A Statistical Numerical Solution for the Time-Independent Schrödinger Equation

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Abstract:- B-transition matrix chains resulting from the Cairo technique numerical statistical solution method have been successfully applied to statistically solve time-dependent partial differential equations in classical physics.

This paper studies the extension of transition matrix chains B to the numerical statistical solution of the time-independent Schrödinger equation.

However, 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 we briefly explain in this article.

We present the numerical solution of matrix B in three illustrative examples, namely the heat diffusion equation, the quadratic potential well and the one-dimensional infinite potential well wherethe numerical results are surprisingly accurate.

I. INTRODUCTION

This paper studies the extension of transition matrix chains B to the numerical statistical solution of the time-independent Schrödinger equation. However, extending physical transition matrix chains B to the solution of the time-independent Schrödinger equation requires some basic clarifications which we briefly explain as follows:

- Statistics transition matrices and chains of statistical transition matrices exist and its modelling works effectively in the solution of partial differential equations.

    At present, we know two of them, namely the mathematical statistical transition matrix of Markov and the transition matrix Bwhich is the subject of this article.

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

- Not all matrix equations "resulting from the solution of PDE viathe transition matrix" are eigen value equations.

    For example, the matrix of the numerical solution of the heat diffusion equation results in a system of non-homogeneous firstorder linear algebraic equations while the matrix of the numerical solution of the Schrödinger equation is homogeneous and results in an eigen value problem with multiple eigen values.

    Multiple eigen values have their corresponding eigenvectors.

Both the time-dependent and time-independent Schrödinger equations are in-depth examples of eigen value equations in quantum mechanics, with their eigen values corresponding to the allowed energy levels of the quantum system.

- A transition matrix, such as the B-statistical transition matrix, must be able to describe the trajectory of the solution through itsown space of solutions for an evolution in time which is the solution of the energy E in the 4-D x-t space.

Generally speaking, in the statistical transition matrix B eigenvalueis the dominant eigenvalue (eigenvalue of maximal absolute value)equal to 1.

Through this article, we examine in detail three different illustrative physical problems in the areas of the heat diffusion equation and the time-independent Schrödinger equation.

The numerical results for heat conduction in a long rod, the steady-state distribution of quantum energy density in a quadratic potential field, and a one-dimensional infinite potential well are surprisingly accurate.

In fact, 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. Many physicists and mathematicians recommend skipping classical quantum mechanics.

By classical quantum mechanics we mean the original QM of the hydrogen atom by N. Bohr in 1913 before the Schrödinger equation and the Bohr/Copenhagen superposition interpretation in 1927.Bohr's original theory of the hydrogen atom introduced for the first time in history the condition of quantization of electronic energy as quantification of the 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 forbidden energy states.

Niels Bohr's original model in 1913 was based entirely on Newton'slaws of motion supplemented by Bohr's quantification hypothesis, ofthe principal quantum number n, namely,

$$mv.2\,\pi.\,Rn{=}n\,h \ldots \qquad (1)$$

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 orthe superposition of quantum states.

He also said nothing about the electron cloud in a quadratic potentialnor about any of the quantization numbers (n, l, m, s) other than the principal quantum number n.

This is what we call classical quantum mechanics, where the electronis considered as a particle whose position x and velocity v are known.

In fact, Bohr's original hypothesis in 1913 introduced a giant steptowards modern quantum mechanics and the Schrödinger equationin1927.

As a result, classical quantum mechanics corresponds to N. Bohr's original QM model of the hydrogen atom and similar models that consider subatomic particles as a point in x-t space, prior to Schrödinger's equation with N. Bohr/Copenhagen super position interpretation.

A second giant step was Bohr's modern theory of the hydrogen a tomin 1927, where he introduced the concept of representing the dynamics of subatomic particles in space as a probability cloud described by the equation of Schrödinger which replaced Newton's laws of motion.

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

We assume that classical quantum mechanics somehow forms the basis of an approach to understanding or a preliminary description of modern quantum mechanics. And, therefore, a professional mathematician/physicist should master classical quantum mechanics before studying modern quantum mechanics, sometimes called full or complete quantum mechanics.

The preceding analysis applies both to the statistical study of the Schrödinger equation and to modern or complete quantum mechanics. And yet, we begin by focusing on classical quantum mechanics and its eigenvalue problems as a preliminary step to the study of modern quantum mechanics.

In other words, we assume that the proposed numerical statistical solution for the time-independent Schrödinger equation is a preliminary step on a long path toward the solution of complete quantum mechanics described by the time-dependent Schrödinger equation.

We recall that, in previous articles [2,3,4] we 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 numerical statistical modelling proposed for the study of time-independent SEs is based on the same chains of transition matrices Band 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 elements of the relationships:

$$E(N) = B0 + B + B2 + B3 + \ldots + BN \ldots \quad (2)$$

Where,
$B0 = I$, the unit matrix.
If N is large enough, we arrive at the time-independent steady state solution,

$$E = 1/(I-B) \ldots \quad (3)$$

For N sufficiently large.

In all cases the transfer matrix D is defined as,

$$D = E - I \ldots \ldots \quad (4)$$

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 procedure is called the Cairo technique (by distinction)[2,3,4].

It is worth mentioning 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 pre requisites in matrix algebra and in statistical transition matrix chains [1,2,3,4].

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

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

Where S is the source/sink term vector and IC is the initial conditions vector.

It should be noted that equation 5 contains a term due to the initial state described by IC. B^N which decreases exponentially with time because the module 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 Eq 5 is the solution of U(x,t) in 4D x-t unitary space where the real time t is completely lost and is replaced by a dimension less 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 inherently 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 of the important reasons for replacing the Schrödinger equation with chains of statistical transition matrices is that you are moving from a field of SE where many questions remainun answered to the field of modern statistical physics where almost all questions have adequate answers.*

We emphasize here that the subject of the statistical equivalence of the Schrödinger equation is not complicated but is a bit long and requires prior knowledge of matrix algebra [1] and the statistical solution of the matrix B to the problems of statistics and classical physics [2, 3,4, 6].

The question arises: is it possible to extend the B matrix chain solution of the Cairo technique to cover time-independent stationary situations in quantum mechanics? In other words, how can we process equation 5 in order to find a statistical equivalence of the Schrödinger equation?

This is the subject of the current article.

II. THEORY

There are two completely different languages for dealing with the subject of quantum mechanics, resulting in two different approaches:

- The time-independent Schrödinger equation, describing the square root of the probability density function ψ in all space, is expressed as follows:
  $$E. \psi(x) = -h^2/2m. \, d/d2x . \psi(x) + V(x) . \psi(x) \ldots \quad (6)$$

- The statistical equivalence approach of Cairo techniques which is in general a time-dependent solution for the energy density $U(x,t)$ as given by equation 5,
  $$U(x,t) = D(N) . (b + S) + IC. B^N \ldots \ldots (5)$$

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:

- If the stationary Schrödinger equation can be interpreted as aneig envalue equation in Hamiltonian space describing the square root of the probability density ψ then the square of ψ can also be interpreted as an eigen value equation in l 'space of matrix B (or any other appropriate space equation) having eigen values (λ^2)

- the square of ψ can also be interpreted as the quantum energy density and that ψ^2 is subject to the classical physical transition matrix B described by equation 5 with secondary modification.

- The modifications required for Equation 5 to describe the time-independent Schrödinger equation are briefly:

  ✓ The vector of boundary conditions b in Eq. 5 must be set equal to 0since the function ψ extends to +/- infinity and is bounded.

  ✓ The source/sink term S in Eq. 5 is conveniently described by afunction of the potential V(x), viz,

  $$S(x) = Constant * V(x) \ldots \quad (7)$$

Equation 7 is very important and can be applied to 2D and 3D geometric configuration, i.e.
  $$S(x,y) = Constant * V(x,y)$$
  $$S(x,y,z) = Constant * V(x,y,z)$$

This means that S = Sx + sy + Sz, which will be explained in more detail in Part III of this article.

Note also that equation 7 applies both to the cases of quadratic potential of the hydrogen atom and to the case of 1D potential wells.

The choice of constants C depends on the size and structure of the matrix B.

It is worth mentioning that the same matrix B which works efficiently for the solution of the time-dependent heat conduction equation is proposed for the solution of the time-independent Schrödinger equation.

The space of matrix B is subject to the condition,

PE/E =RO (where RO are the main diagonal entries of the matrix B[2,3,4]).

RO is the constant of motion and is function of the coefficient of heat diffusion D in the thermal conduction problems.

Note that the study of transition matrix solutions allows all possible values of RO in the interval [0,1] for the solution of the thermal conduction equation whilethe allowed values of RO for quantum mechanics problems are [0,1/2].

The statistical reason is that for RO > ½ Eq 2 would not converge.

It is worth mentioning that the strings of matrix B may be, in some way, more informative than SE itself. Again, the reason why the boundary conditions in Equation 5 are assumed to be zero is that the Schrödinger equation which describes the wave function and energy of the particle throughout space -∞ <x< ∞ must be delimited. 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 three illustrative applications.

III. NUMERICAL RESULTS

A. Heat diffusion/conduction equation

The heat diffusion/conduction equation has particular importance both in modern classical physics (classical physical laws supplemented by the modern definition of transition probability) and in classical and modern quantum mechanics where there are many communities of characteristics.

We start here with the 1D thermal conduction/diffusion equation problem where there is a great similarity between the solution procedure and the use of the transfer matrices D and E of the thermal diffusion/conduction equation and the solution of the Schrödinger equation.

Consider that a long uniform rod is heated under Dirichlet boundary conditions, that is, the near end is kept at unit temperature (T = 1)and the far end is kept at zero (T = 0), as shown in Figure 1.Fig 1- Temperature distribution for long uniform rod subjected to Dirichlet boundary conditions. The 1D x stem space is discretized into 11 free nodes and the11x11 transition matrix B can be applied for any RO element of the closed interval [0,1].
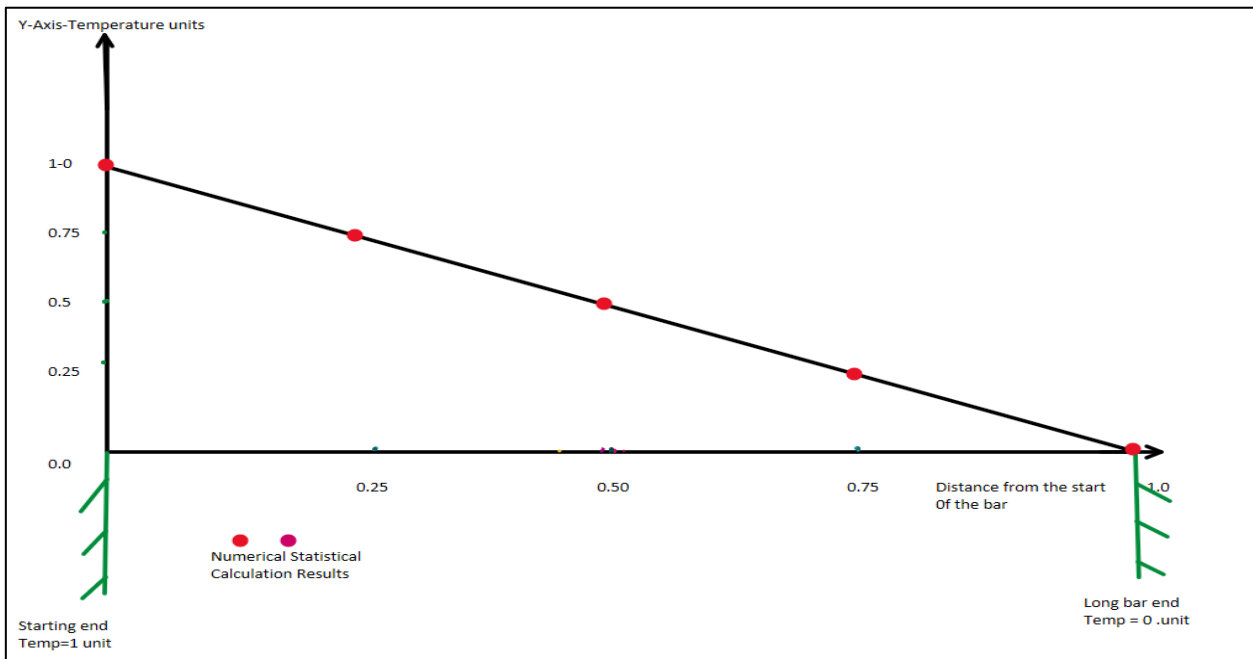

Fig. 1: A long uniform rod is heated under Dirichlet boundary conditions

Finding the solution of the heat equation without going through the partial differential equation of heat is a challenge but rather possible by following the following steps,

> *Step 1*

Construct the 1D B-matrix 11x11 with RO=0.

Note that for the steady state of the heat diffusion problem, all values of the RO element of [0,1] will converge to the same matrix E.

The tri diagonal 1D B-matrix 11x11 is given by[2,3,4],
RO ½-RO/20 0 0 . . . . 0 0
½ -RO/2 RO ½-RO/20 0 . . . 0 0
. . . .

> *Step 2*

Using equation M1 and equation 3, the numerical results forthe transfer matrix E11x11 are given by,

  11/6 5/3 3/2 4/3 7/6 1 5/6 2/3 1/2 1/3 1/6
  5/3 10/3 3 8/3 7/3 2 5/3 4/3 1 2/3 1/3
  3/2 3 9/2 4 7/2 3 5/2 2 3/2 1 1/2
  4/3 8/3 4 16/3 14/3 4 10/3 8/3 2 4/3 2/3
  7/6 7/3 7/2 14/3 35/6 5 25/6 10/3 5/2 5/3 5/6
   1 2 3 4 5 6 5 4 3 2 1
  5/6 5/3 5/2 10/3 25/6 5 35/6 14/3 7/2 7/3 7/6
  2/3 4/3 2 8/3 10/3 4 14/3 16/3 4 8/3 4/3
  1/2 1 3/2 2 5/2 3 7/2 4 9/2 3 3/2
  1/3 2/3 1 4/3 5/3 2 7/3 8/3 3 10/3 5/3
  1/6 1/3 1/2 2/3 5/6 1 7/6 4/3 3/2 5/3 11/6

We call this matrix M2.

Note that the matrix E is equal to its transpose similar to its generating matrix B,

0 0 . . . 0 0 0 0 0 0 ½-RO/2 RO

We call it matrix M1

The preceding matrix M1 is used calculate the time-independent steady state solution of the temperaturedistribution along the bar via the transfer matrices D,E.

In the PDE solution with time-dependent thermal conduction, the RO value can take any value between 0 and 1 determined by the thermal diffusivity value D of the medium butwe emphasize again that the numerical results for the energy density (T) of the time-independent 1D steady-state heat diffusion equation do not depend on the choice of RO.

$B=B^T$

And,
$E = E^T$

Step 3

Calculate the vector of temperature distribution (vector v) alongthe rod from Eq 5,
V=D . (b+S)

when S=0, or from its alternative equation,
V=[E-I] . (b+S) with S=0.

➢ *Step 3*
For the numerical values of the physical situation shown in Figure 1, the 11-element boundary condition vector b is expressed as follows:

b1 =[1 0 0 0 0 0 0 0 0 0 0]T

and the numerical values of the solution vector V1 given by V1=E*b1 are given by,

V1=[11/6 5/3 3/2 4/3 7/6 1 5/6 2/3 ½ 1/3 1/6]^T

➢ *step 4*
The last step 4 consists of dividing the vector V1 by a factor 2 to obtain the temperature distribution vector, namely:

T =[11/12 5/6 3/4 4/6 7/12 1/2 5/12 2/6 ¼ 1/6 1/12]^T

Which is exactly the same as the numerical results shown in Figure 1.

We present Figure 1 to show the linear dependence of T on x.

T is the temperature energy density distribution (y axis) along the rod (x direction).

The reason for dividing by the factor of 2 in step 4 is that we used the transfer matrix E instead of the transfer matrix D. Considering that E=D+I resultsin a doubling of the numerical values of the answer, you must then divide by 2.

B. Application on the Hydrogen atom
Here, the system of linear algebraic equations is homogeneous and its solution satisfies the eigenvalues and eigenvectors of E as explained previously by equations 5,6.

Our goal is to find the admissible energy levels for a quantum particle in an infinite potential well (Fig. 2), as introduced by Bohr's original 1913 model via the use of equation 5.
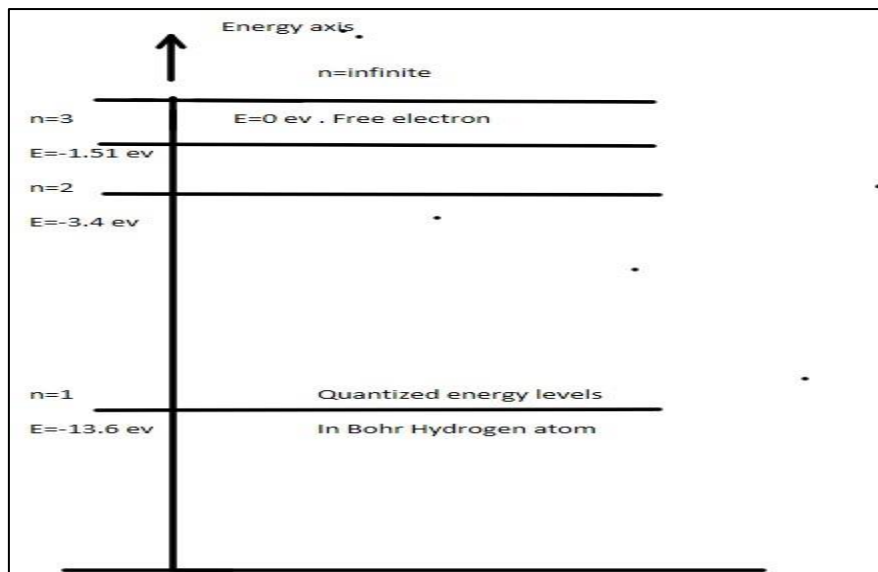

Fig. 2: Energy levels allowed in the classical hydrogen atom

➢ *step 1*
Construct the same 11x11 matrix B 11x11 (or any other nxn square matrix which is an arbitrary choice) for RO=0.

Matrix B= Matrix M1 explained previously in the heat diffusion problem.

➢ *Step 2*
In the case of 1D quantum mechanics problems the matrix M1 must be transformed into matrix M2 where M2 is equal to M1+C1*I.

C1 is equal to 1/11 or 0.091 to close the matrix M2 which describes a closed energy system as required by the Schrödinger equation.

➢ *Step 3*
Construct the proper or eigenmatrix M3 = M2 + C . V(x)*I

By the method of trial and error, the constant C is set to near 0.75 V(x), as equation 7 suggests.

Note that you should predefine appropriate values for V(x) provided that they represent a symmetric quadratic potential field.

Therefore, the eigenmatrix M3 =

0.75*1/36	1/2	0	0	0	0	0	0	0	0	0
1/2	0.75*1/25	1/2	0	0	0	0	0	0	0	0
0	1/2	0.75*1/16	1/2	0	0	0	0	0	0	0
0	0	1/2	0.75*1/9	1/2	0	0	0	0	0	0
0	0	0	1/2	0.75*1/4	1/2	0	0	0	0	0
0	0	0	0	1/2	0.75*1/1	1/2	0	0	0	0
0	0	0	0	0	1/2	0.75*1/4	1/2	0	0	0
0	0	0	0	0	0	1/2	0.75*1/9	1/2	0	0
0	0	0	0	0	0	0	1/2	0.75*1/16	1/2	0
0	0	0	0	0	0	0	0	1/2	0.75*1/25	1/2
0	0	0	0	0	0	0	0	0	1/2	0.75*1/36

> *step 4*

Verify that the vector V(x) is the principal eigenvector with dominant eigenvalue λ. In other words, multiply M3 by the external applied potential (voltage) V(x) where V(x) is the applied quadratic function potential (electric potential of the nucleus on the circulating electron as described by equation 1) given by the symmetric vector,

V(x)=
0.75*1/36
0.75*1/25
0.75*1/16
0.75*1/9
0.75*1/4
0.75*1/1
. . . . .
continue with symmetry,

gives the energy states authorized in the following vector V2,

V2=
889/57600
8341/240000
18083/307200
143/1152
347/768
3/4
347/768
143/1152
18083/307200
8341/240000
889/57600

The values are proportional to the quantized energy for the infinite 1D potential shown in Figure 2.

C. A quantum particle in a 1D infinite potential well

Here, we follow exactly the same procedure of steps as that of the previous application III-b with the only difference that the applied potential vector V(x) is intrinsic and assumed to be symmetrical and linear such that:

V(x)=C . (0 1 2 3 4 5 4 3 2 1 0)

> *step 1*

The 1D statistical B-matrix 11x11 is chosen the same as M1 in cases A and B for RO=0 .

The proper eigen matrix It is expressed by the following M4 and the numerical results are presented in Figure 3.
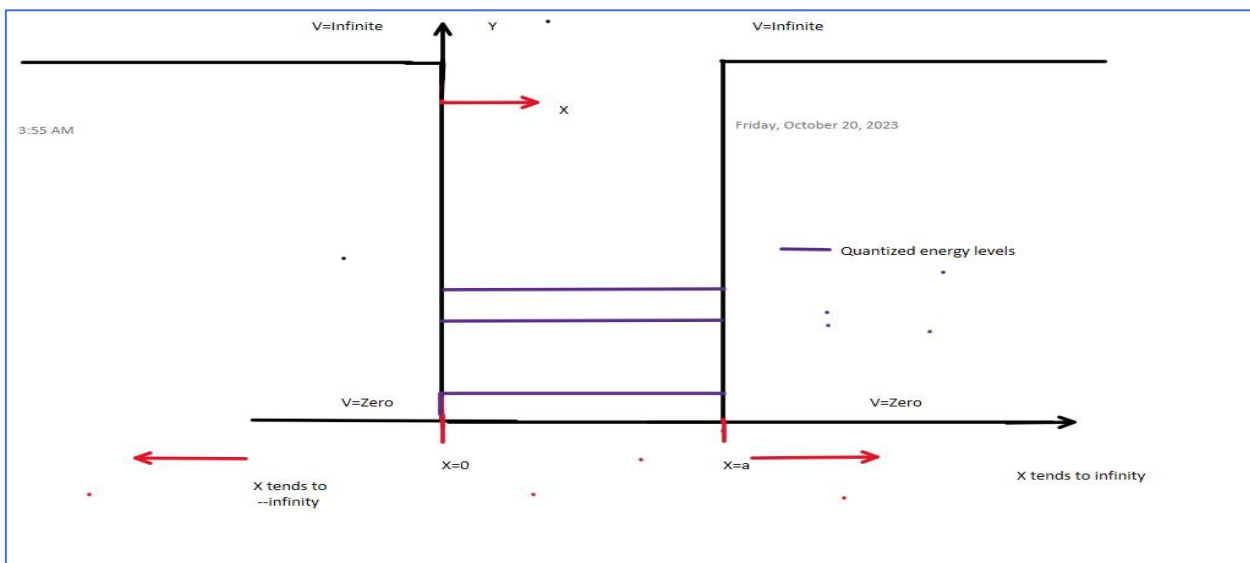

Fig. 3: A quantum particle in a 1D infinite potential well

> *step 2*

Set V(x) equal to,
V(x)=C . (0 1 2 3 4 5 4 3 2 1 0)

➢ *Step 3*

Construct the proper eigen matrix M4 expressed by,

M4=B 11x11 + C . V(x) . I
M4 equals,

```
0.0 1/2   0    0    0    0    0    0    0    0   0
1/2 1/20 1/2   0    0    0    0    0    0    0   0
 0  1/2 2/20 1/2   0    0    0    0    0    0   0
 0   0  1/2 3/20 1/2   0    0    0    0    0   0
 0   0   0  1/2 4/20 1/2   0    0    0    0   0
 0   0   0    0  1/2 5/20 1/2   0    0    0   0
 0   0   0    0    0  1/2 4/20 1/2   0    0   0
 0   0   0    0    0    0  1/2 3/20 1/2   0   0
 0   0   0    0    0    0    0  1/2 2/20 1/2  0
 0   0   0    0    0    0    0    0  1/2 1/20 1/2
 0   0   0    0    0    0    0    0   0  1/2 0.0
```

Where the constant C is replaced by the convenient value 1/20.

➢ *step 4*

Multiply the eigen matrix M4 by the energy eigenvector C.(0 1 2 3 45 4 3 2 1 0) you obtain almost the same eigenvector M4 . 1/20 [0 1 2 3 45 4 3 2 1 0] equals,

1/40
21/400
11/100
69/400
6/25
21/80
6/25
69/400
11/100
21/400
1/40

Which is in good agreement with the intrinsic vector λ V(x) with λ =1 as predicted.

It is worth mentioning that the same transition matrix B is applied for the three situations of thermal conduction, quantum particle inquadratic potential well and 1D infinite potential well.

Also note that all matrices M1, M2, M3 and M4 are obtained via statistical methods bypassing the partial differential equation of heat and the Schrödinger equation itself.

Furthermore, neither the classical variable separation method nor the FDM method are necessary since they are intrinsically included in the chains of matrix B.

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 that we briefly explain in this article.

The present study shows that the statistical chains of matrix B can be applied to the solution of the time-independent Schrödinger equation as a prerequisite for the study of the time-dependent equation.

Here we present the numerical solution of the B matrix in three illustrative physical situations, namely the heat diffusion equation, the quadratic potential well and the one-dimensional infinite potential well where the numerical results are surprisingly accurate.

NB: In the previous calculations, the author used his own double precision algorithm as explained in ref. 8.

No ready-made algorithms such as Python or MATLAB are needed.

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