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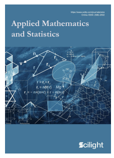

Article

Discretized Infinite Potential Well and Their Associated Coherent States

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Abstract: Since, unlike "traditional" physics, computational physics uses the discretization formalism, in this paper we have focused our attention on the discrete approach in order to solve the Schrödinger as well as the Bloch equations for a free particle and the "quantum gas" of free particles in an infinite quantum well with the finite length, respectively. By applying the so called continuous quantum mechanics limit we recover the corresponding results in continuous-variable quantum mechanics. For the infinite quantum well model we formulated the associated coherent states, which lead to the expression for the coherent qubits, in counterpart to the thermal qubits, obtained as a result of using the thermofield dynamics model. Thus, a "bridge" is created between the infinite quantum well model, coherent states and thermofield dynamics, which ultimately converge towards Quantum Computing.

Keywords: difference equation; quantum well; density matrix; coherent states; qubits

PACS: 02.70.Bf Finite-difference methods; 04.60.Nc Lattice and discrete methods; 05.30.-d Quantum statistical mechanics; 81R30 Coherent states; 81P68 Quantum computation

1. Introduction

As is well known, discrete or discontinuous calculus, also known as discretization, constituted the first step or mathematical basis in the transition to computational physics. This continuous-discrete transition in the examination of physical properties and phenomena appears natural, if we consider that matter itself does not have, at the micro level, a continuous, but discrete structure. Whereas in "usual" quantum mechanics differential equations are used, in which continuous variables intervene, in discrete quantum mechanics and implicitly in computational physics finite difference equations are used instead. Obviously, the latter are programmable on the computer, which offers a much more precise spectrum of solutions. But, at first glance, the results obtained using discrete calculus are different from those we are used to in quantum mechanics which uses continuous variables. Only by applying a discrete-continuous limit will we obtain the results obtained for the continuous case.

The discrete quantum mechanics (dQM) is the counterpart of the ordinary or continuous-variable quantum mechanics (cQM) in which the second order differential time-independent Schrödinger equation is written as a second order difference equation. The dQM was developed by Odake and Sasaki [1]. In this context the dQM can be considered as a generalization (or deformation) of the ordinary or continuous-variable QM, in the sense that a differential equation can be obtained from a difference equation by applying an appropriate limit. In what follows, we will call this limit the continuous quantum mechanical limit ($\lim\limits_{cQM}$). Generally, by applying this limit to the results obtained in dQM, you need to get the appropriate results in cQM.

On the one hand, there are only a few physical models for which the Schrödinger equation, even in one dimension, can be solved analytically, i.e., admit precise analytic solutions. Consequently, the most interesting physical problems must be solved numerically, considering the unprecedented development of computers and their programming languages.

On the other hand, intrinsic structure of matter has a discontinuous character, so an increasing use of discrete models is absolutely desirable. Consequently, the discrete approach is suitable for many different applications in solid state physics, since many physical systems are formed of the crystalline semiconductors, where the distances between atoms or ions are finite. Also, the discrete approach can be successfully used in various nanostructures including quantum wells, wires and dots. These are the fundamental entities used in Theoretical and Computational Physics.

The purpose of the present paper is to show that a discrete finite difference calculus can be successfully applied also to some (simple) quantum mechanical models and that the obtained results tend, at the continuous quantum mechanical limit, to the corrresponding results of the continuous space models.

In the present paper we have chosen a simple physical model: a free particle trapped in an infinite square quantum well. This model is otherwise known as the particle in a box. Even though the quantum dynamics in an infinite well potential represents a rather unphysical limit situation, it is a familiar textbook problem and a simple tractable model for the behavior of a quantum particle. The infinite square quantum potential well model is probably not totally applied to any real situation, but it will be in a certain sense a good approximation to some other simple quantum models. Actually, the same role is played by the harmonic oscillator model: the behavior of real quantum systems (e.g., molecular vibrations) is harmonic only near the equilibrium position.

In order to apply the dQM for some physical models, it will be useful to remember some rules of the discrete calculus and the difference equations (see, [2,3] and the references therein and also [4,5]).

2. Preliminaries Related to the Discrete Operations

As it is well-known, the ordinary (continuous) derivative a function $f(x)$, that is analytic in the neighborhood of a point x, with respect to the continuous variable x is defined as

$$\frac{df(x)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x} \tag{1}$$

where

$$\frac{\Delta f(x)}{\Delta x} = \frac{f(x+\Delta x) - f(x)}{\Delta x} \tag{2}$$

Hovever, the computers cannot deal with the infinitesimal limit $\Delta x \to 0$ and, consequently, it is necessary to define the discrete counterparts of the continuous derivative. So, if the variable x is discrete, i.e., the functions values are available on a discrete set of points, from the map $x \to x_n = a\,n$, where $\Delta x \equiv a$ is a positive constant (the lattice spacing), then for a function $f(x_n)$ which is analytic in the neighborhood of a point x_n it can define their discrete counterpart of the step a as

$$\frac{\Delta}{\Delta x_n} f(x_n) = \frac{f(x_{n+1}) - f(x_n)}{x_{n+1} - x_n} \quad \to \quad \frac{1}{a}\frac{\Delta}{\Delta n} f(n) = \frac{f(n+1) - f(n)}{a}. \tag{3}$$

In fact, it can define three discrete valid counterparts of the continuous derivatives: the forward discrete derivative (FDD), the backward discrete derivative (BDD), and also the central or centered discrete derivative (CDD), since it uses forward, backward or central differencing [2,3]. All these three definitions are equivalent in the continuous case, but lead to different aproximations in the discrete case.

For the purpose of our paper it is useful to use the *centered discrete derivative* defined with the step $2a$ as follows:

$$\frac{\Delta}{\Delta x_n} f(x_n) = \frac{f(x_{n+1}) - f(x_{n-1})}{x_{n+1} - x_{n-1}} \quad \to \quad \frac{1}{a}\frac{\Delta}{\Delta n} f(n) = \frac{f(n+1) - f(n-1)}{2a}. \tag{4}$$

The motivation of the use of centered discrete derivative consists in the fact that, using this kind of derivative, the solutions of the difference Schrödinger equation for the examined case have an oscillatory character [6].

In order to simplify the notations and not to create confusion, we will use the following notation for the discrete forward derivative

$$\frac{\Delta}{\Delta x_n} f(x_n) \equiv \frac{1}{a} \frac{\Delta}{\Delta n} f(n) = \frac{f(n+1) - f(n-1)}{2a} . \tag{5}$$

Consequently, the second central or centered derivative (in what follows we will omit the words “central” or “centered”) is

$$\frac{1}{a^2} \frac{\Delta^2}{\Delta n^2} f(n) \equiv \frac{1}{a} \frac{\Delta}{\Delta n} \left(\frac{1}{a} \frac{\Delta}{\Delta n} f(n) \right) = \frac{f(n+2) - 2f(n) + f(n-2)}{4a^2} . \tag{6}$$

Because we have to deal with physical observables, then it should be paid attention to the dimensions of the physical observables which participate to the difference equations (so, it must appear, to the right place, the the lattice spacing a).

In another train of thoughts, a translation operator with the step a, i.e., $T_a \equiv T_1$ act on an analytical function as follows:

$$T_1 f(x_n) = f(x_{n+1}) \;\; \to \;\; T_1 f(n) = f(n+1) \tag{7}$$

and it has the following properties [4,5]:

$$(T_1)^{-1} = T_{-1} \; ; \quad T_1 T_{-1} = T_{-1} T_1 = 1 \; ; \quad (T_m)^n = T_{m \cdot n} \; , \quad m,n \in \mathrm{N}^* . \tag{8}$$

Consequently, the first and second difference derivatives can be written with the help of the translation operator:

$$\frac{1}{a} \frac{\Delta}{\Delta n} f(n) = \frac{1}{2a} (T_1 - T_{-1}) f(n) \; ; \quad \frac{1}{a^2} \frac{\Delta^2}{\Delta n^2} f(n) = \frac{1}{4a^2} (T_1 - T_{-1})^2 f(n) . \tag{9}$$

As is known, the integral of a continuous function is

$$\int dx\, f(x) = F(x) + C \tag{10}$$

where the function $F(x)$ is the antiderivative function of $f(x)$, i.e.,:

$$\frac{dF(x)}{dx} = f(x) . \tag{11}$$

For the discrete variable $x_n = a\,n$, instead of the integration symbol $\int dx ...$ (which is the inverse of the differentiation symbol $\frac{d}{dx}$), we will use the symbol $\Delta x \frac{\Delta^{-1}}{\Delta x_n} \equiv a \frac{\Delta^{-1}}{\Delta n}$, as the inverse of the discrete differentiation symbol $\frac{\Delta}{\Delta x_n} \equiv \frac{1}{a} \frac{\Delta}{\Delta n}$ where $\frac{\Delta^{-1}}{\Delta x_n} \equiv \frac{\Delta^{-1}}{\Delta n}$ is only the discrete dimensionless integration symbol which evinces that the discrete integrals refer to the variable $x_n = n\,a$. So, it means that

$$\left(\Delta x \frac{\Delta^{-1}}{\Delta x_n} \right) f(x_n) = F(x_n) + C \tag{12}$$

and also

$$\frac{\Delta F(x_n)}{\Delta x_n} = f(x_n) . \tag{13}$$

One way to define the integration is to find the inverse transform of the derivative and this concept is known as finding the antiderivative. If we apply to the above relation to the inverse derivative operator (the integration operator) we recover the antiderivative function:

$$\left(\Delta x \frac{\Delta^{-1}}{\Delta x_n} \right) \frac{\Delta}{\Delta x_n} F(x_n) = F(x_n) = \left(\Delta x \frac{\Delta^{-1}}{\Delta x_n} \right) f(x_n) . \tag{14}$$

So, the indefinite integral from the function $f(x_n)$ is

$$\left(\Delta x \frac{\Delta^{-1}}{\Delta x_n}\right) f(x_n) = F(x_n) \tag{15}$$

while the definite integral becomes:

$$\left(\Delta x \frac{\Delta^{-1}}{\Delta x_n}\right) f(x_n)\Bigg|_{\tilde{x}_m}^{\tilde{x}_M} = F(\tilde{x}_M) - F(\tilde{x}_m). \tag{16}$$

Applying to Equation (14) the derivative operator, we successively obtain:

$$\frac{\Delta}{\Delta x_n}\left(\Delta x \frac{\Delta^{-1}}{\Delta x_n}\right) f(x_n) = f(x_n) = \frac{\Delta}{\Delta x_n} F(x_n) = \frac{F(x_{n+1}) - F(x_{n-1})}{2\Delta x} = \frac{(T_1 - T_{-1}) F(x_n)}{2\Delta x}, \tag{17}$$

from which, applying the inverse difference operator, it results

$$F(x_n) = 2\Delta x (T_1 - T_{-1})^{-1} f(x_n) \tag{18}$$

Finally, discrete integration is performed using the following relationship:

$$\left(\Delta x \frac{\Delta^{-1}}{\Delta x_n}\right) f(x_n) = 2\Delta x (T_1 - T_{-1})^{-1} f(x_n) \tag{19}$$

If we use our short notation, we must take into account the dimensions:

$$a \frac{\Delta^{-1}}{\Delta n} f(n)\Bigg|_m^M = 2a (T_1 - T_{-1})^{-1} f(n)\Big|_m^M. \tag{20}$$

In order to be able to calculate the right hand side of the above relation, we must expand the operator expression in a power series of the translation operator T_1, using their above mentioned properties:

$$(T_1 - T_{-1})^{-1} = -\frac{1}{T_{-1}(1 - T_2)} = -\frac{1}{T_{-1}} \sum_{k=0}^{\infty} T_{2k} = -\sum_{k=0}^{\infty} T_{2k+1}. \tag{21}$$

Supposing that the series is convergent, the discrete integral can be calculated by using the following equation:

$$a \frac{\Delta^{-1}}{\Delta n} f(n)\Bigg|_m^M = -2a \sum_{k=0}^{\infty} T_{2k+1} f(n)\Bigg|_m^M. \tag{22}$$

Let us provide some examples of using the above formula by indicating the results of several discrete integrals that will be useful in the following sections, whose validity can be directly proved by performing the discrete differentiation operations (for brevity we have omitted the quantity a in front). So, the results are:

$$\frac{\Delta^{-1}}{\Delta n} 1 = n, \tag{23}$$

$$\frac{\Delta^{-1}}{\Delta n} \cos n\alpha = \frac{\sin n\alpha}{\sin\alpha}, \quad \frac{\Delta^{-1}}{\Delta n} \sin n\alpha = -\frac{\cos n\alpha}{\sin\alpha} \tag{24}$$

$$\frac{\Delta^{-1}}{\Delta n} \sin^2 n\alpha = \frac{n}{2} - \frac{1}{2}\frac{\sin 2n\alpha}{\sin 2\alpha}. \tag{25}$$

With these mathematical preliminaries we are able to attack the simple quantum-mechanical models which are based upon the resolution of one-dimensional time-independent Schrödinger equation.

3. Foundamental Notions of the Discrete Schrödinger Equation

Let us now remember the main elements (known before, see, [6–8]) of the finite difference calculation applied to solving the Schrödinger equation for the infinite square quantum well. We will then use the obtained results to solve the finite difference Bloch equation, which is the main purpose of the paper.

A simple one-dimensional time-independent differential Schrödinger equation for a particle with the effective mass m^* in a potential field $U(x)$, where x is a continuous variable, i.e.,:

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}\Psi(x)+U(x)\Psi(x)=E\Psi(x) \tag{26}$$

can be written as a difference equation with the following structure

$$-\frac{\hbar^2}{2m^*}\frac{\Delta^2}{\Delta x_n^2}\Psi(x_n)+U(x_n)\Psi(x_n)=E\Psi(x_n) \tag{27}$$

or in a more convenient manner through the central derivative of second order with step $2a$:

$$\frac{1}{4}\left[\Psi(n+2)-2\Psi(n)+\Psi(n-2)\right]+\frac{2m^*}{\hbar^2}a^2\left[E-U(n)\right]\Psi(n)=0\,. \tag{28}$$

In order to work with a dimensionless equation, we can perform the following transformations to use the dimensionless quantities:

$$\frac{2m^*E}{\hbar^2}a^2=\widetilde{E}\,,\qquad \frac{2m^*}{\hbar^2}a^2U(n)=\widetilde{U}(n) \tag{29}$$

Consequently, the discrete Schrödinger equation can be written as

$$\frac{1}{4}\left[\Psi(n+2)-2\Psi(n)+\Psi(n-2)\right]+\left[\widetilde{E}-\widetilde{U}(n)\right]\Psi(n)=0\,. \tag{30}$$

Our task is to apply the discrete version of solving the Schrödinger equation to an analytically solvable quantum-mechanical problem—the infinite square well.

Let us we consider a free quantum particle of the effective mass m^* moving in an asymetric infinitely deep square well potential, i.e., trapped in a spatial region of length $L=N\,a$, where $a=x_{n+1}-x_n$, $n=0,1,2,...,N$, which is defined as follows:

$$U(x_n)=\begin{cases}0, & \text{if } 0\le x_n\le L=N\,a\\ +\infty, & \text{otherwise}\end{cases} \tag{31}$$

Inside of the well, in which $U=0$, the discrete Schrödinger equation becomes

$$\frac{1}{4}\left[\Psi(n+2)-2\Psi(n)+\Psi(n-2)\right]+\widetilde{E}\Psi(n)=0\,. \tag{32}$$

This is a homogenous difference equation of the second order with the constant coefficients.

The use of the central difference formula for the second derivative of the Hamiltonian is justified by the fact that in this manner we lead to the Hermitian Hamiltonian (as is stated also in Ref. [7], which refers to the connection with the tight-binding model). This can be seen immediately, if we transcribe the above equation in the matrix form

$$\frac{1}{4}\begin{pmatrix}-2 & 0 & 1 & 0 & \ddots & 0\\ 0 & -2 & 0 & 1 & \ddots & \ddots\\ 1 & 0 & \ddots & \ddots & \ddots & 0\\ 0 & 1 & \ddots & -2 & \ddots & 1\\ \ddots & \ddots & \ddots & \ddots & \ddots & 0\\ 0 & \ddots & 0 & 1 & 0 & -2\end{pmatrix}\begin{pmatrix}\Psi(0)\\ \Psi(1)\\ \vdots\\ \Psi(n)\\ \vdots\\ \Psi(N)\end{pmatrix}=-\widetilde{E}\begin{pmatrix}\Psi(0)\\ \Psi(1)\\ \vdots\\ \Psi(n)\\ \vdots\\ \Psi(N)\end{pmatrix} \tag{33}$$

where we can observe that this Hamiltonian matrix is three-diagonal, and, of course, Hermitian ($H_{ij} = H_{ji}^*$). This leads to the oscillatory character of solutions [6].

Therefore, we will try the general solution of the difference equation as

$$\Psi(n) = C_1 \cos(n\varphi) + C_2 \sin(n\varphi) \ . \tag{34}$$

In order to find the arbitrary integration constants $C_{1,2}$ we will use the border conditions: at the borders of the infinite square well the eigenfunctions must vanish (particle is confined to a space of the length $L = N\,a$ surrounded by infinite square potential well). So, we have:

$$\begin{aligned} \Psi(n=0) = 0 \quad &\Rightarrow \quad 0 = C_1 \\ \Psi(n=N) = 0 \quad &\Rightarrow \quad 0 = C_2 \sin N\varphi \end{aligned} \ . \tag{35}$$

The last condition leads to the energy quantization, because we must have $N\varphi = n_E \pi$, where $n_E = 0, 1, 2, \ldots$ will play the role of the main (principal) quantum number. From this it follows: $\varphi = \pi \frac{n_E}{N}$ and the eigenfunctions are

$$\Psi_{n_E}(n) = C_2 \ \sin\left(\pi \frac{n_E}{N} n\right) . \tag{36}$$

Introducing this expression in the discrete Schrödinger Equation (32), we obtain

$$\sin[(N+2)\varphi] - 2\sin(N\varphi) + \sin[(N-2)\varphi] + 4\widetilde{E}\sin(N\varphi) = 0 \tag{37}$$

and also, after some trigonometric manipulations and because the coefficient of $\sin(N\varphi)$ must vanish, we must have

$$2\cos 2\varphi + 2 + 4\widetilde{E} = 0 \, . \tag{38}$$

This condition leads to the quantized energy eigenvalues of the free particle in the infinite square well:

$$E_{n_E}^{(d)} = \frac{\hbar^2}{2m^* a^2} \sin^2\left(\pi \frac{n_E}{N}\right), \tag{39}$$

where $n_E = 0, 1, 2, 3, \ldots$ play the role of the main quantum number.

We will point out that this result was obtained earlier by Wolf [8] which used also the central discrete derivative, but with step $a/2$, which confirms that, due to the symmetry in the definition of central discrete derivative, the used step does not play an essential role.

Evidently, this expression is different from their counterpart in the continuous quantum mechanics (cQM) (i.e., there obtained by the resolution of the Schrödinger equation for the continuous variable x). If the number N of lattice points becomes infinite, the spacing between them becomes infinitesimal. Imposing that the quantum well length remains constant and finite, we can perform the following limit [8,9]: $N \to \infty$, $a \to 0$, $aN = L$ (finite). We call this limit the continuous quantum mechanical limit ($\lim\limits_{cQM}$). By applying this limit we can verify the correctness of the obtained results for the discrete case.

For the energy eigenvalues E_{n_E}, by using the l'Hospital rule for the indeterminate forms of limits, this limit leads to the correct result for the continuous case:

$$\lim_{\substack{N\to\infty \\ a\to 0 \\ aN=L}} E_{n_E}^{(d)} \equiv \lim_{cQM} E_{n_E}^{(d)} = \frac{\hbar^2}{2m^*} \lim_{cQM} \left[\frac{\sin\left(\frac{n_E}{aN} \pi\, a\right)}{a} \right]^2 = \frac{\hbar^2}{2m^*} \frac{\pi^2}{(aN)^2} n_E^2 = E_{n_E}^{(c)} \, . \tag{40}$$

In this manner, the expression for the energy eigenvalues of a free particle in a discrete infinite quantum well reduces to the well-known parabolic expression for the energy eigenvalues of a free particle in a continuous infinite quantum well (see, e.g., [10]):

$$E_{n_E}^{(c)} = \frac{\hbar^2 \pi^2}{2m^* L^2} n_E^2 \,. \tag{41}$$

Let us now calculate the normalization constant C_2 from the normalization condition of the discrete eigenfunctions $\Psi(n)$:

$$a\left[\frac{\Delta^{-1}}{\Delta n}\left|\Psi(n)\right|^2\right]\Bigg|_0^N = 1 \,. \tag{42}$$

We have, successively, also Equation (26):

$$\frac{\Delta^{-1}}{\Delta n}\left|\Psi(n)\right|^2 = \left|C_2\right|^2 \frac{\Delta^{-1}}{\Delta n}\sin^2\left(\pi \frac{n_E}{N} n\right) = \frac{1}{2}\left|C_2\right|^2\left[n - \frac{\sin 2\pi \frac{n_E}{N} n}{\sin 2\pi \frac{n_E}{N}}\right]. \tag{43}$$

Consequently, the definite integral is then:

$$a\left[\frac{\Delta^{-1}}{\Delta n}\left|\Psi(n)\right|^2\right]\Bigg|_0^N = \frac{a}{2}\left|C_2\right|^2\left[N - \frac{\sin 2\pi \frac{n_E}{N} N}{\sin \pi \frac{n_E}{N}}\right] = \frac{a}{2}\left|C_2\right|^2 N = 1 \,, \tag{44}$$

so that we obtain the same value for the normalization constant C_2 as in the continuous case:

$$\left|C_2\right| = \sqrt{\frac{2}{aN}} = \sqrt{\frac{2}{L}} \,. \tag{45}$$

Finally, the normalized eigenfunctions for the discrete case are identical to those of the continuous one:

$$\Psi_{n_E}(n) = \sqrt{\frac{2}{L}} \sin\left(\pi \frac{n_E}{N} n\right), \tag{46}$$

i.e., it is the solution of sinusoidal stationary waves along the x-axis, with $0 \le x_n \le L$ and $n_E = 0, 1, 2, \ldots, \infty$.

4. The Discretized Bloch Equation for the Infinite Square Well

Let us consider a "quantum gas" of the free particles trapped in the infinite discrete quantum well which are in the thermodynamical equilibrium with the "reservoir" (confined by the infinitely higher walls) at the temperature T (with $T = (\beta k_B)^{-1}$, where k_B is the Boltzmann's constant). Obviously, such a gas is in a mixed quantum state described by the statistical or density operator ρ or, in some representation, say ξ, by the density matrix $\rho(\xi, \xi'; \beta)$.

For the quantum system described by the Hamiltonian H and which obeys the canonical distribution, the canonical density operator ρ is an exponential operator

$$\rho = e^{-\beta H} \tag{47}$$

and satisfies the quantum Bloch equation with the initial condition:

$$-\frac{\partial}{\partial \beta}\rho = H\rho \,, \;\; \rho(\beta = 0) = 1 \,. \tag{48}$$

The canonical (or unnormalized) density matrix $\rho(\xi, \xi'; \beta)$ can be normalized to unity and the corresponding normalized density matrix $\tilde{\rho}(\xi, \xi'; \beta)$ is

$$\tilde{\rho}(\xi, \xi'; \beta) = \frac{1}{Z(\beta)} \rho(\xi, \xi'; \beta), \ \int \rho(\xi, \xi; \beta) d\xi = Z(\beta), \tag{49}$$

where $Z(\beta)$ is called partition function or statistical sum or statistical integral, the last two names depending generally on the discrete or continuous character of the energy of examined quantum system.

Generally, the canonical density matrix $\rho(\xi, \xi'; \beta)$ can be obtained in two ways:

- directly, if we know the energy eigenvalues E_{n_E} of the system's Hamiltonian H, then we can use the general definition:

$$\rho(\xi, \xi'; \beta) = \sum_{n_E=0}^{\infty} e^{-\beta E_{n_E}} \Psi_{n_E}(\xi) \Psi^*_{n_E}(\xi'). \tag{50}$$

- indirectly, if we do not know the energy eigenvalues E_{n_E}, then we must try to solve the Bloch equation for the canonical density matrix [11]:

$$-\frac{\partial}{\partial \beta} \rho(\xi, \xi'; \beta) = H(\xi) \rho(\xi, \xi'; \beta) \tag{51}$$

with the initial condition:

$$\lim_{\beta \to 0} \rho(\xi, \xi'; \beta) \equiv \rho(\xi, \xi'; 0) = \delta(\xi - \xi'). \tag{52}$$

It is true that the Bloch equation (like the Schrödinger equation), even in one dimension, admits precious analytic solutions only for a few quantum systems. Fortunately, for the infinite (continuous and discrete) quantum well this is possible.

In the continuous case, in the coordinate representation x, the canonical density matrix is defined as

$$\rho(x, x'; \beta) = \sum_{n_E=0}^{\infty} e^{-\beta E^{(c)}_{nE}} \Psi_{n_E}(x) \Psi^*_{n_E}(x'). \tag{53}$$

Because, in this case, the density matrix is a real function, it is symmetric with respect to two coordinates: $\rho(x, x'; \beta) = \rho(x', x; \beta)$.

Similarly, for the discrete space, assuming that $x \to x_n = a\,n$ and $x' \to x_n' = a\,n'$ their counterpart will be:

$$\rho(n, n'; \beta) = \sum_{n_E=0}^{\infty} e^{-\beta E^{(d)}_{nE}} \Psi_{n_E}(n) \Psi^*_{n_E}(n'), \tag{54}$$

With $Z^{(c)}(\beta)$ and $Z^{(d)}(\beta)$ we will denote the continuous, respectively discrete statistical sums, defined by normalizing the density matrix to unity:

$$Z^{(c)}(\beta) = \int_0^L \rho(x, x; \beta) dx = \sum_{n_E=0}^{\infty} e^{-\beta E^{(c)}_{nE}} = \sum_{n_E=0}^{\infty} \left(e^{-\beta \frac{\hbar^2 \pi^2}{2m^* L^2}} \right)^{n_E^2}, \tag{55}$$

$$Z^{(d)}(\beta) = a \frac{\Delta^{-1}}{\Delta n} \left[\rho(n, n; \beta) \right]_0^N = \sum_{n_E=0}^{\infty} e^{-\beta E^{(d)}_{nE}} = \sum_{n_E=0}^{\infty} e^{-\beta \frac{\hbar^2}{2m^* a^2} \sin^2\left(\frac{\pi}{N} n_E\right)}. \tag{56}$$

The partition function is a quantity of maximal informational importance, because all the thermodynamic functions can be expressed through the partition function. But, in the case of free particle in an infinite quantum well (or, precisely, for such a "quantum gas"), due to their mathematical structure, these quantities cannot be expressed analytically and must be calculated numerically or adopted some approximations. In the Appendix A, we have drawn some considerations regarding the partition function.

However, for the continuous case, the partition function can be evaluated also analytically. So, as an example, let us consider a free electron (with mass $m^* = 9.1 \cdot 10^{-31}$ kg), in an infinite quantum well with length $L = 10^{-9}$ m and equilibrium temperature T = 300 K. With $\hbar$ = 1.054·10^{-34} J·s and k_B = 1.38 · 10^{-23} J·K^{-1}, the exponential into the sum, for $n_E = 1$ becomes $\exp(-\beta E_1) \approx \exp(-30) \approx 10^{-13}$, i.e., extremely small. So, we can replace the sum with the integral by replacing $y = l\, n_E$, where we take into account the dimensional aspects:

$$\sum_{n_E=0}^{\infty} \ldots \to \frac{1}{l}\int_0^{\infty} dy \ldots \tag{57}$$

In this manner, we obtain:

$$\begin{gathered} Z^{(c)}(\beta) = \lim_{\substack{N\to\infty \\ a\to 0 \\ aN=L}} Z^{(d)}(\beta) \equiv \lim_{cQM} Z^{(d)}(\beta) = \sum_{n_E=0}^{\infty}\left(e^{-\beta \frac{\hbar^2\pi^2}{2m^* L^2}}\right)^{n_E^2} \to \\ \to \frac{1}{l}\int_0^{\infty} e^{-\beta \frac{\hbar^2\pi^2}{2m^* L^2}\frac{1}{l^2}y^2} dy = \frac{1}{l}\frac{1}{2}\sqrt{\frac{\pi}{\beta \frac{\hbar^2\pi^2}{2m^* L^2}\frac{1}{l^2}}} = L\sqrt{\frac{m^*}{2\pi\beta\hbar^2}} \end{gathered} . \tag{58}$$

The last result is the same as in [11].

Let us solve the Bloch equation for a free particle of mass m^* in an infinite quantum well. In coordinate x—representation for the continuous case this equation reads:

$$-\frac{\partial}{\partial\beta}\rho(x, x'; \beta) = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}\rho(x, x'; \beta) \tag{59}$$

with the initial condition $\rho(x, x'; 0) = \delta(x - x')$.

By passing to the discrete space $x \to x_n = a\,n$ this equation becomes

$$-\frac{\partial}{\partial\beta}\rho(n, n'; \beta) = -\frac{\hbar^2}{2m^* a^2}\frac{\Delta^2}{\Delta n^2}\rho(n, n'; \beta) \tag{60}$$

which is a differential-difference equation.

We try to solve this equation by using a new less dimensional thermal variable: $f = \beta\frac{\hbar^2}{2m^* a^2}$. So, we have:

$$\frac{\partial}{\partial f}\rho(n, n'; f) = \frac{\Delta^2}{\Delta n^2}\rho(n, n'; f) \tag{61}$$

or, equivalently

$$\frac{\partial}{\partial f}\rho(n, n'; f) = \frac{1}{4}\left[\rho(n+2, n'; f) - 2\rho(n, n'; f) + \rho(n-2, n'; f)\right] \tag{62}$$

which is an differential-difference equation with partial derivatives.

We will try to solve this equation by the separation variable method (similarly as we did for the Bloch equation for the Morse potential, see [12]), i.e.,:

$$\rho(n, n'; f) = \sum_{n_E=0}^{\infty} A_{n_E}(n)\, B_{n_E}(n'; f)\,. \tag{63}$$

By substituting it into the Bloch equation, we obtain:

$$\sum_{n_E=1}^{\infty} A_{n_E}(n)\frac{\partial}{\partial f}B_{n_E}(n'; f) = \frac{1}{4}\sum_{n_E=1}^{\infty}\left[A_{n_E}(n+2) - 2A_{n_E}(n) + A_{n_E}(n-2)\right]B_{n_E}(n'; f) \tag{64}$$

which means that

$$\frac{1}{B_{n_E}(n';f)}\frac{\partial}{\partial f}B_{n_E}(n';f)=\frac{1}{4}\frac{A_{n_E}(n+2)-2A_{n_E}(n)+A_{n_E}(n-2)}{A_{n_E}(n)}=-p_{n_E} \tag{65}$$

where p_{n_E} is a positive constant which will be determined later.

Now we have to solve the differential equation:

$$\frac{1}{B_{n_E}(n';f)}\frac{\partial}{\partial f}B_{n_E}(n';f)=-p_{n_E} \tag{66}$$

$$\frac{\partial}{\partial f}B_{n_E}(n';f)+0\frac{\partial}{\partial n'}B_{n_E}(n';f)=-p_{n_E}B_{n_E}(n';f), \tag{67}$$

meaning that we should have:

$$\frac{dB_{n_E}(n';f)}{B_{n_E}(n';f)}=-p_{n_E}df \tag{68}$$

$$B_{n_E}(n';f)=B_{n_E}(n';0)e^{-f\,p_{n_E}}, \tag{69}$$

where, at the moment, $B_{n_E}(n';0)$ is an arbitrary function, constant with respect to variable f, which will be determined later, from the symmetry condition of the density matrix (which, in our case is a real function).

The second equation

$$A_{n_E}(n+2)-2\left(1-2p_{n_E}\right)A_{n_E}(n)+A_{n_E}(n-2)=0 \tag{70}$$

is a difference equation like the Schrödinger equation for a free particle in the infinite quantum well. For this reason, we can perform the identification and the quantization condition:

$$p_{n_E}=\frac{2m^*E_{n_E}^{(d)}}{\hbar^2}a^2=\sin^2\frac{\pi}{N}n_E. \tag{71}$$

Also, from the previous resolution of the Schrödinger equation, we take the solution:

$$A_{n_E}(n)=\widetilde{C}\sin\left(\frac{\pi\,n_E}{N}n\right). \tag{72}$$

Consequently, the density matrix becomes

$$\rho(n,n';f)=\widetilde{C}\sum_{n_E=0}^{\infty}e^{-f\,p_{n_E}}\sin\left(\frac{\pi\,n_E}{N}n\right)B_{n_E}(n';0). \tag{73}$$

Because the eigenfunctions $\Psi_{n_E}(n)$ are real functions, the density matrix is symmetric, so the function $B_{n_E}(n';0)$ must be:

$$B_{n_E}(n';0)=\widetilde{C}\sin\left(\frac{\pi\,n_E}{N}n'\right). \tag{74}$$

If we return to the old notations

$$fp_{n_E}=\beta\frac{\hbar^2}{2m^*a^2}\tan^2\frac{\pi}{N}n_E=\beta E_{n_E}^{(d)} \tag{75}$$

the density matrix becomes

$$\rho(n, n'; \beta) = \widetilde{C}^2 \sum_{n_E=0}^{\infty} e^{-\beta E_{n_E}^{(d)}} \sin\left(\frac{\pi n_E}{N} n\right) \sin\left(\frac{\pi n_E}{N} n'\right) . \tag{76}$$

Having in mind the expression of the discrete eigenfunctions $\Psi_{n_E}(n)$, it follows that we have $\widetilde{C} = C_2 = \sqrt{\frac{2}{L}}$ and so, the canonical density matrix becomes:

$$\rho(n, n'; \beta) = \frac{2}{L} \sum_{n_E=0}^{\infty} e^{-\beta E_{n_E}^{(d)}} \sin\left(\frac{\pi n_E}{N} n\right) \sin\left(\frac{\pi n_E}{N} n'\right) , \tag{77}$$

i.e., exact the same mathematical structure as the one obtained from the general definition of the discrete canonical density matrix.

Like the density matrix for the continuous case, their counterpart for the discrete one can be also normalized to unity and consequently, the discrete integral from the canonical density matrix is just the partition function $Z^{(d)}(\beta)$:

$$a \frac{\Delta^{-1}}{\Delta n} \rho(n, n; \beta) \Big|_0^N = \frac{2}{L} \sum_{n_E=0}^{\infty} e^{-\beta E_{n_E}^{(d)}} a \frac{\Delta^{-1}}{\Delta n} \left[\sin^2\left(\frac{\pi n_E}{N} n\right)\right] \Big|_0^N = Z^{(d)}(\beta) . \tag{78}$$

The discrete integral in the above relation was previously calculated (see Equation (44)) and their value is $N/2$. Consequently, we obtain the correct expression for the partition function $Z^{(d)}(\beta)$.

In this manner, the normalized discrete density matrix becomes

$$\widetilde{\rho}(n, n'; \beta) \equiv \frac{1}{Z^{(d)}(\beta)} \rho(n, n'; \beta) = \frac{2}{L} \frac{1}{Z^{(d)}(\beta)} \sum_{n_E=0}^{\infty} e^{-\beta E_{n_E}^{(d)}} \sin\left(\frac{\pi n_E}{N} n\right) \sin\left(\frac{\pi n_E}{N} n'\right) . \tag{79}$$

On the other hand, the canonical density matrix (i.e., the solution of the Bloch equation) can fulfill the initial condition with respect to the variable β. So, we have:

$$\lim_{\beta \to 0} \rho(n, n'; \beta) = \frac{2}{L} \sum_{n_E=0}^{\infty} \sin\left(\frac{\pi n_E}{N} n\right) \sin\left(\frac{\pi n_E}{N} n'\right) = \frac{1}{a} \delta(n - n') , \tag{80}$$

where we have used the Fourier series representation for the Dirac delta function [13]:

$$\delta(x - x') = \frac{2}{L} \sum_{k=0}^{\infty} \sin\left(\frac{k\pi}{L} x\right) \sin\left(\frac{k\pi}{L} x'\right), \qquad L > 0 . \tag{81}$$

Let us apply the continuous limit to the canonical discrete density matrix $\rho(n, n'; \beta)$. We obtain:

$$\begin{aligned} \rho(x, x'; \beta) &= \lim_{\substack{N \to \infty \\ a \to 0 \\ aN = L}} \rho(n, n'; \beta) \equiv \lim_{cQM} \rho(n, n'; \beta) = \\ &= \frac{2}{L} \sum_{n_E=1}^{\infty} \lim_{cQM} \left[e^{-\beta E_{n_E}^{(d)}} \right] \sin\left(\frac{\pi n_E}{L} x\right) \sin\left(\frac{\pi n_E}{L} x'\right) = \frac{2}{L} \sum_{n_E=0}^{\infty} e^{-\widetilde{\beta} n_E^2} \sin(\alpha n_E) \sin(\alpha' n_E) \end{aligned} \tag{82}$$

where $\widetilde{\beta} \equiv \beta \frac{\hbar^2 \pi^2}{2m^* L^2}$, $\alpha \equiv \frac{\pi}{L} x$ and $\alpha' \equiv \frac{\pi}{L} x'$.

As we have seen earlier, the quantity $\widetilde{\beta} \equiv \beta \frac{\hbar^2 \pi^2}{2m^* L^2}$ is very small and we can replace the sum with respect to n_E by integral with respect to a continuous variable, say $y = l n_E$ as earlier. If we develop the sinus products using the Euler's formulae

$$\sin(\alpha n_E) \sin(\alpha' n_E) = \frac{1}{4} \left[e^{\mathrm{i}(\alpha - \alpha') n_E} + e^{-\mathrm{i}(\alpha - \alpha') n_E} - e^{\mathrm{i}(\alpha + \alpha') n_E} - e^{-\mathrm{i}(\alpha + \alpha') n_E} \right] \tag{83}$$

then we have to calculate four integrals of the following kind:

$$\lim_{cQM}\rho(n, n'; \beta) = \frac{1}{2L}\left[I_1^- + \left(I_1^-\right)^* - I_2^+ - \left(I_2^+\right)^*\right] \tag{84}$$

where:

$$I_1^- \equiv \frac{1}{l}\int_0^\infty e^{-\frac{\tilde{\beta}}{l^2}y^2 + \mathrm{i}\frac{(\alpha-\alpha')}{l}y}dy = \frac{1}{2}\sqrt{\frac{\pi}{\tilde{\beta}}}\, e^{-\frac{(\alpha-\alpha')^2}{4\tilde{\beta}}} = L\sqrt{\frac{m^*}{2\pi\beta\hbar^2}}\, e^{-\frac{m^*}{2\beta\hbar^2}(x-x')^2} \tag{85}$$

$$I_2^+ \equiv \frac{1}{l}\int_0^\infty e^{-\frac{\tilde{\beta}}{l^2}y^2 + \mathrm{i}\frac{(\alpha+\alpha')}{l}y}dy = \frac{1}{2}\sqrt{\frac{\pi}{\tilde{\beta}}}\, e^{-\frac{(\alpha+\alpha')^2}{4\tilde{\beta}}} = L\sqrt{\frac{m^*}{2\pi\beta\hbar^2}}\, e^{-\frac{m^*}{2\beta\hbar^2}(x+x')^2} . \tag{86}$$

These integrals are of the following kind (see, 3.323/2 of Ref. [14]):

$$\int_0^\infty e^{-p^2\left(y\pm \mathrm{i}\frac{q}{2p^2}\right)^2}dy = \frac{1}{2}\sqrt{\frac{\pi}{p^2}}\, e^{-\frac{q^2}{4p^2}} . \tag{87}$$

Note that the integrals do not depend on the sign in front of $(\alpha \pm \alpha')$ and thus, $I_1^- = \left(I_1^-\right)^*$ and $I_2^+ = \left(I_2^+\right)^*$. Apart from this, the last two integrals, I_2^+ and $\left(I_2^+\right)$, which finally contain the sum $(x + x')^2$, do not lead to the Dirac delta function at the limit $\beta \to 0$, so they have no significance.

Finally, we obtain the same results as in [11]:

$$\rho(x, x'; \beta) = \sqrt{\frac{m^*}{2\pi\beta\hbar^2}}\, e^{-\frac{m^*}{2\beta\hbar^2}(x-x')^2} . \tag{88}$$

By normalizing this density matrix, we obtain the same expression of the partition function as the one obtained by applying the continuous limit (see, Equation (57) to the discrete partition function $Z^{(d)}(\beta)$:

$$Z^{(c)}(\beta) = \int_0^L \rho(x, x; \beta)dx = L\sqrt{\frac{m^*}{2\pi\beta\hbar^2}} = e^{-\beta F} , \tag{89}$$

where F is the free energy of the quantum gas in the infinite quantum well [11].

This is another proof of the correctness of the calculations made for the discrete case of the free quantum particle in the infinite quantum well.

The normalized density matrix then becomes:

$$\tilde{\rho}(x, x'; \beta) = \frac{1}{L}e^{-\frac{m^*}{2\beta\hbar^2}(x-x')^2} . \tag{90}$$

Let us we calculate now the thermal expectation of the Hamiltonian $H = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}$ of free particle trapped in the infinite square quantum well, by using the canonical density matrix $\rho(x, x'; \beta)$.

In the cQM this is given by the expression [11]:

$$< H >^{(c)} = -\frac{\hbar^2}{2m^*}\left\langle \frac{\partial^2}{\partial x^2}\right\rangle = -\frac{\hbar^2}{2m^*}\frac{1}{Z_c(\beta)}\int_0^L dx\left[\frac{\partial^2}{\partial x'^2}\rho(x, x'; \beta)\right]_{x'=x} \tag{91}$$

where we must perform the following succession of operations: first we carry out the differentiation with respect to the variable x', then we replace x' with x and finally we integrate with respect to the variable x.

Then, in the dQM, the corresponding expression will be

$$< H >^{(d)} = -\frac{\hbar^2}{2m^*}\left\langle \frac{1}{a^2}\frac{\Delta^2}{\Delta n^2}\right\rangle = -\frac{\hbar^2}{2m^*}\frac{1}{Z_c(\beta)}\left\{ a\frac{\Delta^{-1}}{\Delta n}\left[\frac{1}{a^2}\frac{\Delta^2}{\Delta n'^2}\rho(n,n';\beta)\right]\Bigg|_{n'=n}\right\}\Bigg|_0^N \quad (92)$$

with the same succession of operations as earlier.

The discrete differentiation is easy to be performed if we use the Bloch equation (4.14), i.e., if we observe the operator equality which are applied to the function $\rho(n,n';\beta)$:

$$\frac{\partial}{\partial\beta} = \frac{\hbar^2}{2m^* a^2}\frac{\Delta^2}{\Delta n^2} \quad (93)$$

Then the expectation value becomes

$$< H >^{(d)} = -\frac{\hbar^2}{2m^*}\left\langle \frac{1}{a^2}\frac{\Delta^2}{\Delta n^2}\right\rangle = -\left\langle\frac{\partial}{\partial\beta}\right\rangle = -\frac{1}{Z_d(\beta)}\left\{ a\frac{\Delta^{-1}}{\Delta n}\left[\frac{\partial}{\partial\beta}\rho(n,n';\beta)\right]\Bigg|_{n'=n}\right\}\Bigg|_0^N =$$
$$= -\frac{1}{Z_d(\beta)}\frac{2}{N}\frac{\partial}{\partial\beta}\sum_{n_E=0}^{\infty} e^{-\beta E_{n_E}^{(d)}}\left\{\frac{\Delta^{-1}}{\Delta n}\left[\sin^2(n\varphi)\right]\right\}\Bigg|_0^N = -\frac{\partial}{\partial\beta}\ln Z_d(\beta) \quad (94)$$

where we have used the notation $\varphi = \frac{n_E}{N}\pi$ and Equation (26).

In this manner, for dQM we have obtained the correct results, like for cQM.

5. Infinite Quantum Wells and Their Associated Coherent States

Previously, the Wigner and Q-distribution functions, which are characteristics of usual coherent states, were also defined for the discrete case [15]. Also, in a previous paper, Fiset and Hussin showed that particles in a quantum well have many properties specific to coherent states [16]. In this section, let's see what is the expression of the coherent states associated with a particle embedded in a potential well of infinite height.

In a previous paper we showed that this model can be associated with the quantum group SU(1, 1), with the Bargmann index $k = 1/2$ whose generators are $K_\pm$ and K_0 [17]. They act on the Fock vectors $| n_E >,\ n_E = 0,1,2,...$ as follows:

$$K_+ | n_E >= (n_E+1) | n_E+1 > ,\quad K_- | n_E >= n_E | n_E-1 > ,\quad K_0 | n_E >= \left(n_E+\frac{1}{2}\right) | n_E > \quad (95)$$

For a Hamiltonian with the eigenequation $H | n_E >= E_{n_E}^{(c)} | n_E >$, with energy eigenvalues $E_{n_E}^{(c)} = \frac{\hbar^2\pi^2}{2m^* L^2} n_E^2 \equiv E_1^{(c)}\, e(n_E)$, the coherent states can be defined in the Barrt-Girardello manner [18], i.e., as the eigenvectors of the annihillation operator.

$$K_- | z >= z | z > ,\quad z = | z | \exp(i\varphi) \quad (96)$$

Their expansion on the Fock vector's basis, after normalization is [17]

$$| z >= \frac{1}{\sqrt{I_0(2|z|)}}\sum_{n_E}\frac{z^{n_E}}{\sqrt{\rho(n_E)}} | n_E >= \frac{1}{\sqrt{I_0(2|z|)}}\sum_{n_E}\frac{z^{n_E}}{n_E!} | n_E > \quad (97)$$

where $I_0(2|z|)$ is the modified Bessel function of the first kind, and $\rho(n_E)$ is the structure constant of the coherent states, defined as

$$\rho(n_E) = \prod_{j=1}^{n_E}\rho(j) = e(1)e(2)...e(n_E) = 1^2\cdot 2^2\cdot ...\cdot (n_E)^2 = (n_E!)^2 \quad (98)$$

Any set of coherent states must satisfy some minimal conditions (named "Klauder's prescriptions" [19]). They form a complete set, i.e., the identity operator can be resolved as

$$\int d\mu(z) | z >< z | = 1 \tag{99}$$

where $d\mu(z)$ is the integration measure. For our problem this is expressed in terms of the modified Bessel functions, of the first and second order [17].

$$d\mu(z) = 2\frac{d\varphi}{2\pi} d\left(| z |^2\right) I_0(2| z |) K_0(2| z |) \tag{100}$$

Multiplying the previous relation by $| n_E >$, we obtain

$$| n_E >= \int d\mu(z) \frac{1}{\sqrt{I_0(2| z |)}} \frac{\left(z^*\right)^{n_E}}{n_E !} | z > \tag{101}$$

This relation shows that the information contained in the Fock state $| n_E >$ has been redistributed towards the coherent state $| z >$, that is, "divided" into an infinity of copies, with a different weight, because the spectrum of the variable z contains an infinity of values, z being a continuous variable.

If we represent the base Fock vectors in the form of column and row matrices, that is

$$| n_E >= \begin{pmatrix} \left.\begin{matrix} 0 \\ \vdots \\ 0 \end{matrix}\right\} n_E - 1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \ < n_E | = \begin{pmatrix} \underbrace{0 \ \ldots \ 0}_{n_E} & 1 & 0 \ \ldots & 0 \end{pmatrix} \tag{102}$$

then, in particular, we will have

$$| 0 > \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ | 1 > \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{103}$$

A qubit $| \Psi >$ can be represented as a given point over the Bloch sphere (a sphere with unitary radius), by means of the spherical coordinates (θ, φ) i. e. as a linear combination of these two states

$$| \Psi > = a_0 | 0 > + a_1 | 1 >, \ a_0 = \cos(\theta / 2), \ a_1 = e^{i\varphi}, \ | a_0 |^2 + | a_1 |^2 = 1 \tag{104}$$

Assuming that the particle in the potential well is a system with two energy levels, E_1 and E_2, then we will have

$$| 0 >= \int d\mu(z) \frac{1}{\sqrt{I_0(2| z |)}} | z > , \ | 1 >= \int d\mu(z) \frac{1}{\sqrt{I_0(2| z |)}} z^* | z > \tag{105}$$

so the expression of the qubit becomes

$$| \Psi >= \int d\mu(z) \frac{1}{\sqrt{I_0(2| z |)}} \left(a_0 + a_1 z^*\right) | z > \tag{106}$$

This relationship shows that any qubit can be expanded into associated coherent states, which allows us to manage quantum information for the most general evolution of the system states.

Conversely, using the general expression of coherent states, Equation (97), for the case of systems with two energy levels, the coherent states will be

$$| z >^{(2)} = \frac{1}{\sqrt{I_0(2| z |)}} \sum_{n_E=0}^{1} \frac{z^{n_E}}{n_E !} | n_E > \ \rightarrow \ | z >^{(2)} = \frac{1}{\sqrt{I_0(2| z |)}} | 0 > + \frac{z}{\sqrt{I_0(2| z |)}} | 1 > \tag{107}$$

$$I_0(2|z|)=\sum_{n_E=0}^{1}\frac{(|z|)^{n_E}}{(n_E!)^2} \quad \rightarrow \quad I_0(2|z|)=1+|z|^2 \tag{108}$$

Finally, we obtain

$$|z>^{(2)}=\frac{1}{\sqrt{1+|z|^2}}|0>+\frac{z}{\sqrt{1+|z|^2}}|1> \tag{109}$$

Calculating the sum of the squares of the complex coefficients, we will have

$$\begin{aligned} {}^{(2)}<z|z>^{(2)} &= \left(\frac{1}{\sqrt{1+|z|^2}}<0|+\frac{z^*}{\sqrt{1+|z|^2}}<1|\right)\left(\frac{1}{\sqrt{1+|z|^2}}|0>+\frac{z}{\sqrt{1+|z|^2}}|1>\right)= \\ &= \frac{1}{1+|z|^2}+\frac{|z|^2}{1+|z|^2}=1 \end{aligned} \tag{110}$$

By concluding, this expression has exactly the structure of a qubit. In other words, a two-level particle embedded into an infinite potential quantum well is just a qubit. To highlight this type of qubit, which depends on the complex variable z , characteristic of coherent states, we will call it the coherent qubit.

With this, we have concrete proof of the connection between the model of a particle embedded in an infinite potential well with rectangular walls and the basic elements of quantum computing.

Thus, coherent states become a very important entity in quantum computing.

Assuming that a quantum message $|M>$ is represented by a tensor product of a finite number of qubits, it can be written in two equivalent ways:

$$\begin{aligned} |M> &= \bigotimes_{j=1}^{N}|\Psi_j>=|\Psi_1>\otimes|\Psi_2>\otimes...\otimes|\Psi_N>\equiv \\ &\equiv \bigotimes_{j=1}^{N}|z_j>=|z_1>\otimes|z_2>\otimes...\otimes|z_N> \end{aligned} \tag{111}$$

The Hilbert space H associated with the message |> is a tensor product of the Hilbert spaces associated with the individual qubits: $\mathsf{H} = \bigotimes_{j=1}^{N}|\mathsf{H}_j>=|\mathsf{H}_1>\otimes|\mathsf{H}_2>\otimes...\otimes|\mathsf{H}_N>$.

Other aspects of the connection between coherent states and qubits the readers can find in our previous paper [20].

In principle, the discretization method can also be applied to the case of a more realistic or finite potentials, for which in a certain region of space the potential (outside the quantum well) is $U_j \neq 0$, $1\leq j\leq N$. The appropriate discretization method is also that of centered finite differences. This assumes that the discretized Hamiltonian is also a tridiagonal matrix, but which, for these cases, has the elements on the main diagonal equal to $\frac{\hbar^2}{m(\Delta x)^2}+U_j$, and the off-diagonal ones equal to $-\frac{\hbar^2}{m(\Delta x)^2}$. Of course, unlike the potential well with infinite walls, there will also be a tunneling phenomenon, with a non-zero probability of finding the particle even outside the potential pit. Consequently, the boundary conditions for the wave function will be written $\Psi_0\left(-\frac{L}{2}\right)=0$ and $\Psi_{N+1}\left(+\frac{L}{2}\right)=0$, where $L\leq\infty$ is a sufficiently wide spatial coordinate, outside the potential well [7,9,21].

As a general remark, if you compare the centered difference method with the similar forward / backward methods, for solving finite difference equations (therefore Schrodinger's equation), it is found that the first one brings more accuracy, that is, it produces smaller errors for a chosen Δx step. Implicitly, the computational efficiency is higher due to the fact that, although it uses the same number of points (adjacent neighbors), the stability is higher. In addition, in the case of using the method with centered differences, the precision is higher, compared to that of the forward / backward methods, being of the order of $O\left[(\Delta x)^2\right]$ [22].

Also, some properties of coherent states, particularly associated with a particle (or quantum particle gas) confined in a infinite potential well can be connected with the thermofield dynamics (TFD) approach. At the same time this constitute the nowest application of this method.

It is known that, in general, quantum computers need to be cold, due to their fundamental quantum elements—qubits, which can exist simultaneously in multiple states, a phenomenon called superposition. These elements are very sensitive to the environment and any type of interaction with it (thermal, electromagnetic or vibrational) can lead to the collapse of the initial states or, in happier cases, the device's operation slows down, freezes, or even stops unexpectedly.

That is why research is being developed with the aim of finding new cooling methods and improving the stability of quantum systems to handle larger quantum processors in the future. Methods that allow computers to function at the lowest possible temperatures (ideally, as close to absolute zero as possible).

In this sense, it is necessary to establish a connection between the phenomena occurring at non-zero temperatures and those corresponding to temperatures close to theoretical absolute zero. This step is performed by the thermofield dynamics (TFD) theory or model. In essence, TFD is a formalism in quantum field theory that extends the theory formulated from zero temperature phenomena to corresponding phenomena involving finite temperatures. In this formalism description of thermal effects and phenomena at temperature $T \to 0$ is extended to respective phenomena at non-zero temperatures $T \neq 0, T = (k_B \beta)^{-1}$, where k_B is the Boltzmann constant, and $\beta = (k_B T)^{-1}$ is the temperature parameter. TFD is a natural way to studying quantum states at finite temperatures by doubling the degrees of freedom in a Hilbert space and applying a temperature-dependent Bogoliubov transformation. In the TFD theory, the physical quantities at equilibrium are represented by their thermal expectation values. The central idea in TFD is to express this ensemble average as an expectation value over just one state $|\Psi(\beta)> \equiv |0(\beta)>$, called the thermofield double vacuum state or the thermal vacuum state. Their expression is [23]

$$|0(\beta)>= \sqrt{\frac{e^{-\beta \hat{H}}}{Z(\beta)}} \sum_{n=0}^{\infty} |n, \tilde{n}> = \sum_{n=0}^{\infty} \sqrt{\frac{e^{-\beta E_n}}{Z(\beta)}} |n, \tilde{n}> \tag{112}$$

Just in general terms, let's mention the connection between TFD and quantum computing. If we consider the case when the particle confined in the infinite quantum well is a two-level, where the ground energy level is zero, i.e., $E_0 = 0$ (as in the case of the particle embedded in an infinite rectangular potential well), the expression of the fundamental entity from TFD, i.e., the thermal vacuum, will be

$$|0(\beta)>= \sum_{n=0}^{1} \sqrt{\frac{e^{-\beta E_n}}{Z(\beta)}} |n, \tilde{n}>= \sqrt{\frac{1}{Z^{(2)}(\beta)}} |0, \tilde{0}> + \sqrt{\frac{e^{-\beta E_1}}{Z^{(2)}(\beta)}} |1, \tilde{1}> \tag{113}$$

where the partition function is $Z^{(2)}(\beta) = 1 + e^{-\beta E_1}$, so that finally we have

$$|0(\beta)>^{(2)} = \frac{1}{\sqrt{1+e^{-\beta E_1}}} |0, \tilde{0}> + \frac{1}{\sqrt{1+e^{+\beta E_1}}} |1, \tilde{1}> \tag{114}$$

It can be verified that the sum of the squares of the coefficients is equal to 1, so we identify $|0, \tilde{0}> \equiv |0>$ and $|1, \tilde{1}> \equiv |1>$. It can therefore be seen that the thermal vacuum of TFD $|0(\beta)>$ is identical to the so-called thermal vacuum qubit or thermal qubit:

$$|0(\beta)>^{(2)} = c_0 |0> + c_1 |1> \quad , \quad c_0^2 + c_1^2 = 1 \tag{115}$$

This clearly shows the connection between thermofield dynamics and quantum computing [24–26].

6. Concluding Remarks

In the present paper, we presented a type of treatement of the infinite square quantum well in discrete quantum mechanics using a central difference second-derivatives approach. The results obtained by discretization of both the Schrödinger and the Bloch equations could be of certain interest in a different context, especially in the condensed matter physics.

The aim of our paper was to solve the Bloch equation for quantum non interacting particles trapped in a square quantum well of discretized space of the length L. For this purpose, at the beginning, we recalled some (earlier known) methods and results regarding the solving of the Schrödinger equation of a quantum particle trapped in the square infinite well, in the discrete space. The depth of the quantum well is considered infinite $U \to \infty$ so, inside the well the potential is zero.

If we compare the two approaches (discrete and continuous) for the purpose of studying the behavior of the free particle (or the "quantum gas" of free particles) in the infinite quantum well of the same length, we can observe some fundamental differences. The paper lead to the conclusion that, for the problems which include the resolution of the Schrödinger equation (respectively, the Bloch equation) in the discrete space for a particle (respectively, non interacting particle gas) trapped in an infinite square well, the most useful form of the discrete derivatives (between forward, backward and central variants) is the central difference formula, because this approach is consistent with the oscillatory behaviour of the wave functions of the examined problem. The main difference refers to the energy spectrum and, consequently, to the band structure. If in the continuous case the energy has parabolic dependence on the main or principal quantum number n_E, in the discrete case this dependence is more complicated, being achieved by means of the square sinus function $\sin^2\left(\pi \frac{n_E}{N}\right)$.

By applying the continuous quantum mechanical limit ($\lim\limits_{cQM}$) to the physical quantities or formulae regarding the discrete case, we lead to the corresponding quantities or formulae for the continuous case.

As we pointed out, the main purpose of the paper was to solve the discretized Bloch equation for the free particle in the infinite quantum well which is, in our opinion, a completely new approach which had not appeared yet in the scientific literature.

The discretized approach is appropriate for many problems e.g., in condensed matter physics, because in this scientific area many physical systems are achieved from crystalyne materials wherein the spacing between atoms is finite.

On the other hand, the discretization approach can be used successfully in different nanostructures including quantum wells, wires and dots, i.e., in the physical systems containing a finite number of atoms.

In the last part of the paper, we showed how the formalism of coherent states, in particular those associated with a particle embedded in the infinite quantum square well, leads to an important connection with quantum computation. In this way, the coherent state—qubits connection provides a new and important application example of the coherent state concept.

In conclusion, together with other works examining some aspects of the quantum infinite square well, for example tight-binding models [7,9], or coherent states [20,26], we believe that our paper will be a small step forward and will contribute to a better understanding of the phenomena involving quantum infinite square well, especially as regarded of quantum computation and quantum information.

Finally, we can say that the paper presents a theoretical connection from the model of the particle confined in an infinite potential well ($\infty - QW$), treated under continuous-discrete aspect, the formalism of associated coherent states (CSs), aspects of thermofield dynamics (TFD) and up to quantum computing (QC).

The ideas presented in this paper can be summarized in the following} block diagram:

$$\infty - QW \left\{ \begin{matrix} CSs & \Leftrightarrow & coherent\,qubits & |\,z>^{(2)} = \frac{1}{\sqrt{1+|\,z\,|^2}}\,|\,0> + \frac{z}{\sqrt{1+|\,z\,|^2}}\,|\,1> \\ \Updownarrow & & \Updownarrow & \\ TFD & \Leftrightarrow & thermal\,qubits & |\,0(\beta)>^{(2)} = \frac{1}{\sqrt{1+e^{-\beta E_1}}}\,|\,0> + \frac{1}{\sqrt{1+e^{+\beta E_1}}}\,|\,1> \end{matrix} \right\} QC$$

Institutional Review Board Statement

Not applicable.

Informed Consent Statement

Not applicable.

Data Availability Statement

All data generated or analyzed during this study are included in this published article and can be accessed without restrictions.

Acknowledgments

This work is dedicated to the memory of Academician Bratislav S. Tošić (1935–2010), an eminent man and teacher, supporter and promoter of the finite difference calculus applications in quantum physics.

Conflicts of Interest

The author declares no conflict of interest.

Use of AI and AI-Assisted Technologies

No AI tools were utilized for this paper.

Appendix A

The evaluation in an analytical manner of the partition function of the canonical partition function, both for the discrete and also for the continuous case would be an extremely difficult task [8]. Therefore, we try to express the canonical partition function of the discrete case in an approximate manner, by reteining only two terms of the sum. This is motivated by the fact that in the low temperature limit, the exponent is exceedingly small, so only the first two terms make a most important contribution (see the numerical example in the Section 4). So, we can consider that the particle is a two-level system, with energies $E_0^{(d)}=0$ and $E_1^{(d)}=\frac{\hbar^2}{2m^*a^2}\sin^2\left(\frac{\pi}{N}\right)$.

We denote this approximation with $Z_d^{(2)}(\beta)$, where $E_0^{(d)}=0$:

$$Z_d^{(2)}(\beta)=1+e^{-\beta E_1^{(d)}} \tag{A1}$$

Let us use this expression in order to calculate the molar heat capacity at the constant volume $C_V^{(2)}$, defined as:

$$C_V^{(2)}=\frac{1}{\nu}\frac{\partial}{\partial T}\left(N_{tot}<H>^{(d)}\right)=R\beta^2\frac{\partial^2}{\partial\beta^2}\ln Z_d^{(2)}=R\beta^2\left[\frac{1}{Z_d^{(2)}}\frac{\partial^2 Z_d^{(2)}}{\partial\beta^2}-\left(\frac{1}{Z_d^{(2)}}\frac{\partial Z_d^{(2)}}{\partial\beta}\right)^2\right]. \tag{A2}$$

After some simple algebraic calculations we arrived at an interesting final expression:

$$\frac{C_{V,(d)}^{(2)}}{R}=\left[\frac{\beta\frac{E_1^{(d)}}{2}}{\cosh\left(\beta\frac{E_1^{(d)}}{2}\right)}\right]^2=\left[\frac{\beta\frac{\hbar^2}{4m^*a^2}\sin^2\left(\frac{\pi}{N}\right)}{\cosh\left(\beta\frac{\hbar^2}{4m^*a^2}\sin^2\left(\frac{\pi}{N}\right)\right)}\right]^2 \tag{A3}$$

where the argument of hyperbolic function is:

$$\beta\frac{E_1^{(d)}}{2}=\beta\frac{\hbar^2}{2m^*a^2}\sin^2\left(\frac{\pi}{N}\right). \tag{A4}$$

As a matter of fact we indicate that the continuous canonical partition function $Z^{(c)}(\beta)$ (55) can be evaluated, up to an additional constant, by the help of the Jakobi theta function which is an integral functions defined as follows [27]:

$$\vartheta_3(z,\mu)=\sum_{n_E=-\infty}^{\infty}\exp\left\{-\mathrm{i}2z\,n_E-\mu n_E^2\right\}=\sqrt{\frac{\pi}{\mu}}\sum_{n_E=-\infty}^{\infty}\exp\left\{-\frac{(z-\pi n_E)^2}{\mu}\right\}. \tag{A5}$$

For $z=0$ we have $\vartheta_3(0,\mu)\equiv\vartheta_3(\mu)$, i.e., [15]:

$$\vartheta_3(\mu)=\sum_{n_E=-\infty}^{\infty}\exp\left\{-\mu n_E^2\right\}=\sqrt{\frac{\pi}{\mu}}\sum_{n_E=-\infty}^{\infty}\exp\left\{-\frac{\pi^2}{\mu}n_E{}^2\right\}=\sqrt{\frac{\pi}{\mu}}+O\left(e^{-\frac{\pi^2}{\mu}}\right). \tag{A6}$$

For $\mu<<1$ we can neglect the correction terms to order $e^{-\frac{\pi^2}{\mu}}$ and so, we have

$$\vartheta_3(\mu)=\sqrt{\frac{\pi}{\mu}}. \tag{A7}$$

Consequently, by identifying $\mu=\beta\frac{\hbar^2\pi^2}{2m^*L^2}$, the continuous partition function $Z^{(c)}(\beta)$ becomes:

$$Z^{(c)}(\beta)=\sum_{n_E=1}^{\infty}e^{-\beta\frac{\hbar^2\pi^2}{2m^*L^2}n_E^2}=\frac{1}{2}\left(\sum_{n_E=-\infty}^{\infty}e^{-\beta\frac{\hbar^2\pi^2}{2m^*L^2}n_E^2}-1\right)=\frac{1}{2}\left[\vartheta_3\left(\beta\frac{\hbar^2\pi^2}{2m^*L^2}\right)-1\right]=L\sqrt{\frac{m^*}{2\pi\hbar\beta}}-\frac{1}{2} \quad \text{(A8)}$$

Thus, with an accuracy up to a constant term, which does not contribute to the heat capacity value, we obtained in another way Equation (58).

For the case of two-level system, the partition function is

$$Z_c^{(2)}(\beta)=1+e^{-\beta E_1^{(c)}} \quad , \qquad E_1^{(c)}=\frac{\hbar^2\pi^2}{2\,m^*L^2} \quad \text{(A9)}$$

Formally, the expression of molar heat capacity at the constant volume $C_V^{(2)}$ is identical

$$\frac{C_{V,(c)}^{(2)}}{R}=\left[\frac{\beta\frac{E_1^{(d)}}{2}}{\cosh\left(\beta\frac{E_1^{(d)}}{2}\right)}\right]^2=\left[\frac{\beta\frac{\hbar^2\pi^2}{4\,m^*L^2}}{\cosh\left(\beta\frac{\hbar^2\pi^2}{4\,m^*L^2}\right)}\right]^2 \quad \text{(A10)}$$

respecting the limit:

$$\lim_{\substack{N\to\infty\\ a\to 0\\ aN=L}}\frac{C_{V,(d)}^{(2)}}{R}\equiv\lim_{cQM}\frac{C_{V,(d)}^{(2)}}{R}=\frac{C_{V,(c)}^{(2)}}{R} \quad \text{(A11)}$$

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