A 3D Numerical Statistical Solution for the Time-Independent Schrödinger Equation

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Abstract:- In previous papers we have studied the extension of transition matrix chains B to the numerical statistical solution of the time-independent Schrödinger equation in one two dimensions x,y.

In this paper we examine the extension of B-transition matrix chains to the numerical statistical solution of the time-independent Schrödinger equation in the three dimensions x, y, z.

However, extending the physical transition matrix chains B to the solution of the time-independent Schrödinger equation requires respecting certain limitations of the bases which we briefly explain in this article.

We present the numerical statistical solution via B-matrix chains in two illustrative examples, namely the three-dimensional time-dependent heat diffusion equation and the quantum particle in a three-dimensional infinite potential well. The numerical results are surprisingly accurate.

I. INTRODUCTION

In two previous articles, we studied the extension of transition matrix chains B to the numerical statistical solution of the time-independent Schrödinger equation in one and two dimensions x, y. In this paper, we propose the extension of transition matrix chains B to the numerical statistical solution of the time-independent Schrödinger equation in the 3D geometric space x, y, z.

Note that extending the chains of the physical transition matrix B for the solution of the thermal and time-independent Schrödinger equations requires the explanation of some basic physical and mathematical terms or concepts which we briefly explain in the following ten:

- Square matrices are a subset of mathematical matrices and physical square matrices that have physical meaning (such as transition matrix B) are a subset of square matrices.

- Statistical transition matrices and Chains of statistical transition matrices exist and its modeling works effectively in the solution of partial differential equations. At present, we know of two, namely the mathematical and statistical Markov transition matrix and the transition matrix B which is the subject of this article. However, in Markov matrix chains we do not care about the energy density, boundary conditions, source term, average properties of the medium, etc., whereas in the case of B matrix chains we do that .

- A physical transition matrix chain B for energy density U exist and can be defined by the recurrence relation,

$$U (x, t+ dt) = B. U(x,t)$$

NB: The transition matrix B has a place for the boundary conditions BC and the source term S which are essential in the solution of the heat diffusion equation and the Schrödinger equation respectively.

Therefore, a chain transition matrix B emerges and must be able to describe the solution trajectory through its own solution space for a given time evolution which is the energy solution E in 4-D x-t. space.

- The matrix solution for the energy density U(x,y,z,t) in time dependent and time-independent PDE appears in matrix equation form. All matrix equations "resulting from the solution of PDE via the transition matrix" are not eigenvalue equations. For example, the matrix equation of the numerical solution of the heat diffusion equation results in a system of non-homogeneous first-order linear algebraic equations while the matrix equation of the numerical solution of the Schrödinger equation is homogeneous and results in an eigenvalue problem with multiple eigenvalues. Several eigenvalues have their corresponding eigenvectors. The time-dependent and time-independent Schrödinger equations are in-depth examples of eigenvalue equations in quantum mechanics, with their eigenvalues corresponding to the allowed energy levels of the quantum system. Generally speaking, in the statistical transition matrix B, the eigenvalue is the dominant eigenvalue (eigenvalue of the maximum absolute value) equal to 1.

- What is the Schrödinger equation and what is the time-independent Schrödinger equation?

  ✓ The time-dependent equation is
  ✓ $i\hbar(d\psi/dt) = \hat{H}\psi$,
  ✓ and the time-independent equation is
  ✓ $E\psi = \hat{H}\psi$.

  Showing that the Schrödinger equation is a second-order linear PDE in the so-called wave function $\psi(x,t)$ and is a way to probabilistically describe the time evolution of

energy, momentum and the position of quantum particles in space. His time-independent equation for ψ(x) describes the equilibrium state that occurs when evolutionary time tends to infinity. It should be noted that another way to describe quantum particle dynamics is to use statistical transition matrices that completely ignore the Schrödinger equation and the wave function ψ as if they never existed in the same way that one solves the heat diffusion equation without going through the thermal EDP.

Obviously it is ψ2 and not ψ itself which is replaced by the energy density U to be the subject of the study in the matrix chains B.

- What is a Numerical and/or Statistical Solution!

The numerical solution replaces the analytical solution of the time-dependent PDE by discretizing space and time into dx and dt and replacing the differentials dy/dx by [y+dy-2y +y-dy]/2dx And d ^2 y/dx ^ 2 by [y+dy-2y +y-dy]/dx^2. etc.

In other words, the numerical solution method reduces the PDE to a system of algebraic equations via the finite difference method FDM.

On the other hand, calculus methods such as (FDM) are not necessary in transition matrices of statistical solutions since FDM techniques inherently exist in statistical chains of transition matrices.

- This means that, in a way, the numerical statistical solution is a subset of the numerical solution in which the differential calculus is ignored and replaced by the statistics of the transition matrix.
- In addition, the method of separating variables W(x,y,z,t)=X(x)Y(y)Z(z) f(t) is also not necessary because it is intrinsically included in the unit 4D inseparable space x-t of the B matrix strings.
- The numerical (technical) method of Monte Carlo is the closest to the Cairo technical method. However, the numerical Monte Carlo method is a bit old and requires generating a random numerical variable thousands of times. This makes the interpretation of its numerical results long and tedious.
- Finally, it should be mentioned that today we only know one physical transition matrix which is the transition matrix B resulting from the so-called Cairo technique.

Through this article, we examine in detail two different illustrative 3D physics problems in the areas of the heat diffusion equation and the time-independent Schrödinger equation.

Namely, we present numerical results for time-dependent thermal diffusion in a three-dimensional thermal energy field and the steady-state distribution of quantum energy density in a 3D potential box.

II. THEORY

In practice, the field of modern quantum mechanics relies entirely on the Schrödinger equation and its derivatives which constitute a subset of physics but not physics as a whole. Bohr's original theory of the hydrogen atom introduced the condition of quantization of electronic energy as quantification for the first time in history. circular orbits of the electron around the nucleus in orbits called allowed orbits. The so-called authorized orbits give rise to authorized atomic energy states, as opposed to prohibited energy states. Niels Bohr's original model in 1913 was based entirely on Newton's laws of motion supplemented by Bohr's quantification hypothesis, of the principal quantum number n, namely,

$$mv. \ 2\pi. \ Rn=nh. \ . \ . \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(1)$$

n=1,2,3. . , infinity

Where Rn is the nth radius of electrons circulating around the nucleus.

At the time, N. Bohr did not say a word about the electronic cloud or the superposition of quantum states. Nor did he say about the electron cloud in a quadratic potential nor about any of the quantization numbers (n, l, m, s) other than the principal quantum number n.

This is called classical quantum mechanics, where the electron is considered as a particle whose position x, speed v and trajectory in space are known. Although old and classical, Bohr's original hypothesis in 1913 introduced a giant step towards modern quantum mechanics and the Schrödinger equation to come in 1927.

Accordingly, we introduce the term classical quantum mechanics which corresponds to the original model of quantum mechanics developed by N. Bohr's theory of the hydrogen atom in 1913 and to similar models which considered subatomic particles as a point in the x-t space.

Modern quantum mechanics was supplemented by the 1927 Schrödinger equation and the Bohr/Copenhagen interpretation. This interpretation is known as the principle of superposition of quantum states. It is considered the second giant leap emerging Bohr's modern theory of the hydrogen atom in 1927.

N. Bohr introduced the concept of representing the dynamics of subatomic particles in space as a probability cloud described by the Schrödinger equation which replaced Newton laws of motion. In this article we describe how to apply the chains of the matrix B to describe the quantized dependence of the total energy E on a principal quantum number n (in order not to go further to other quantum numbers l, m, s)

The quantum hypothesis of energy and angular momentum can be, in some way, replaced by the quantification of time inherent in matrix chains B.

The concept of a quantum point particle and a quantum particle path subject to Newton's laws of motion has been radically overturned.

We recall that, in previous articles [2,3,4] we had introduced numerical statistical solutions to time-dependent partial differential equations such as Poisson and Laplace partial differential equations, sound intensity and time of reverberation in audio rooms. , digital integration and differentiation, etc. Our proposed numerical statistical modeling for the study of time-independent SEs is based on the same chains of transition matrices B and its derived transfer matrices D, E. The basic entries of the statistical transition matrix B (i, j) are well defined in 1D, 2D and 3D configuration space problems via four statistical conditions [2,3,4] and the resulting transfer matrices D ,E are well defined via the following relation elements:

$$E(N) = B0 + B + B2 + B3 + . . . + B^N. . . . . ……….…..(2)$$

Where,

B0 = I, the unitary matrix.

If N is sufficiently large, we arrive at the time-independent steady state solution,

$$E = 1/(I-B) . . . . ……………………………………. (3)$$

For N sufficiently large.

In all cases, the transfer matrix D is defined as,

$$D = E-I . . . .. ……………………………….….... (4)$$

Equation 3 is the reason why we introduced the transfer matrix E to use in the first step, and then calculated the transfer matrix D from equation 4 in the second step. This matrix calculation procedure is called the Cairo technique (by distinction) [2,3,4].

We emphasize again that the Cairo technical procedure for solving the time-dependent PDE in classical physics and its proposed extension to cover QM problems is not complicated but rather lengthy and requires mastery of some prerequisites in matrix algebra [1] and in statistical transition matrix chains [2,3,4].

In the Cairo techniques approach, the time-dependent solution of the PDE energy density U (x, t) is given by,

$$U (x, t)=D(N) . (b + S) + IC . B^N . . . . . ……………..(5)$$

Where S is the vector of the source/sink term and IC is the vector of the initial conditions. Equation 5 is used as a time dependent statistical PDE equivalence matrix which has been used in the solution of classical physics problems such as heat conduction PDE and it is now proposed to find a solution to the equation of Schrödinger 3D geometric shapes.

It should be noted that equation 5 contains a term due to the initial state conditions described by IC. B^N which decreases exponentially with time because the modulus of matrix B is less than 1. This term tends towards zero with time and is therefore not treated in the present case of the steady state in the remainder of this article. Note that equation 5 is the solution of U(x,t) in a 4D unit space x-t where the real time t is completely lost and is replaced by a dimensionless integer N.

It is also worth mentioning that discretizing time t into forbidden and allowed where t = N dt and N is an integer is itself a quantification of time. Again, the integer N is the number of iterations which is the number of time steps or time jumps dt. One important reason to replace the Schrödinger equation with chains of statistical transition matrices is that you are moving from an area of SE where many unanswered questions remain to the area of modern statistical physics where almost all questions have adequate answers.

The question arises how to extend the B matrix chain solution of the Cairo technique to cover time-independent stationary situations in 3D quantum mechanical problems.

In other words, how can we process Equation 5 in order to find the statistical equivalence of the 3D Schrödinger equation? This is the subject of the current article.

The time-independent Schrödinger equation, describing the square root of the probability density function ψ in all space, is expressed as follows:

$$E. \psi(x,y,z) = -h^2/2m. \text{Nabla}^2 \psi(x,y,z) + V(x,y,z) .\psi(x,y,z) . . . (6)$$

Considering that the statistical equivalence approach of the Cairo techniques which is in general a time-dependent solution for the energy density U(x,t) as given by equation 5,

$$U(x, t)=D(N) . (b + S) + IC. B^N . . . . . .……………(5)$$

Eq 7 is very important as it defines the spatio-temporel evolution of the energy density U in space and time in matrix form.

The similarity between Equation 5 and Equation 6 is obvious and the application of Equation 5 to solving quantum mechanical problems seems natural.

➢ *In Order to apply Equation 5 as a Substitution for Equation 6, we Propose two Important Natural Assumptions:*

- We first assume an intrinsic and/or extrinsic landscape potential V(x,y,z) which must be symmetrical and imply zero BC.
- We assume that the matrix B must be completed by a diagonal matrix V representing the source term S, that is to say

S(x,y,z,t)=Constant. V(x,y,z,t) . . . .………………………… (7)

Where S is a source term.

The constant in equation 7 is found by trial and error.

Equation 7 is a breakthrough because it characterizes the physical domain of validity of SE and suggests a statistical solution to 3D SE that circumvents SE itself.

There is a simple way to solve the matrix statistical equivalence of SE,

[B(x,y,z)] + C [V(x,y,z)] . . . . .….………………….……… (8)

This involves assuming in advance the potential landscape V (x, y, z) first, then working backward to find the eigenvalues and eigenvectors of the energy. This may be a way to resolve the SE, while it's easier to go back and look for a solution.

This is exactly what happens even when solving the 1D, 2D and 3D Schrödinger equation via B-matrix statistical chains, while it is better to first assume the potential landscape before solve.

We also assume that the solution of matrix chains B may be, in some way, more informative than SE itself, a claim which will be explored in more detail when describing solutions to Schrödinger's equations in 4D.

It is worth mentioning that B-matrix string theory is not entirely new and has been working effectively since 2020 [2,3,4].

In order not to worry too much about the details of the theory, let's move on to the following numerical results.

III. NUMERICAL RESULTS

A. 3A Heat Diffusion Equation

The heat diffusion/conduction equation is of particular importance both in modern classical physics (classical physical laws supplemented by the modern definition of transition probability) and in quantum mechanics where we find numerous communities of characteristics.

In the previous parts of this article I, II, we solved the thermal conduction/diffusion equation in 1D and 2D via chains of 1D and 2D B matrices. In this third part of the paper, we use 3D B-matrix chains to find a numerical statistical solution for the spatiotemporal heat diffusion flow in solid shapes and test the correctness and precision of the numerical statistics of the method.

Consider the simple case of a rectangular cube shown in Figure 1 with 27 equidistant free nodes, u1, u2, u3, ... u27 and 52 Dirichlet boundary conditions BC1 to BC52. These conditions of 52 BC are reduced to just 27 BC when using the ruler,

- BC(1)=BC1X+BC1Y+BC1Z

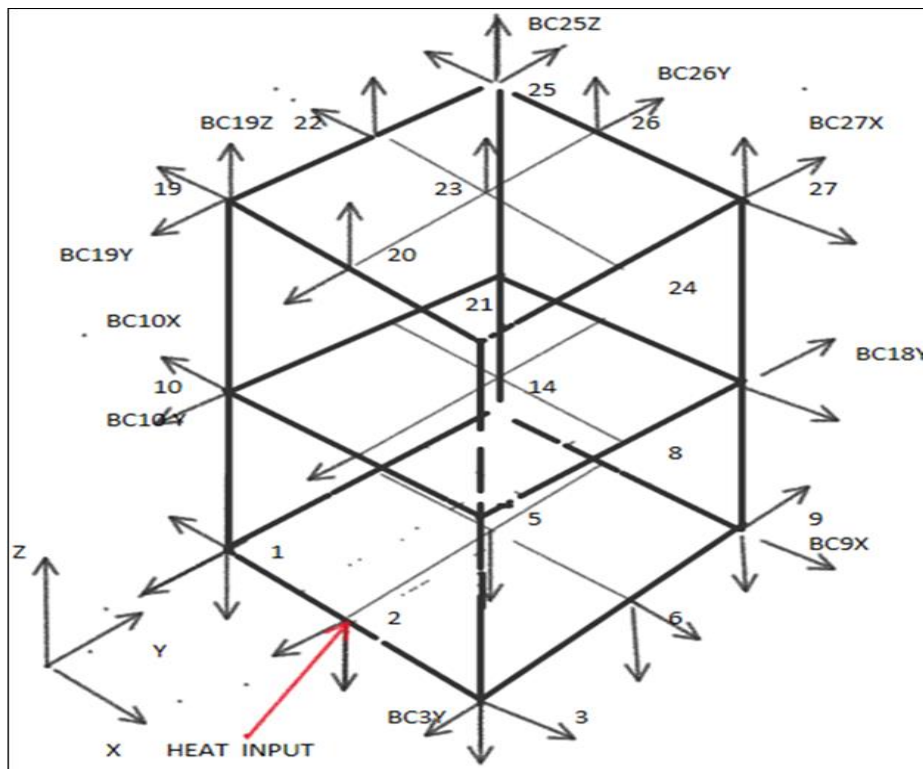- BC(2)=BC2X+BC2Y+BC2Z

- BC(27)=BC27X+BC27Y+BC27Z

Fig 1 Heat Diffusion Flow in a Rectangular Cube with 27 Equally Spaced Free Nodes

As shown in Figure 1 A 3D rectangular cube domain with 27 equally spaced free nodes subjected to Dirichlet BC.

Again, the 52 boundary conditions in Figure 1 can be reduced only to 27 modified BCs for the 7 boundary nodes as follows:

- BC(1)=BC1X+BC1Y+BC1Z

- BC(2)=BC2X+BC2Y+BC2Z

- BC(27)=BC27X+BC27Y+BC27Z+ BC9Y

➢ *Step 1*

The first step consists of constructing the 27x27 B transition matrix so as to satisfy the conditions i-iv [2,3,4] and to set the presupposed value of RO.

For an arbitrary RO, the 27x27 matrix B is given by,

27X27 B-Matrix inputs

- Line1 RO 1/6-RO/6 0.0000 1/6- RO 1/6-RO/6 0.0000 0.0000 0.0000 0.00001/6-RO/6 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000.0000 0.00000.00000.0000 0.0000 0.0000 0.0000 0.0000 0.0000

- Line 2 1/6-RO/6 RO 1/6-RO/6 0.0000 1/6-RO/6 0.0000 0.0000 0.0000 0.0000.00001/6-RO/6 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000.00000.00000.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

- Line 3 0.0000 1/6-RO/6 RO 0.0000 0.0000 1/6RO/6 0.0000 0.00000.00000.00000.0000 1/6-RO/6 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000.00000.00000.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

- Line 14 0.0000 0.0000 0.0000 0.0000 1/6-RO/6 0.0000 0.00000.00000.00000.0000 1/6-RO/6 0.0000 1/6-RO/6 RO 1/6-RO/6 0.00001/6-RO/60.00000.0000 0.0000 0.0000 0.0000 1/6-RO/6 0.0000 0.0000 0.00000.0000

- Line 25 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000.00000.00000.0000 0.0000 0.0000 0.0000 1/6-RO/6 0.0000 0.00000.00000.00000.0000 1/6-RO/6 0.0000 0.0000 RO 1/6-RO/6 0.0000

- Line 26 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000.00000.00000.0000 0.0000 0.0000 0.0000 0.0000 1/6-RO/6 0.00000.00000.00000.0000 0.0000 1/6-RO/6 0.0000 1/6-RO/6 RO 1/6-RO/6

- Line 27 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000.00000.00000.0000 0.0000 0.0000 0.0000 0.0000 0.0000 1/6-RO/60.00000.00000.0000 0.0000 0.0000 1/6-RO/6 0.0000 1/6-RO/6 RO

- *We Call this Matrix M1.*

Note that a given numerical value of RO uniquely defines the thermal diffusivity of the medium, e.g. RO = 0.22 for legal carbon steel and 0.13 for high purity aluminum, as shown in reference 5.

➢ *Step 2*

Choose the appropriate values of the boundary conditions vector b and the source/sink term S corresponding to a given set of experiments.

Here we set S=0 for all 27 free nodes, except node 2 which is set to 100 units. The 27 boundary condition inputs b, are all set to zero as for Zeiga modeling in 2021[6].

The initial conditions vector IC is set equal to zero for all 27 free nodes.

➢ *Step 3*

Use equations 2 and 4 to calculate D(N) for different N for a given RO parameter, then use equation 5 { U(x, t)=D(N). (b + S) + IC * BN} to calculate the spatio-temporal evolution of the temperature field. Zeiga [6] classically solved the same thermal system shown in Figure 1 via the MATLAB technique and obtained a space-time distribution of the temperature field similar to that of the B-matrix chain solution.

However, it should be mentioned that the numerical results in reference 6 are not related to the thermal properties of the support material.

Numerical results for the thermal system in the following table,

N= 1

0.000	100.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000					

- *Axial Temperature 0.000   0.000   0.000*

EXP RISE/DECAY ALPHA = -0.4302

N=5

24.107	139.25	24.107	7.42	25.387	7.427
1.280	3.903	1.280	7.427	25.387	7.427
2.560	7.80	2.560	0.379	1.280	0.379	1.280
3.903	1.280	0.379	1.280	0.379	0.000	0.190
0.000					

- *Axial Temperature   25.387   7.806   1.280*

EXP DECAY ALPHA = -0.405

N=10

27.359   143.910   27.359   10.833   30.383
10.833   3.024   6.429   3.024   10.833   30.383
10.833   6.048   12.859   6.048   2.026   3.768
2.026   3.024   6.429   3.024   2.026   3.768   2.026
0.744   1.295   0.744

- *Axial Temperature   30.383   12.859   3.768*

EXP DECAY ALPHA = -0.405

N=15

27.921   144.707   27.921   11.570   31.426   11.570
3.505   7.110   3.505   11.570   31.426   11.570   7.009
14.220   7.009   2.649   4.651   2.649   3.505
7.110   3.505   2.649   4.651   2.649   1.147   1.865
1.147

- *Axial Temperature   31.426   14.220   4.651*

EXP DECAY ALPHA = -0.364

N= 20

28.053   144.893   28.053   11.753   31.684   11.753
3.631   7.289   3.631   11.753   31.684   11.753   7.262
14.578   7.262   2.825   4.899   2.825   3.631   7.289
3.631   2.825   4.899   2.825   1.268   2.037   1.268

- *Axial Temperature   31.684   14.578   4.899*

EXP DECAY ALPHA = -0.382

Where the axial points are nodes 5,14,23 and Alpha parameter represents the exponential coefficient in the formula:

$T(x,y,z,t)=F(x,y,z).\text{Exp-Alpha} . t$ . . . . Cooling curve,

$T(x,y,z,t)=F(x,y,z).(1-\text{Exp-Alpha} . t)$ . . . . Heating curve

WE present the Temperature T along the central axis as a function of time t=n. dT in Figure 2.
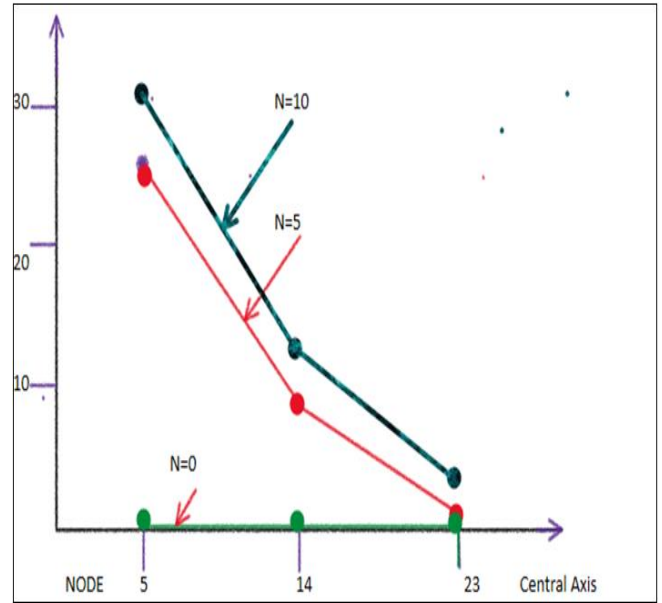
Temperature T

Fig 2 Temperature along the Central Axis as a Function of Time

Here the numerical value of Alpha which is a function of the size and shape of the object considered as well as the thermal diffusivity coefficient is invariant and is almost equal to 0.37 in SI units.

B. A Quantum Particle in a 3D Potential box (Fig.1)

Interestingly, the same transition matrix B used to solve classical physics problems such as heat diffusion PDE is also valid for the solution of the time-independent Schrödinger equation with minor modifications [7,8,9].

➢ *Step 1*

- Construct the B-matrix 27x27 with RO=0.
- We call this matrix M2.

➢ *Step 2*

- Construct the proper matrix M3=M2+CV(x,y,z). I
- Such that V(x,y,z) is symmetrical about the center of mass (node 14) and tends to zero at the boundaries.
- The 27x27 eigenmatrix is given by,

3/16 1/6 0.0 1/6 0.0 0.0 0.0 0.0 0.0 1/6 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

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0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1/6 0.0 0.0 0.0 0.0 0.0 1/6 0.0 1/6 3/16

Note that we used an integer multiplication factor for the 27 diagonal entries M3 (I,i) of, 3 4 3 4 6 4 3 4 3 3 4 6 4 6 8 . . . etc

➢ *Step 3*
Verify that V(x,y,z) is an eigenvector of M3 with an eigenvalue equal to 1.

- *V(x,y,z)=*
- ✓ 635/256
- ✓ 63/16
- ✓ 635/256
- ✓ 63/16
- ✓ 641/96
- ✓ 63/16
- ✓ 635/256
- ✓ 63/16
- ✓ 635/256
- ✓ 193/48
- ✓ 641/96
- ✓ 63/16
- ✓ 641/96
- ✓ 45/4
- ✓ ..etc..

- *M3 . V(x,y,z)=*
- ✓ 635/256
- ✓ 63/16

- ✓ 635/256
- ✓ 63/16
- ✓ 641/96
- ✓ 63/16
- ✓ 635/256
- ✓ 63/16
- ✓ 635/256
- ✓ 193/48
- ✓ 641/96
- ✓ 63/16
- ✓ 641/96
- ✓ 45/4
- ✓ ..etc..

- *Showing that $M3 . V(x,y,z)=V(x,y,z)$ is almost exact !*

IV. CONCLUSION

Extending the physical transition matrix chains B to the solution of the time-independent Schrödinger equation is not complicated but it is a bit long and requires respecting certain limitations of the bases which are briefly explained in this article. The present study shows that the statistical chains of matrix B can be applied to the solution of the time-dependent 3D heat equation and the time-independent 3D Schrödinger equation. We present the numerical solution via the statistical transition matrix B in two illustrative situations, namely the 3D thermal diffusion equation and the quantum particle in a three-dimensional box where the numerical results are of excellent precision.

- *NB: In the previous calculations, the author used his own double precision algorithm as explained in ref. 10.*
- *No ready-made algorithms such as Python or MATLAB are needed*

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