$ of $\gamma 42$][$\beta = \alpha 1$ of $\gamma 38$]
$\gamma 41$	ami113ficO[$\beta = \alpha 0$ of $\gamma 40$]
$\gamma 42$	Cst1[$\beta = \alpha 1$ of $\gamma 40$]
$\gamma 43$	Sin[$\alpha 0 = \beta$ of $\gamma 44$][$\beta = \alpha 1$ of $\gamma 37$]
$\gamma 44$	ami1N[$\beta = \alpha 0$ of $\gamma 43$]

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Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version at

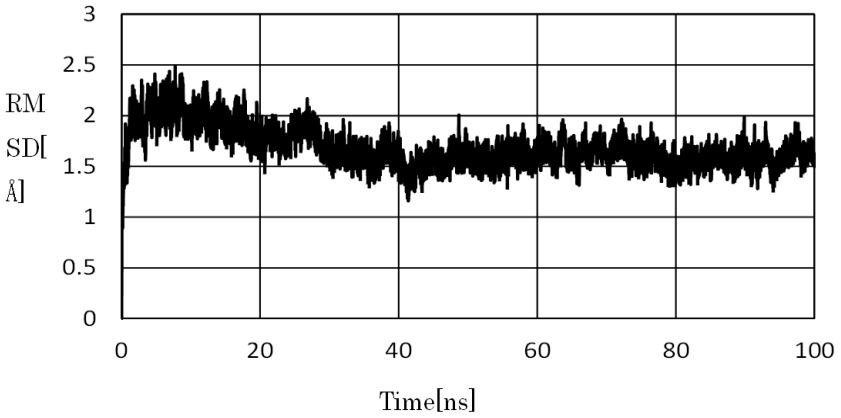


Figure S1.: RMSD between the successive simulations.

Table S1: The selected tetrapeptides.

(a)	(b)
Ser–Ser–Ile–Arg	Met–Gly–Lys–Gln
Arg–Cys–Lys–Arg	Lys–Cys–Arg–Gln
His–Cys–Arg–Ala	Gln–Ser–Arg–Asn
Arg–Asn–Arg–Asn	Arg–Ser–Lys–Lys
Thr–Asn–Arg–Arg	Gln–Ala–Arg–Asn
His–Gly–Leu–Gly	Arg–Ala–Val–Val
Arg–Gln–Arg–Arg	Lys–Gly–Lys–Val
Asn–Ser–Lys–Gln	His–Gly–Arg–Asn
Leu–Gly–Arg–Asn	Arg–Asp–Arg–Pro
Met–Asp–Ile–Arg	Lys–Ala–Lys–Lys

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Table S2: Affinity of the 100 tetrapeptides in the active region of the average structure of locally modified ficin (Y113F).

Ser–Ser–Ile–Arg	NA3	Lys–Gly–Ile–Gln	NA4	Arg–Gly–Lys–Leu	NA2	Arg–Gly–Lys–Asn	NA4
Arg–Cys–Lys–Arg	NA2	Gln–Gly–Ile–Gln	NA4	Gln–Gly–Lys–Lys	NA4	Arg–Gly–Arg–Thr	NA4
His–Cys–Arg–Ala	NA3	Gln–Gly–Leu–Gln	NA4	Arg–Gly–Gln–Leu	NA2	Arg–Gly–Arg–Asn	NA2
Arg–Asn–Arg–Asn	NA2	Lys–Gly–Val–Gln	NA4	Arg–Gly–Asn–Leu	NA1	Val–Trp–Cys–Gly	NA4
Thr–Asn–Arg–Arg	NA3	Arg–Gly–Val–Leu	NA1	Arg–Gly–Ser–Lys	NA4	Met–Arg–Ile–Phe	NA4
His–Gly–Leu–Gly	NA4	Lys–Gly–Ile–Leu	NA4	Arg–Gly–Pro–Lys	NA3	Met–Gly–Glu–Arg	NA3
Arg–Gln–Arg–Arg	NA3	Arg–Gly–Lys–Met	NA3	Met–Gly–Val–Lys	NA4	Arg–Gly–Glu–Leu	NA4
Asn–Ser–Lys–Gln	NA1	Lys–Gly–Val–Leu	NA3	Arg–Gly–Ala–Leu	NA3	Lys–Gly–Gln–Arg	NA4
Leu–Gly–Arg–Asn	NA4	Arg–Gly–Val–Gln	NA2	Arg–Gly–Lys–Gln	NA3	Arg–Gly–Thr–Ile	NA3
Met–Asp–Ile–Arg	NA3	Arg–Gly–Arg–Gln	NA1	Arg–Gly–Gln–Gln	NA4	Ile–Gly–Asp–Arg	NA4
Met–Gly–Lys–Gln	NA3	Arg–Gly–Pro–Gln	NA4	Arg–Gly–Gln–Ile	NA4	Arg–Gly–Asp–Leu	NA4
Lys–Cys–Arg–Gln	NA4	Arg–Gly–Arg–Lys	NA3	Arg–Ser–Lys–Ile	NA3	Ile–Gly–Glu–Arg	NA4
Gln–Ser–Arg–Asn	NA4	Lys–Gly–Pro–Ile	NA2	Arg–Ser–Lys–Leu	NA4	Arg–Gly–Gln–Lys	NA1
Arg–Ser–Lys–Lys	NA2	Arg–Gly–Leu–Lys	NA4	Arg–Ala–Gln–Leu	NA2	Arg–Gly–Thr–Leu	NA1
Gln–Ala–Arg–Asn	NA3	Arg–Ala–Gln–Lys	NA4	Arg–Gly–Asn–Ile	NA1	Leu–Gly–Glu–Arg	NA3
Arg–Ala–Val–Val	NA1	Arg–Gly–Leu–Val	NA4	Gln–Asp–Lys–Arg	NA3	Arg–Gly–Ser–Ile	NA2
Lys–Gly–Lys–Val	NA4	Arg–Cys–Leu–Leu	NA4	Lys–Ser–Leu–Arg	NA3	Arg–Gly–Ser–Leu	NA1
His–Gly–Arg–Asn	NA4	Arg–Ser–Leu–Lys	NA1	Arg–Asp–Lys–Arg	NA1	Arg–Gly–Ile–Lys	NA3
Arg–Asp–Arg–Pro	NA4	Arg–Ser–Ile–Lys	NA4	Gln–Asp–Ile–Arg	NA4	Arg–Gly–Val–Arg	NA4
Lys–Ala–Lys–Lys	NA4	Arg–Gly–Leu–Ile	NA2	Lys–Ser–Ile–Arg	NA1	Arg–Ser–Gln–Arg	NA4
Arg–Gly–Val–Ile	NA3	Arg–Gly–Asn–Lys	NA1	Arg–Cys–Lys–Lys	NA2	Arg–Ser–Val–Arg	NA2
Arg–Gly–Pro–Leu	NA1	Arg–Gly–Lys–Pro	NA3	Arg–Gly–Thr–Lys	NA2	Arg–Ser–Ile–Arg	NA3
Lys–Gly–Pro–Gln	NA3	Arg–Ala–Leu–Lys	NA3	Arg–Gly–Asn–Val	NA1	Arg–Ser–Leu–Arg	NA3
Lys–Gly–Leu–Gln	NA1	Arg–Gly–Lys–Lys	NA3	Arg–Ala–Lys–Asn	NA4	Arg–Ser–Pro–Arg	NA2
Arg–Gly–Pro–Ile	NA1	Arg–Gly–Ile–Met	NA3	Arg–Cys–Arg–Asn	NA3	Arg–Gly–Lys–Arg	NA3

Table S3: The 38 especially incompatible tetrapeptides.

His–Gly–Leu–Gly	Gln–Gly–Lys–Lys
Leu–Gly–Arg–Asn	Arg–Gly–Ser–Lys
Lys–Cys–Arg–Gln	Met–Gly–Val–Lys
Gln–Ser–Arg–Asn	Arg–Gly–Gln–Gln
Lys–Gly–Lys–Val	Arg–Gly–Gln–Ile
His–Gly–Arg–Asn	Arg–Ser–Lys–Leu
Arg–Asp–Arg–Pro	Gln–Asp–Ile–Arg
Lys–Ala–Lys–Lys	Arg–Ala–Lys–Asn
Lys–Gly–Ile–Gln	Arg–Gly–Lys–Asn
Gln–Gly–Ile–Gln	Arg–Gly–Arg–Thr
Gln–Gly–Leu–Gln	Val–Trp–Cys–Gly
Lys–Gly–Val–Gln	Met–Arg–Ile–Phe
Lys–Gly–Ile–Leu	Arg–Gly–Glu–Leu
Arg–Gly–Pro–Gln	Lys–Gly–Gln–Arg
Arg–Gly–Leu–Lys	Ile–Gly–Asp–Arg
Arg–Ala–Gln–Lys	Arg–Gly–Asp–Leu
Arg–Gly–Leu–Val	Ile–Gly–Glu–Arg
Arg–Cys–Leu–Leu	Arg–Gly–Val–Arg
Arg–Ser–Ile–Lys	Arg–Ser–Gln–Arg

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Table S4: Affinity of the 17 tetrapeptides in the active region of the snapshot structures of locally modified ficin (Y113F).

	max	min
Arg-Ala-Val-Val	NA3	NA3
Arg-Asp-Lys-Arg	NA1	NA1
Arg-Gly-Arg-Gln	NA1	NA3
Arg-Gly-Asn-Ile	NA1	NA1
Arg-Gly-Asn-Leu	NA1	NA1
Arg-Gly-Asn-Lys	NA1	NA1
Arg-Gly-Asn-Val	NA1	NA1
Arg-Gly-Gln-Lys	NA2	NA3
Arg-Gly-Pro-Ile	NA1	NA3
Arg-Gly-Pro-Leu	NA3	NA3
Arg-Gly-Ser-Leu	NA1	NA3
Arg-Gly-Thr-Leu	NA3	NA4
Arg-Gly-Val-Leu	NA1	NA3
Arg-Ser-Leu-Lys	NA2	NA3
Asn-Ser-Lys-Gln	NA3	NA1
Lys-Gly-Leu-Gln	NA3	NA3
Lys-Ser-Ile-Arg	NA2	NA3

Table S5: Explanation of the acronyms. (α: Input β: Output).

Add[α0][α1][β]	β = arithmetic addition of α0 and α1
Sub[α0][α1][β]	β = subtraction of α1 from α0
Mul[α0][α1][β]	β = arithmetic multiplication of α0 and α1
Div[α0][α1][β]	β = division of α0 by α1
Fmod[α0][α1][β]	β = remainder after division of α0 by α1
Log[α0][β]	β = natural logarithm of α0
Log10[α0][β]	β = common logarithm of α0
Sin[α0][α1][α2][β]	β = arithmetic multiplication of α0 and X, where X is sine of division of α1 by α2
Cos[α0][α1][α2][β]	β = arithmetic multiplication of α0 and X, where X is cosine of division of α1 by α2
If[α0][α1][α2][β]	β = if α0 = true then α1 else α2
Equal[α0][α1][β]	β = if α0 = α1 then true else false
NotEqual[α0][α1][β]	β = if α0 = α1 then false else true
GT[α0][α1][β]	β = if α0 > α1 then true else false
GE[α0][α1][β]	β = if α0 ≥ α1 then true else false
And[α0][α1][β]	β = logical multiplication of α0 and α1
Or[α0][α1][β]	β = logical addition of α0 and α1
Not[α0][β]	β = logical negation of α0
Fmod2[α0][β]	β = remainder after division of α0 by 4
Sqrt[α0][β]	β = square root of α0
ami γ	4 amino acids in a tetrapeptide, γ = 1-4 from the N-terminus to the C-terminus
ami γ C	the number of carbon atoms in ami γ
ami γ N	the number of nitrogen atoms in ami γ
ami γ O	the number of oxygen atoms in ami γ
ami γ S	the number of sulfur atoms in ami γ
ami γ AC	the number of aromatic carbon atoms in ami γ
ami113ficC	the number of carbon atoms in 113~th amino acid of ficin
ami113ficN	the number of nitrogen atoms in 113~th amino acid of ficin
ami113ficO	the number of oxygen atoms in 113~th amino acid of ficin
ami113ficS	the number of sulfur atoms in 113~th amino acid of ficin
ami113ficAC	the number of aromatic carbon atoms in 113~th amino acid of ficin
domainDist	the distance between domains of ficin (0:minimum, 1:average, 2:maximum)
CST δ	a constant integer number δ (δ = 0-9)
TRUE	a boolean value 1
FALSE	a boolean value 0
ficin_Y113F_ave	the average structure of ficin_Y113F
ficin_Y113F_max	the snapshot structure of ficin_Y113F when distance between its domains is at a maximum
ficin_Y113F_mini	the snapshot structure of ficin_Y113F when distance between its domains is at a minimum

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Gaps and Errors of the Schrödinger Equation

By Stanislav Ordin

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Abstract- "Quantum" World, within the framework of which "outstanding" scientific discoveries are being made now, is built on initially laid nonsense. Quantum Theory was initially built on incorrect adjustment by Schrodinger of two-dimensional "solutions" of the One-Dimensional Harmonic Oscillator equation. These are the consequences of this fitting and "excite Minds". This is the reason why Quantum Mechanics is not necessary to UNDERSTAND, but it is necessary to ACCEPT. But they accepted and canonized, as it is shown in this work, non-physical, rough, approximate solutions. And it is on the basis of these solutions that electron orbitals, widely used in fundamental and applied science, are constructed.

But simply a rigorous mathematical analysis of the Two-Dimensional Oscillator equation in a rotational paraboloid gives reasons to believe that it is the Planck-Einstein Quantization moved away by the "evolvability" that gives a correct description of the parameter hidden for macroscopic measurements - de Broglie matter waves.

Keywords: *classical harmonic oscillator, rotation paraboloid, quantization, de broglie waves, two-dimensional model, resolved states.*

GJSFR-A Classification: *DDC Code: 530 LCC Code: QC23*



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But simply a rigorous mathematical analysis of the Two-Dimensional Oscillator equation in a rotational paraboloid gives reasons to believe that it is the Planck-Einstein Quantization moved away by the "evolvability" that gives a correct description of the parameter hidden for macroscopic measurements - de Broglie matter waves.

Keywords: classical harmonic oscillator, rotation paraboloid, quantization, de broglie waves, two-dimensional model, resolved states.

I. Introduction

The qualitative description by Quantum Mechanics of the Periodic Table of Mendeleev and the chemical bond [1] overshadowed the catastrophic discrepancies between the experimentally obtained Ionization Potentials [2, 3] and the energy position of the allowed levels obtained from the Schrödinger equation. Be that as it may, the Schrödinger equation was canonized to such an extent that even Richard Feynman, who came close to the original Planck-Einstein Quantization in his path integrals, did not dare to declare his approach to correcting the canonized equation [4, 5]. And as Bob Laughlin said in his Nobel lecture: To describe any quantum phenomenon, it is enough to take the Schrödinger equation and solve it under new boundary conditions [6]. And his solutions give no less serious discrepancies with the shape of electron orbitals [7, 8 9] and with experimentally measured phonon spectra [10]. And, as follows from the analysis of basic models [11], a huge number of earlier works, including mine, built on the canonized "Quantum Representations", are simply fitting the results of experiments to quantum mechanical calculations. Whereas ELEMENTARY ANALYSIS, as will be shown below, shows that the Schrödinger equation itself is a very rough fit to Bohr's atomic model.

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The return of Mathematics to Physics by the senior telegrapher Havyside was actually a return to Newton's Physics, where they were UNITS. It helped both Maxwell in combing his Electrodynamics and Schroedinger in applying the operator method to describe the microcosm. So the very use of the operator method was undoubted progress, pushing both Dirac to build vector Quantum Mechanics and von Neumann to prove its Completeness. But the Completeness was obtained abstractly, for a set of operators, and was taken concretely as referring to Schrödinger solutions, which, as shown above, simply do not fit the careful characterization given by Einstein: "Some equations of Classical Physics allow rewriting in operator form". Einstein subtly sensed the dissonance of the equations with Reality, both some obtained by himself and some obtained by Schroedinger. That's what the analysis he conducted was pushing away from the verification of the Classical Equations rewritten by Schroedinger, from which Einstein himself (in the Theory of Relativity) was repelled by Bo with the phrase that he was taking on the role of God in determining the RIGHTness of the Classical Equations used. But God in Science is Logic, which must be followed, commensurate conclusions with Reality.

II. Analysis of Propositions and Solutions of the Schrödinger Equation

Einstein, pushed aside together with Planck, who laid the FOUNDATIONS of QUANTUM [12, 13], correctly formulated the method introduced by Schrödinger (actually for Schrödinger): “Some equations of classical physics can be rewritten in operator form.” But Schrödinger, using the Hamiltonian of the One-Dimensional Equation

$$\frac{m\left(x'[t]\right)^2}{2}+\frac{\kappa\left(x[t]\right)^2}{2}\equiv \mathrm{E}\Rightarrow \quad \Omega=\sqrt{\frac{k}{m}} \qquad (1)$$

and with the help of the introduction of the mystical wave function, he “got” the Stationary, again one-dimensional Equation in the “operator form”:

$$-\frac{h^2}{2m}\frac{\partial^2}{\partial x^2}\varphi[x]+\frac{m\omega^2x^2}{2}\varphi[x]=E\varphi[x] \qquad (2)$$

At the same time, Schrödinger acted as a professional fortune-teller, giving out the desired result and inventing all sorts of fables to “substantiate” it. He

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fitted, with phenomenological errors, Two-dimensional solutions - mystical wave functions of this, in principle, One-Dimensional Equation. Adjusted so that both quanta were (in the radial part of the solution) and two-dimensional orbits - orbitals (these solutions are given in all textbooks on "Quantum Mechanics"). In fact, he used Newton's method of separation of variables to find the wave function, which gives only a particular solution [14]. But on the radial and angular parts, which corresponds not to the One-Dimensional Parabola, but, in fact, to the Paraboloid of rotation (Fig. 1).

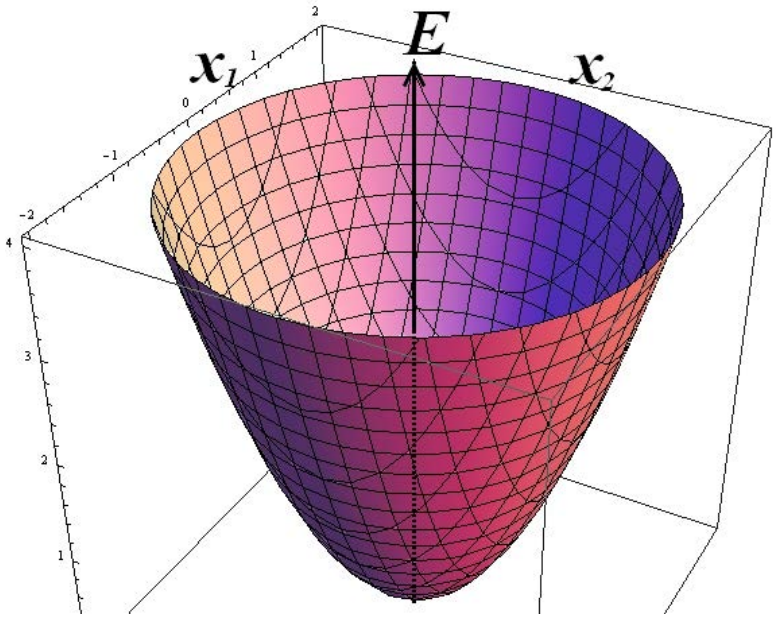


Fig. 1: True Hamiltonian "implied" by Schrödinger

The Schrödinger equation in its usual form (f.2) has a strict one-dimensional (radial), but not at all harmonic solution (f.3):

$$\frac{h^2}{2m}y''[x]+\frac{m\omega^2}{2}x^2y[x]=Ey[x] \quad (3)$$

$$y=C[2]ParabolicCylinderD\left[-\frac{1}{2}-\mathsf{E}^*,ix^*\right]+ \quad (4)$$

$$C[1]ParabolicCylinderD\left[-\frac{1}{2}+\mathsf{E}^*,x^*\right]$$

Where $\mathsf{E}^*=\frac{E}{h\omega}, \Lambda=\frac{h^2/2m}{h\omega}$ ™ $x^*=\frac{x}{\Lambda}$

The complete solution is the interference of two terms, depending on the real x purely real and complex, depending on the imaginary x.
And it is the real term that has the property

$$y=ParabolicCylinderD[n,x] \quad (5)$$

– The function is not equal to zero only in the area of origin only for integer values of n (Fig. 2).

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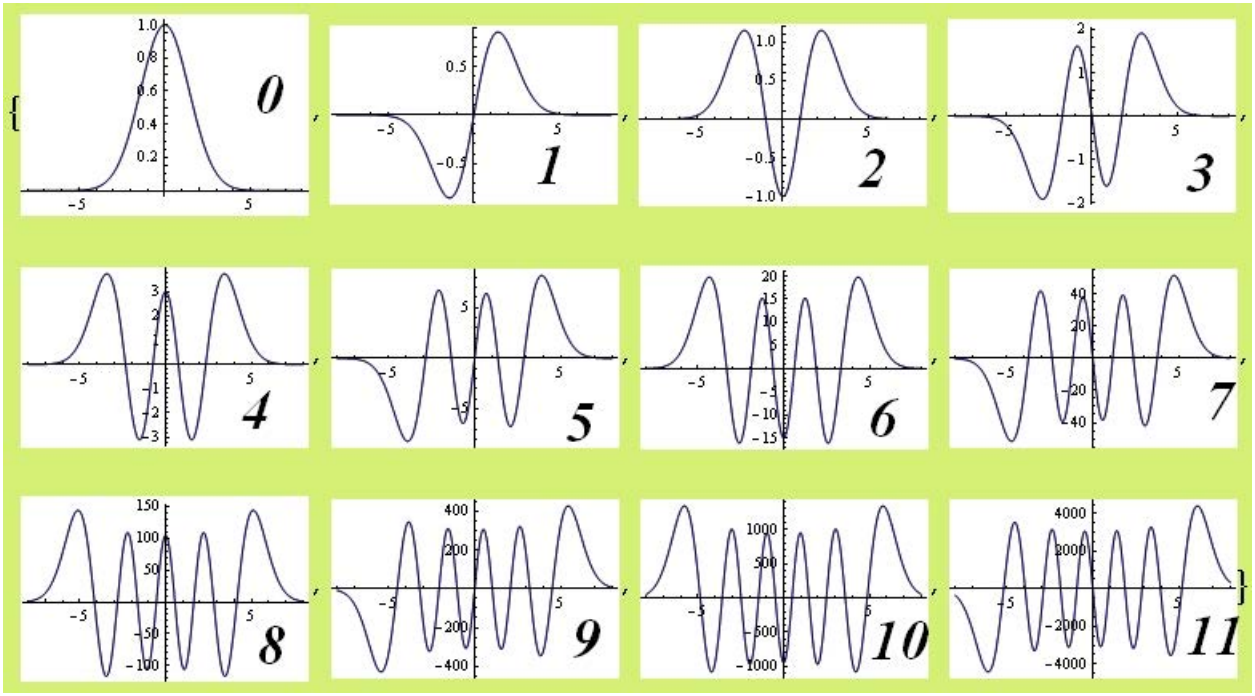


Fig. 2: Unnormalized functions of a parabolic cylinder converging at infinity for integer values.

Those. for the radial part of the wave function, we have the values of "allowed" (guessed by Schrödinger) energies, with the non-physical half of the "zero oscillations"

$$-\frac{1}{2}+E^{*}=n \quad \Rightarrow \quad E^{*}=n+\frac{1}{2} \tag{6}$$

This purely mathematical, abstract solution is not, strictly speaking, physical, since the function obtained, which describes the movement along a parabolic cylinder, when passing from one parabola of the cylinder section to another, undergoes a discontinuity of the derivative (Fig. 3).

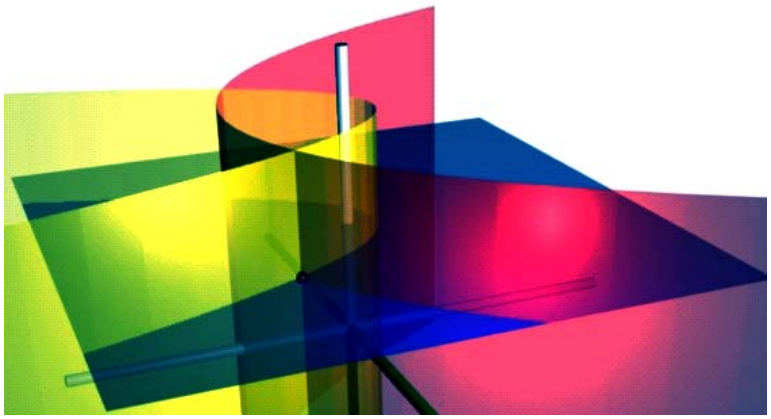


Fig. 3: Parabolic cylinder

The functions shown in Fig. 2 are not normalized, but in fact these are strictly obtained solutions for each "quantum" energy level, similar to those obtained approximately, but normalized "wave functions" of Schrödinger (Fig. 4).

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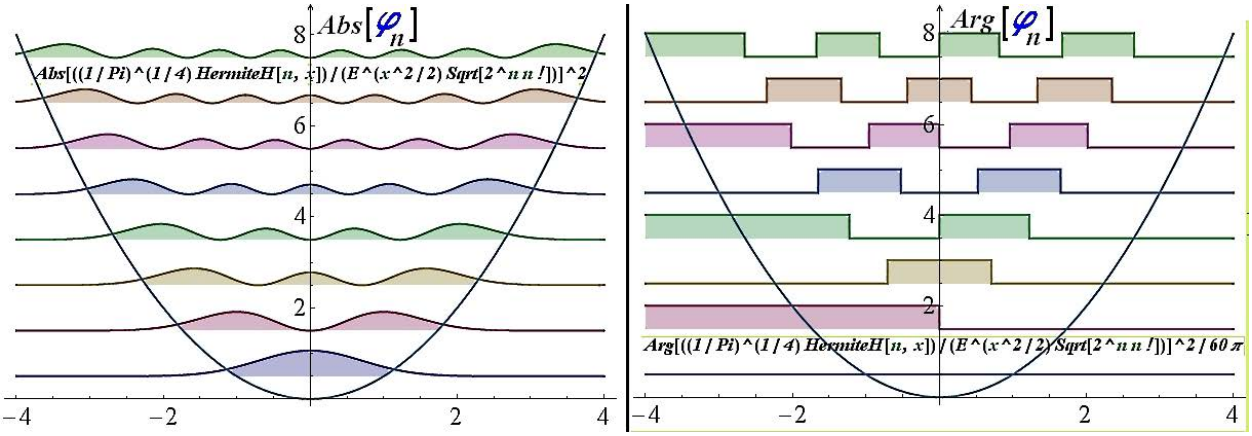


Fig. 4: Normalized "wave functions of the Quantum (one-dimensional) Oscillator" by Schrödinger: on the left - their absolute values, and on the right - their corresponding phases

As can be seen from Fig. 4, Schrödinger's fitting of solutions, in principle, to the incorrect equation of the "Quantum Oscillator", gave only absolute values of "wave functions" similar to physical functions (Fig. 4, on the right), which were interpreted by "quantum physicists" . But the phases corresponding to them are both absurd in magnitude and contain non-physical jumps - discontinuities in the derivatives.

The resulting abstract but rigorous solution is smooth (physical) dependences both on the actual values of the coordinate (shown in Fig. 2) and smooth dependences of the absolute value and phase for the term depending on the imaginary coordinate (f. 4). So, purely it is useful for initial, qualitative analysis.

First, as can be seen from Fig. 2, there are no halves of a quantum (Schrödinger). As can be seen from Fig. 4, the first level corresponds to zero energy. And the maximum of the hidden parameter of the particle is observed in the center, with its minimum bounce, which can be physically related to the fact that the minimum oscillation amplitudes near zero (Fig. 2, first inset) are smaller than the particle size. To be more precise, as follows from Pontryagin's dualism, even for an ideal Newton particle, its spatial uncertainty is less (the article "Analysis of Newton's Elementary Particle" in the book [13]). So, in relation to the electron orbitals of the atom, this term can be safely discarded.

Secondly, the first (and not one-and-a-half, as in Schrödinger) quantum level physically quite corresponds to finding a particle (somewhat blurred), but on a distinguished classical orbit, which will be analyzed in detail in the next part of the work "Correction of the Schrödinger Equation). We will not analyze the quantum levels following from formula 5, in accordance with formula 6, and so on, because taking into account its second, depending on the imaginary coordinate, term of the strict solution (f.4) gives the real and imaginary parts of the function limited in space, but not for all the numbers from formula (6), and also gives a number of additional numbers that also do not fit in any way into the canonized series of permitted levels according to Schrödinger.

III. Conclusion

It was from MISSION that the mysticism of two-dimensional mathematical solutions for a one-dimensional model was hidden behind the mystical parameter "wave function", to which the entire "understanding" of Quantum Theory was reduced to various interpretations. Thus, the correction of the original Classical Equation rewritten by Schrödinger in the operator form (correction of the Quantum Oscillator model) is required, and, possibly, the correction of the operators used by him. The correction of electronic atomic and molecular orbitals, which were directly associated with Schrödinger's solutions, will make it possible to solve the problems of many areas of science and technology associated with Physics. In the second, planned part of the work, within the framework of a two-dimensional model, ELEMENTARY Quantization based on harmonic de Broglie waves will be demonstrated.

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Effect of a Carbon Nanotube on Ballistic Conduction through Single-Quantum-Dot

By Thiago Lobo, Minos A. Neto, Marcio G. da Silva & Octavio D. R. Salmon

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Abstract- We will study the competitive effect between the transport of a quantum dot adsorbed to a ballistic channel and laterally coupled to a single-walled carbon nanotube (SWNT). We will use the “tight-binding" approach to analytically write the SWNT Green's function and the quantum dot will be solved by the atomic method for $U \to \infty$. We will present curves of the electronic density of states for some different sizes of nanotubes. The results for the conductance curves will be presented as a function of E_f and for different values of n and hopping between the nanotube and the quantum dot.

Keywords: *Kondo effect, single wall carbon nanotubes, quantum dot, conductance.*

GJSFR-A Classification: *PACS: 71.10-w, 71.10.-w, 74.70.Tx, 74.20.Fg, 74.25.Dw*



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I. Introduction

In the last few decades, low-dimension systems have been the focus of great interest on the part of the scientific community [1]. Due to their extraordinary physical properties, these carbon-based systems have applications in areas ranging from medicine: such as DNA nanosensors [2], to nanoelectronics: with quantum dot systems interacting with graphene [3] and carbon nanotubes [4].

Quantum mechanics combined with epitaxial molecular growth and chemical deposition techniques are of fundamental importance in understanding and making quantum dots. An example of this device is the tunnel diode [5], which can play an important role in the development of quantum dot circuits [6, 7].

From the theoretical point of view [9], these low dimensional systems have revealed several fundamental aspects in the understanding of the interaction between light and matter, such as the development of circuits in Quantum Electrodynamics-QED Circuits[10]. In addition, quantum dots have electronic properties at low temperatures governed by the Kondo effect, which can be observed both in the study of theoretical models [11] as well as in experimental results [12,13].

Recently, quantum junctions - a combination of a quantum dot coupled to a carbon nanotube – have demonstrated a probe for transferring charges between discrete and continuous [14]. This type of coupling was presented in systems that can be used in high conductance devices, laterally connecting a quantum dot with a sheet of graphene [3].

In this work, we present a device that combines with a quantum dot adsorbed in a ballistic channel, coupled laterally to a carbon nanotube. We are interested in the properties of transport through the ballistic channel, which at low temperatures is governed by the Kondo effect at the quantum dot. The carbon nanotube, connected to the quantum dot through a hopping energy, also affects these transport properties, since it injects conduction electrons into the system that produce a destructive effect at the Kondo peak.

We apply the atomic approach [15] to model the quantum dot and use the Dyson's equation to connect the quantum dot to the ballistic channel and carbon nanotube, as schematically represented in Fig. 1.

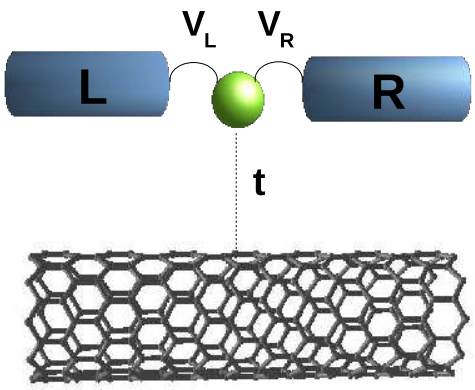


Fig. 1: Quantum dot adsorbed in a ballistic channel laterally coupled to a carbon nanotube

In Section 2 we present the model and the formalism of Green's function (GF). The results and discussions are described in Section 3. As a final point, the last section is devoted to final remarks and conclusions.

II. Model and Formalism

The quantum dot was modeled by the atomic approach [16,15] and the leads at the points (L and R) were represented by two square bands where the Green's function can written as

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$$G_c^0(\mathbf{k},z)=\frac{-1}{z-E(\mathbf{k})} \quad (1)$$

where *E*(k) is the energy of the free electrons with wave vector $\mathbf{k}$, which must be integrated for all k values, in the range from *-D* to *D*, where *D* is the half-width of the conduction band.

The GF of the zigzag nanotube is calculated analytically, adopting a single $\pi-$band tight-binding Hamiltonian approach [17].

$$G_{jj'}^{SWNT}(z)=\frac{1}{n}\sum_l \frac{a\sqrt{3}}{2\pi}\int_{-\pi/a\sqrt{3}}^{\pi/a\sqrt{3}} dk_x \frac{z.e^{i.\vec{k}.(\vec{R_j}-\vec{R_{j'}})}}{z^2-\epsilon^+(\tilde{k_x})} \quad (2)$$

where the energy dispersion relation $\epsilon^{\pm}(\tilde{k}_x)$ for the zigzag nanotube, may be written as[18]

$$\epsilon^{\pm}(\tilde{k}_x)=\pm t\sqrt{1+4\cos\left(\tilde{k}_y\right)\cos(\tilde{k}_x)+4\cos^2\left(\tilde{k}_y\right)}. \quad (3)$$

with $\tilde{k}_x = k_x a\sqrt{3}/2$, $\tilde{k}_y = k_y a/2$ and for $-\pi/\sqrt{3} < k_x\, a < \pi/\sqrt{3}$. For the zigzag nanotube $(n,\ 0)$, the $k_y = \frac{2\pi l}{an}$ is quantized, where $l = 1,...,n$, a is the lattice parameter, whose approximate value is of 2:46 Å and t is the electronic hopping between the carbon atoms, whose value we consider equal to the unit.

The density of states (DOS) from the nanotube's conduction band is calculated using

$$\rho_c(z)=-\frac{1}{\pi}Im\left(G_{jj}^{SWNT}(z)\right) \quad (4)$$

The quantum dot adsorbed in the ballistic channel, in the absence of the carbon nanotube, can be modeled by the Anderson impurity model with infinite Coulomb repulsion ($U\to\infty$). The coupling between the nanotube and the quantum dot will be carried out later with the Dyson's equation method. The Hamiltonian is given by

$$\mathcal{H}=\sum_{\alpha\mathbf{k},\sigma}E_{\alpha\mathbf{k},\sigma}c^{\dagger}_{\alpha\mathbf{k},\sigma}c_{\alpha\mathbf{k},\sigma}+\sum_{\sigma}E_{f,\sigma}X_{f,\sigma\sigma}$$

$$+\sum_{\alpha\mathbf{k},\sigma}V_{\alpha\mathbf{k}}\left(X^{\dagger}_{f,0\sigma}c_{\alpha\mathbf{k},\sigma}+H.c.\right), \quad (5)$$

where the first term represents the conduction electrons (c-electrons) from the left ($\alpha = L$) and right ($\alpha = R$) electrodes, the second describes the quantum dot characterized by a localized *f* level $E_{f,\sigma}$ and the last one corresponds to the interaction between the *c*-electrons and the quantum dot. For the sake of simplification, we consider a constant hybridization $V_{\alpha\mathbf{k}} = V$.

For the case with infinite Coulomb repulsion ($U\to\infty$), Hubbard operators [20] are employed to project out the double occupation state $|f,2\rangle$ from the local states at the quantum dot. Local projectors into the states $|f,a\rangle$ at the quantum dot, must respect the following identity: $X_{f,00}+X_{f,\sigma\sigma}+X_{f,\overline{\sigma}\overline{\sigma}}=I$, where $\overline{\sigma}=-\sigma$. Being that $a=0$, σ or $\overline{\sigma}$, the occupation numbers on the quantum dot $n_{f,a}=\langle X_{f,aa}\rangle$ should then satisfy the "completeness" relation

$$n_{f,0}+n_{f,\sigma}+n_{f,\overline{\sigma}}=1. \quad (6)$$

a) The quantum dot

The quantum dot's GF $(G_{qd,\sigma})$ presented in this study is based on the Hubbard cumulative expansion technique, using hybridization as a perturbation [20,21]. Considering M_{σ}^{eff} as an effective cumulant that cannot be separated by cutting a single edge from Feynmann diagram (irreducible diagram) and $G_c^{0,\alpha}(\mathbf{k},z))$ as the GF of the conduction electrons of electrodes ($\alpha=L,R$), We can write the exact GF for the *f* electron located at the quantum dot as follows

$$G_{qd,\sigma}=M_{\sigma}^{eff}+M_{\sigma}^{eff}VG_c^{0,\alpha}VM_{\sigma}^{eff}$$

$$+M_{\sigma}^{eff}VG_c^{0,\alpha}VM_{\sigma}^{eff}VG_c^{0,\alpha}VM_{\sigma}^{eff}+.... \quad (7)$$

$$G_{qd,\sigma}=M_{\sigma}^{eff}\left[1+G_c^{0,\alpha}V^2M_{\sigma}^{eff}+\left(G_c^{0,\alpha}V^2M_{\sigma}^{eff}\right)^2+...\right]. \quad (8)$$

The term in square brackets represents the infinite sum of a geometric progression, with a ratio equal to $G_c^{0,\alpha}V^2M_{\sigma}^{eff}$. The final result is given by

$$G_{qd,\sigma}(z)=\frac{M_{\sigma}^{eff}(z)}{1-M_{\sigma}^{eff}(z)V^2\sum_{\alpha\mathbf{k}}G_c^{0,\alpha}(\mathbf{k},z)}. \quad (9)$$

where the sum over the two identical channels α results in multiplier 2.

The calculation of the exact value of $M_{\sigma}^{eff}(z)$ is an impracticable task, however, we will replace it by an atomic cumulant $M_{\sigma}^{at}(z)$, obtained from the exact solution of the Anderson's impurity in the atomic limit, when the band of uncorrelated electrons has zero width (atomic model).

The atomic solution will be obtained in the next section. We call the replacement of $M_{\sigma}^{eff}(z)$ by $M_{\sigma}^{at}(z)$ an "atomic approach".

b) The atomic solution

The atomic solution of Anderson's impurity problem at the limit of infinite Coulomb repulsion $U\to\infty$, can be obtained by diagonalizing the Hamiltonian Eq.(5) by the states $|f,c\rangle$, where the possibilities are $|f\rangle=0,\uparrow,\downarrow$ and $|c\rangle=0,\uparrow,\downarrow,\uparrow\downarrow$. The GF of the atomic model is obtained by the Zubarev equation [22]

$$G^{at}(z)=e^{\beta\Omega}\sum_n\sum_{jj'}e^{-\beta E_{n,j}}+e^{-\beta E_{n-1,j'}}$$

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$$\times \frac{|\langle n-1, j' \,|X_\mu|\, n, j\rangle|^2}{z-(E_{n,j}-E_{n-1,j'})}, \tag{10}$$

where Ω is the thermodynamical potential and the eigenvalues $E_{n,j}$ and eigenvectors $|nj\rangle$ correspond to the complete solution of the Hamiltonian Eq.(5). The different transitions occur between states with n and $n+1$ particles that satisfy $\langle n-1, j'|X_\mu|n, j\rangle \neq 0$. The final result is the following:

$$G^{at}(z) = e^{\beta\Omega}\sum_{i=1}^{8}\frac{m_i}{z-u_i}. \tag{11}$$

The complete calculation of all poles u_1 and residues m_i is detailed in reference [15].

c) The atomic approach

On the other hand, following the same procedure described for obtaining $G_{qd,\sigma}(z)$, the exact atomic f GF has the same form of Eq.(9) and can be written as [21]:

$$G_\sigma^{at} = M_\sigma^{at} + M_\sigma^{at} V G_c^o V M_\sigma^{at}$$

$$+M_\sigma^{at} V G_c^o V M_\sigma^{at} V G_c^o V M_\sigma^{at} + ... \tag{12}$$

$$G_\sigma^{at} = M_\sigma^{at}\left[1 + G_c^o V^2 M_\sigma^{at} + \left(G_c^o V^2 M_\sigma^{at}\right)^2 + ...\right]. \tag{13}$$

$$G_\sigma^{at}(z) = \frac{M_{2,\sigma}^{at}(z)}{1 - M_{2,\sigma}^{at}(z)\mid V\mid^2 \sum_{\mathbf{k}} G_{c,\sigma}^{o\bar{e}}(\mathbf{k}, z)}, \tag{14}$$

where $G_{c,\sigma}^{o\bar{e}}(\mathbf{k}, z) = -1/(z-\varepsilon(\mathbf{k}))$. From this equation we then obtain an explicit expression for $M_{2,\sigma}^{at}(z)$ in terms of $G_{ff,\sigma}^{at}(z)$

$$M_\sigma^{at}(z) = \frac{G_\sigma^{at}(z)}{1 + G_\sigma^{at}(z) V^2 \sum_{\mathbf{k}} G_{c,\sigma}^o(\mathbf{k}, z)}, \tag{15}$$

where G_σ^{at} was calculated analytically and is given by Eq.(11).

The atomic approach consists in substituting $M_\sigma^{eff}(z)$ in Eq. (9) by the $M_\sigma^{at}(z)$, given by Eq.(15). Finally, the approximate GF of the quantum dot connected to leads *L* and *R* is written as

$$G_{qd,\sigma}(z) = \frac{M_\sigma^{at}(z)}{1 - M_\sigma^{at}(z)\Delta^2 \sum_{\alpha,\mathbf{k}} G_{c,\sigma}^o(\mathbf{k}, z)}, \tag{16}$$

where $G_{c,\sigma}^o(\mathbf{k},z)$ is the GF of the leads and must be integrated in the range from *-D* to *D*, which is the width of the conduction band. With the atomic approach, the different energies $E_{k,\sigma}$ of the c-electrons, which should contribute to the propagators of the effective cumulant $M_\sigma^{eff}(z)$, are now replaced by the contribution of a single E_c energy value in $M_\sigma^{at}(z)$. Thus, it is essential to replace the constant V^2 by Δ^2, decreasing the contribution of the *c*-electrons with was overestimated by concentrating them at a single energy level. We use $\Delta = \pi V^2/2D$ like the Kondo peak width, where *D* is the half conduction bandwidth.

d) Connection with the nanotube

The system formed by the quantum dot and the leads (site 0) must still be connected with the nanotube (site 1). We will use the Dyson's equation method to make this. Let's use hybridization operator $\hat{V} = |0\rangle\mathbf{t}\langle 1| + |1\rangle\mathbf{t}\langle 0|$, where t is the hopping between the carbon nanotube and the quantum dot and will be given in units of V, from the Hamiltonian of Eq.(5). Dressed GF at site of quantum dot $G_{00,\sigma}$ can be written in terms of the localized undressed GF G_{jj}^{SWNT} of the carbon nanotube Eq.(2), and in terms of the undressed GF $G_{qd,\sigma}$ of the quantum dot with the leads Eq.(16).

$$\hat{G} = \hat{g} + \hat{g}\hat{V}\hat{G},$$

$$G_{00,\sigma} = g_{00,\sigma} + g_{00,\sigma}\mathbf{t}G_{10,\sigma} + g_{01,\sigma}\mathbf{t}G_{00,\sigma},$$

$$G_{10} = g_{10,\sigma} + g_{10,\sigma}\mathbf{t}G_{11,\sigma} + g_{11,\sigma}\mathbf{t}G_{00,\sigma}. \tag{17}$$

After solving this system of equations, and considering $g_{10,\sigma} = g_{01,\sigma} = 0$, we can write

$$G_{00,\sigma} = \frac{g_{00,\sigma}}{(1 - g_{00,\sigma}\mathbf{t}^2 g_{11,\sigma})}, \tag{18}$$

and finally

$$G_{00,\sigma} = \frac{G_{qd,\sigma}}{(1 - G_{qd,\sigma}\mathbf{t}^2 G_{jj}^{SWNT})}. \tag{19}$$

III. Results and Discussions

In the set of Fig. 2 - Fig. 3 we will present the density of states curves of the conducting electrons of the nanotube, for different values of n, as well as its importance in the DOS of the electrons localized at the quantum dot, when the hopping between the SWNT and the system formed by QD + balistic channel is $\mathbf{t} = 0.5V$.

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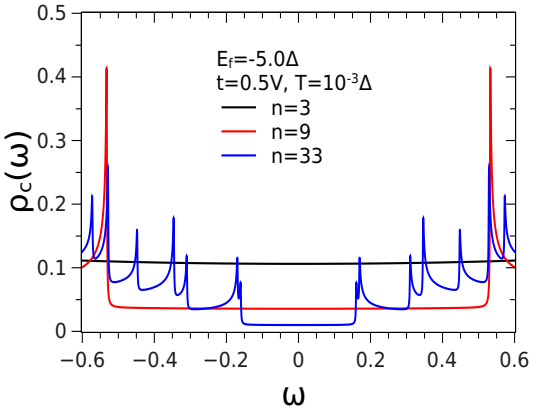


Fig. 2: The density of states of the conduction electrons ρ_c as a function of the ω (multiplied by $\Delta = 0.01$) and for $n = 3$, $n = 9$ e $n = 33$.

In Fig. 2 we show the density of states of the conducting electrons of the carbon nanotube for different values of n. The carbon nanotube of the zig zag type will be metallic for values multiple of 3. We can see in the figure that as the size of the tube increases, represented by the increase in n, the height of the DOS at the Fermi level ($E_F = 0$) decreases.

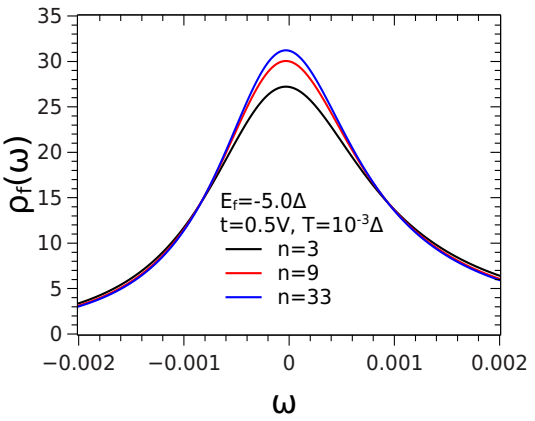


Fig. 3: The density of states of the localized f level ρ_f as a function of the ω (multiplied by $\Delta = 0.01$) and for $n = 3$, $n = 9$ $en = 33$. $E = -5.0\Delta$, $\mathbf{t} = 0.5V$ and $T = 0.001\Delta$. Detail of the height of kondo peak.

In Fig. 3 we show the density of states of the localized electrons of the quantum dot (QD) for different values of n. The figure shows the detail of the Kondo peak, located on the chemical potential $\mu = 0$. We verified that the height of the Kondo peak increases with the increase of n, thus showing a behavior that is the opposite of that presented by the density of conduction electron states at the Fermi level.

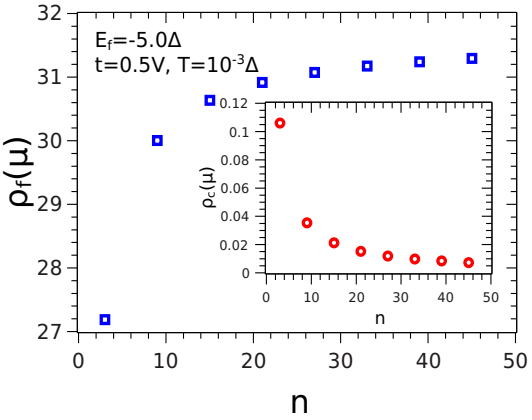


Fig. 4: The density of states of the localized f level ρ_f at the chemical potential $\mu = 0$ as a function of n, for $E_f = -5.0\Delta$, $\mathbf{t} = 0.5V$ and $T = 0.001\Delta$.

In Fig. 4 we show the density of states of the localized electrons and of the conduction electrons at the chemical potential $\mu = 0$. We can verify the inverse behavior between the height of the conduction band and the height of the Kondo peak.

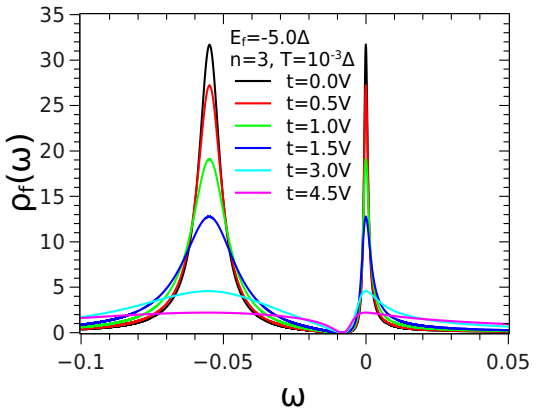


Fig. 5: The density of states of the localized f level ρ_f as a function of the ω (multiplied by $\Delta = 0.01$) and different values of $\mathbf{t}$. $E_f = -5.0\Delta$, $T = 0.001\Delta$ and $n = 3$.

In Fig. 5 we present the density of states of the felectrons localized at the QD for different values of *t,* which is the hopping between the nanotube and the QD, keeping all other parameters constant and for $n = 3$.

We observed that an increase in t produces a decrease in the height of the two peaks, which correspond to the localized level $Ef = -5.0\Delta$ (left peak) and the Kondo peak (right peak), localized at the chemical potential $\mu = 0$. As the interaction between the nanotube and the QD increases, the Kondo effect will be destroyed. This can be explained by the coupling geometry (T-shape ligation), which produces a destructive interference between the electrons of the nanotube and the QD.

The changes produced at the Kondo peak will produce changes in the transport properties of the

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system. These changes can be seen in the calculation of the conductance at site 0 of the nanotube.

At low temperatures and bias voltage the electronic transport is coherent and the conductance is calculated according to the Landauer equation [23]:

$$G = \frac{2e^2}{\hbar}\int\left(-\frac{\partial\Theta_F}{\partial\omega}\right)S(\omega)d\omega, \tag{20}$$

Θ_F is the Fermi function and $S(\omega)$ is the transmission probability of an electron with energy $\hbar\omega$ and is given by

$$S(\omega) = \gamma^2 \mid G_{00}^{\sigma} \mid^2, \tag{21}$$

where γ corresponds to the coupling strength, which is proportional to the kinetic energy of the electrons in the site 0 and G_{00} was obtained previously and is given by Eq. (19).

In the set of curves shown in Fig. 6, we show the conductance calculated at site 0 as a function of the level localized at the quantum dot E_f, for various values of *t*, which is the hopping that connects the QD to the carbon nanotube. We present four graphs, referring to the four values of $n = 3, 9, 15, 21$, which is proportional to the diameter of the nanotube.

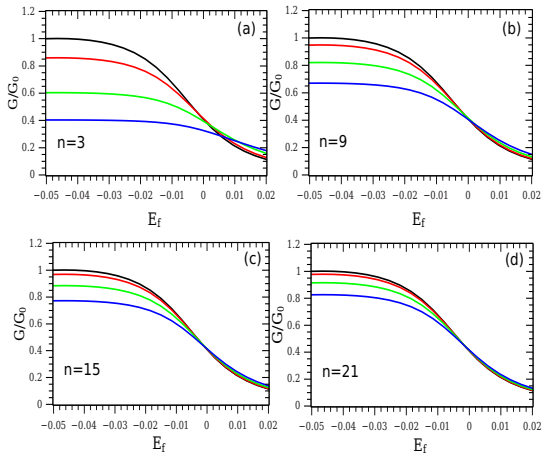


Fig. 6: Condutance as a funtion E_f (multiplied by $\Delta = 0.01$) for different values of hopping $\mathbf{t} = 0.0V$ (black line); $\mathbf{t} = 0.5V$ (red line); $\mathbf{t} = 1.0V$ (green line) and $\mathbf{t} = 1.5V$ (blue line), with $T = 0.001\Delta$ and for different values of n.

First, we can observe in the four figures, for t = 0 (black line), the conductance has a unit value for $E_f = -5.0\Delta$, indicating that the Kondo resonance produces a ballistic transmission channel for the electrons coming from the leads. With the increase in E_f, the conductance drops smoothly until it approaches zero in the empty region ($E_f > 0.0\Delta$). This behavior is known and is in agreement with results presented in previous studies [11].

As we connect the carbon nanotube to the (QD + leads) system, that is, for $t = 0.5V$, $1.0V$, $1.5V$, we observe a destructive interference between the electrons coming from the metallic tube and the quantum dot. The Kondo peak is reduced in height (see Fig. 5, implying a decrease in conductance in the Kondo region ($E_f < 0.0\Delta$). This reduction in conductance is more important in tubes of smaller diameter (*n* small). This can be explained by the height of the conduction band at the chemical potential μ, which is higher in small tubes and smaller in larger tubes, as seen in Fig. 2.

As the value of *n* increases, that is, for increasingly larger diameters, the colored lines get closer and closer, indicating a reduction in destructive interference between the electrons from the nanotube and the QD, caused by the reduction in the amount of electrons coming from the nanotube.

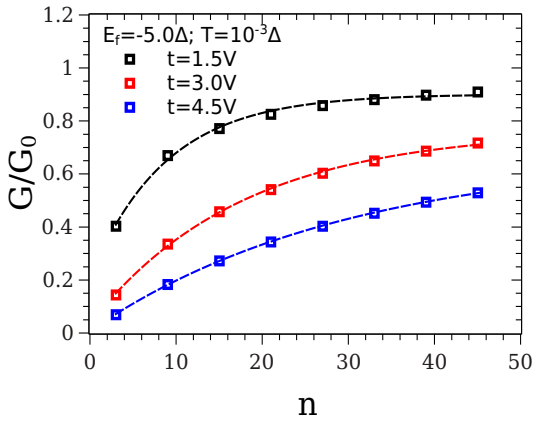


Fig. 7: Condutance as a funtion n for different values t. $E_f = -5.0\Delta$ and $T = 0.001\Delta$.

In Fig. 7 we represent the condutance as a function of *n* for different values of hopping *t*. Although we do not present it in the figure, we know that for a zero hopping, that is, when the nanotube is disconnected from the system, the conductance has its unit value for any value of *n*. We can verify the inuence of hopping in the destruction of the Kondo Effect. As the value of *t* increases, the conductance curve shifts downwards.

IV. Conclusions

In this study, we present a quantum dot system embedded in a ballistic channel and laterally coupled to a carbon nanotube of the zigzag type. The method used was the atomic approximation, which has great reliability in the low temperature regime, satisfying Friedel's sum rule.

We present density of states curves, both for the conduction band of the nanotube and for the electrons localized *f*. We found that an increase in the diameter of the nanotube produces a decrease in the height of the conduction band in the chemical potential

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$\mu = 0$. This decrease, in turn, produces an increase in the height of the Kondo peak, located in the same energy region ($\mu = 0$). This inverse relationship is due to the geometry of the connection between the nanotube and the quantum dot, which are connected laterally.

We also looked at the role of hopping t that links the quantum dot to the carbon nanotube. We verified through the density of electron states f that the Kondo Peak decreases with the increase of t, again indicating the destructive interference characteristic between the electrons from the nanotube to the quantum dot, when the coupling is lateral.

As the variation of n and t changes the height of the Kondo peak, that is located in the chemical potential, the transport properties will also be affected. We observed this effect on the conductance curves.

We found that when $t = 0$, that is, when the nanotube is disconnected from the system, the conductance is ballistic at $E_f = -5.0\Delta$, indicating that the Kondo effect is present and that the Kondo peak produces a conduction channel for the electrons coming of leads. As t increases, the conductance tends to decrease, as the electrons coming from the nanotube conduction band become more and more abundant. We also found that small diameter nanotubes are more sensitive to changes in hopping for conductance calculation.

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Acknowledgments

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Manuscript Style Instruction (Optional)

- Microsoft Word Document Setting Instructions.
- Font type of all text should be Swis721 Lt BT.
- Page size: 8.27" x 11'", left margin: 0.65, right margin: 0.65, bottom margin: 0.75.
- Paper title should be in one column of font size 24.
- Author name in font size of 11 in one column.
- Abstract: font size 9 with the word "Abstract" in bold italics.
- Main text: font size 10 with two justified columns.
- Two columns with equal column width of 3.38 and spacing of 0.2.
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- Large images must be in one column.
- The names of first main headings (Heading 1) must be in Roman font, capital letters, and font size of 10.
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The recommended size of an original research paper is under 15,000 words and review papers under 7,000 words. Research articles should be less than 10,000 words. Research papers are usually longer than review papers. Review papers are reports of significant research (typically less than 7,000 words, including tables, figures, and references)

A research paper must include:

a) A title which should be relevant to the theme of the paper.
b) A summary, known as an abstract (less than 150 words), containing the major results and conclusions.
c) Up to 10 keywords that precisely identify the paper's subject, purpose, and focus.
d) An introduction, giving fundamental background objectives.
e) Resources and techniques with sufficient complete experimental details (wherever possible by reference) to permit repetition, sources of information must be given, and numerical methods must be specified by reference.
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g) Suitable statistical data should also be given.
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Design has been recognized to be essential to experiments for a considerable time, and the editor has decided that any paper that appears not to have adequate numerical treatments of the data will be returned unrefereed.

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The abstract is the foundation of the research paper. It should be clear and concise and must contain the objective of the paper and inferences drawn. It is advised to not include big mathematical equations or complicated jargon.

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One should start brainstorming lists of potential keywords before even beginning searching. Think about the most important concepts related to research work. Ask, “What words would a source have to include to be truly valuable in a research paper?” Then consider synonyms for the important words.

It may take the discovery of only one important paper to steer in the right keyword direction because, in most databases, the keywords under which a research paper is abstracted are listed with the paper.

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Verbs have to be in agreement with their subjects. In a research paper, do not start sentences with conjunctions or finish them with prepositions. When writing formally, it is advisable to never split an infinitive because someone will (wrongly) complain. Avoid clichés like a disease. Always shun irritating alliteration. Use language which is simple and straightforward. Put together a neat summary.

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15. Never start at the last minute: Always allow enough time for research work. Leaving everything to the last minute will degrade your paper and spoil your work.

16. Multitasking in research is not good: Doing several things at the same time is a bad habit in the case of research activity. Research is an area where everything has a particular time slot. Divide your research work into parts, and do a particular part in a particular time slot.

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23. Upon conclusion: Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print for the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects of your research.

Informal Guidelines of Research Paper Writing

Key points to remember:

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- Write your paper in the form which is presented in the guidelines using the template.
- Please note the criteria peer reviewers will use for grading the final paper.

Final points:

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

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Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study with the subsequent elements in any summary. Try to limit the initial two items to no more than one line each.

Reason for writing the article—theory, overall issue, purpose.

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- To-the-point depiction of the research.
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Approach:

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- Simplify—detail how procedures were completed, not how they were performed on a particular day.
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Approach:

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Use standard style in this and every other part of the paper—avoid familiar lists, and use full sentences.

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The page length of this segment is set by the sum and types of data to be reported. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.

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- In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation of an exacting study.
- Explain results of control experiments and give remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or manuscript.

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- Give details of all of your remarks as much as possible, focusing on mechanisms.
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- Recommendations for detailed papers will offer supplementary suggestions.

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References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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