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Coherent States Formalism Applied to the Quantum Well Model

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The different nanostructures (quantum dots, wires and wells) have specific properties which differ from those of the corresponding bulk structures. This fact leads to many applications in several branches of physics. In the paper we examine the behavior of a quantum system (a free particle and a quantum free particle gas) trapped inside the infinite quantum well, by using the coherent states formalism. Our approach is based on the fact that the dynamical group associated with the infinite quantum well is SU(1, 1), with the Bargmann index $k = 1/2$. These coherent states always have the sub-Poissonian behavior. There is a similarity between the energy main quantum number n and the absolute value of the complex variable z which labels the coherent states. This allows us to make a useful approximation in order to calculate the partition function and some thermodynamic characteristics of a canonical non interacting particle gas embedded in the infinite square quantum well.

Keywords: Infinite Quantum Well, Coherent States, Density Matrix.

1. INTRODUCTION

Long time the quantum well has be seen only as a first theoretical model used for teaching purposes to familiarize students with the concept of energy quantization. But, in the last decades, due to the development of the nanoscience and nanotechnology the quantum well model has been reconsidered as a particular kind of heterostructure consisting of one thin "well" layer, surrounded by two "barrier" layers, of certain, practically of some finite height, but which, under certain conditions, can be considered as infinite.

As it is well-known, the properties of nanostructures (quantum dots, wires and wells) are different from those of the corresponding bulk structures and this fact lead to many applications in condensed matter, optoelectronic devices, sensors, electronic and light emitting components (lasers). Consequently, it is of interest to examine the behavior of the particles in quantum wells. In the paper we examine the behavior of a quantum system (an individual free particle and a quantum free particle gas) trapped inside the infinite quantum well (QW) $0 \le x \le L$ by using the coherent states (CSs) formalism, according to the sequence: nanoparticles → QW → CSs.

2. MOTION IN AN INFINITE SQUARE POTENTIAL QUANTUM WELL

Let we consider a quantum particle with effective mass m^* trapped inside an infinite square potential quantum well potential along the x-axis with width L and recall some well-known results regarding the motion of the particle. The corresponding Schrödinger equation for stationary states

$$H\,\Psi_n(x) = E_n \Psi_n(x), \quad H = -\frac{\hbar^2}{2\,m^*}\frac{d^2}{dx^2} \tag{1}$$

with the boundary conditions: $\Psi_n(0) = \Psi_n(L) = 0$ leads to the following normalized eigenfunctions and corresponding energy eigenvalues:

$$\Psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right), \quad E_n = \frac{\hbar^2\pi^2}{2\,m^* L^2}n^2 \equiv \hbar\omega n^2$$
$$\omega \equiv \frac{\hbar\pi^2}{2\,m^* L^2} \tag{2}$$

The normalized eigenfunctions are real and we insert here the well-known relation from the quantum mechanics textbooks fulfilled by them, by virtue of the general conditions of the orthogonality of wave functions:

$$\sum_{n=0}^{\infty}\Psi_n(x)\,\Psi_n(x') = \frac{2}{L}\sum_{n=0}^{\infty}\sin\left(\frac{n\,\pi}{L}\,x\right)\sin\left(\frac{n\,\pi}{L}\,x'\right) = \delta(x - x') \tag{3}$$

Generally, this equation can be regarded also as a consequence of the boundary condition for the canonical density operator in the coordinate representation

$$\rho(x, x'; \beta) = \sum_{n=0}^{\infty} e^{-\beta E_n}\Psi_n(x)\Psi_n(x') \tag{4}$$

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whose limit is

$$\lim_{\beta\to 0}\rho(x,x';\beta)=\sum_{n=0}^{\infty}\Psi_n(x)\Psi_n(x')=\delta(x-x') \tag{5}$$

In order to construct the coherent states, it is not less important to emphasize that the particle motion in an infinite quantum well is stationary and their energy is quantized, the difference between the energy levels is not equal, but increases with increasing principal quantum number n, i.e., $\Delta E_n = E_{n+1}-E_n=\hbar\omega(2n+1)$. This means that the transition of particle between the superior energy levels is more difficult that between than between lower levels. By considering an electron trapped inside an infinite quantum well of width $L=10^{-2}$ m, the "variable quanta" $\hbar\omega$ is approximately $0.3\cdot 10^{-38}$ J, while for the width of atomic dimension order $L=10^{-9}$ m, this value is $0.3\cdot 10^{-17}$ J.

3. SU(1, 1) GROUP

The quantum SU(1, 1) group and the corresponding su(1, 1) algebra have a great relevance due to their applications to many physical systems coherent and squeezed states.

The SU(1, 1) group generators are K_+, K_- and K_3, which are defined by the commutation relations

$$[K_-,K_+]=2K_3,\quad [K_3,K_\pm]=\pm K_\pm \tag{6}$$

and by the following actions on the complete basis of Fock vectors $|n;k\rangle$ from the infinite-dimensional Hilbert space, where $n=0,1,2,\ldots$ and $k=1/2,1,3/2,\ldots$ is the Bargmann index labeling the irreducible representation:

$$\begin{aligned}K_+|n;k\rangle &= \sqrt{(n+1)(n+2k)}|n+1;k\rangle\\ K_-|n;k\rangle &= \sqrt{n(n+2k-1)}|n-1;k\rangle\end{aligned} \tag{7}$$

$$K_3|n;k\rangle=(n+k)|n;k\rangle \tag{8}$$

Some years ago, by using the factorization method, Lemus and Frank have demonstrates that the dynamical group associated with the infinite quantum well is just SU(1, 1), with the Bargmann index $k=1/2$.[1,2] Then the group generators act on the Fock basis vectors $|n;1/2>\equiv|n>$ in the following manner:

$$\begin{aligned}K_+|n>&=(n+1)|n+1>,\quad K_-|n>=n|n-1>\\ K_3|n>&=\left(n+\frac{1}{2}\right)|n>\end{aligned} \tag{9}$$

These generators ensure that the energy eigenvalues of a particle of mass m^* trapped inside infinite square quantum well (ISQW) assumes a simple form:

$$E_n\equiv<n|H|n>=\frac{\hbar^2\pi^2}{2m^*L^2}<n|K_+K_-|n>=\hbar\omega\, n^2 \tag{10}$$

We observe that the Hamiltonian operator H is expressed as the normal ordering product of the creation K_+ and annihilation K_- operators (in the sense that into an operator product, the creation operators K_+ are placed in the left and the annihilation operators K_- are placed on the right each other). With these elements we are able to define the coherent states of the infinite square quantum well.

4. COHERENT STATES

We define the coherent states for the infinite quantum well in the Barut-Girardello manner in the usual way, i.e., as the eigenvalues of the lowering operator K_- and we denote these states as BG-CSs:[3]

$$K_-|z>=z|z> \tag{11}$$

where $z=|z|\exp(i\varphi)$ is the complex variable labeling CSs.

There are some manners to perform realizations of the SU(1,1) generators, depending on the specific problems or quantum systems. Particularly, we consider such a realization of the SU(1,1) algebra in terms of one dimensional harmonic oscillator (HO-1D) creation and annihilation operators a^+ and a[4]:

$$K_+=\sqrt{N}a^+;\quad K_-=a\sqrt{N};\quad K_3=N+\frac{1}{2}\equiv a^+a+\frac{1}{2} \tag{12}$$

Evidently that this realization can be regarded as a nonlinear with respect to the HO-1D creation and annihilation operators a^+ and a, so that the above defined BG-CSs for the ISQW are in fact a version of nonlinear CSs of the usual (canonical) CSs for the HO-1D. Consequently, in the next we will shortly denote these CSs as BG-NCSs for the ISQW.

Recalling that the Fock vectors $|n>$ satisfies the completeness relation

$$\sum_{n=0}^{\infty}|n><n|=1 \tag{13}$$

after some straightforward calculations we obtain the development of the BG-NCSs for the ISQW as the superposition of the complete orthonormal Fock-vectors basis $|n>$:

$$|z>=\frac{1}{\sqrt{I_0(2|z|)}}\sum_{n=0}^{\infty}\frac{z^n}{n!}\;|\;n> \tag{14}$$

where $I_0(x)$ is the modified Bessel function of the first kind defined as:

$$I_0(2|z|)=\sum_{n=0}^{\infty}\frac{1}{(n!)^2}|z|^{2n} \tag{15}$$

As all CSs, the above defined BG-NCSs for the ISQW are also normalized but non orthogonal, so the overlap of two such states is

$$\langle z|z'\rangle=\frac{I_0(2\sqrt{z^*z'})}{\sqrt{I_0(2|z|)I_0(2|z'|)}} \tag{16}$$

Moreover, a crucial property of any set of CSs is that they allow the decomposition (or resolution) of the unity operator, namely:[5]

$$\int d\mu(z)|z><z|=1 \tag{17}$$

where $d\mu(z)=(d\varphi/2\pi)d(|z|^2)h(|z|)$ is the integration measure whose weight function $h(|z|)$ must be determined in the next.

By substituting Eqs. (14) and using (13) we successively obtain:

$$\sum_{n,m=0}^{\infty}\frac{|n><m|}{n!m!}\int_0^{\infty}d(|z|^2)h(|z|)\frac{1}{I_0(2|z|)}\int_0^{2\pi}\frac{d\varphi}{2\pi}z^n(z^*)^m=1 \tag{18}$$

The result of the angular integration is $(|z|^2)^n\delta_{nm}$, so that, in order to accomplish the completeness relation (13), we must have

$$\int_0^{\infty}d(|z|^2)h(|z|)\frac{1}{I_0(2|z|)}(|z|^2)^n=(n!)^2 \tag{19}$$

If we perform the function change, as well as the exponent change:

$$g(|z|) \equiv h(|z|)\frac{1}{I_0(2|z|)}, \quad n = s-1 \tag{20}$$

we come to the Stietjes moment problem[6]

$$\int_0^{\infty} d(|z|^2) g(|z|)(|z|^2)^{s-1} = [\Gamma(n+1)]^2 \tag{21}$$

where $\Gamma(x)$ is the Euler's gamma function.[6]

The solution of this integral equation is $g(|z|) = 2K_0(2|z|)$, where $K_0(x)$ is the modified Bessel function of the second kind and, consequently, the integration measure becomes:

$$d\mu(z) = 2\frac{d\varphi}{2\pi} d(|z|^2)\, I_0(2|z|)K_0(2|z|) \tag{22}$$

With these elements, we can express the expectation value of a certain operator A, in the representation of the BG-NCSs for the ISQW as follows:

$$\langle z|A|z\rangle = \frac{1}{I_0(2|z|)} \sum_{n=0}^{\infty} \frac{z^n (z^*)^m}{n!m!} \langle m|A|n\rangle \tag{23}$$

We will focus our attention especially on those operators which are diagonal in the Fock-vectors basis, such as the Hamiltonian H or particle number operator $N = K_3 - 1/2$, the latter having the following eigenequations:

$$N|n> = n|n>, \quad N^s|n> = n^s|n>, \quad s = 1, 2, \ldots \tag{24}$$

Their expectation values in the BG-NCSs for the ISQW representation are

$$\begin{aligned}\langle z|N^s|z\rangle &= \frac{1}{I_0(2\,|z|)} \sum_{n=0}^{\infty} \frac{(|z|^2)^n}{(n!)^2} n^s \\ &= \frac{1}{2^s}\frac{1}{I_0(2|z|)}\left(|z|\frac{d}{d|z|}\right)^s I_0(2|z|)\end{aligned} \tag{25}$$

For different values of the power index s, in order to express the above differentiation operator we can use an ansatz elaborated in the Appendix B of our previous paper.[7]

For the expectation value of the Hamiltonian operator in the BG-NCSs for the ISQW representation we obtain:

$$\begin{aligned}E_{|z|^2} \equiv \langle z|H|z\rangle &= \frac{\hbar^2\pi^2}{2m^*L^2}\langle z|K_+K_-|z\rangle \\ &= \frac{\hbar^2\pi^2}{2m^*L^2}|z|^2 = \hbar\omega|z|^2\end{aligned} \tag{26}$$

where we have used the following properties of the modified Bessel functions:[6,8]

$$\frac{d}{dx}I_0(x) = I_1(x), \quad \frac{d}{dx}[xI_1(x)] = xI_0(x) \tag{27}$$

Now it is interesting to examine the behavior of the field of the BG-NCSs for the ISQW and for this purpose it is useful to examine the values of the Mandel parameter as function of variable $|z|$. The Mandel parameter is defined as:[9]

$$Q_{|z|} = \frac{V_{|z|}}{<z|N|z>} - 1 \equiv \frac{\langle z|N^2|z\rangle - (<z|N|z>)^2}{<z|N|z>} - 1 \tag{28}$$

Depending of the values of the Mandel parameter, the field of CSs is as follows:

$$Q_{|z|}\begin{cases} <0 & \text{sub-Poissonian field} \rightarrow \text{sub-Poissonian statistics} \\ =0 & \text{Poissonian field} \rightarrow \text{Poissonian statistics} \\ >0 & \text{super-Poissonian field} \rightarrow \text{super-Poissonian statistics}\end{cases}$$

By using Eqs. (25) and (27), the Mandel parameter BG-NCSs for the ISQW is

$$Q_{|z|} = |z|\left[\frac{I_0(2|z|)}{I_1(2|z|)} - \frac{I_1(2|z|)}{I_0(2|z|)}\right] - 1 \tag{29}$$

As we can see from Figure 1, the Mandel parameter BG-NCSs for the ISQW is always negative, i.e., the field of the BG-NCSs for the ISQW is always sub-Poissonian and these states obeys the sub-Poissonian statistics. This means that the variance $V_{|z|} = \langle z|N^2|z\rangle - (\langle z|N|z\rangle)^2$ of these states is always less than the mean value in the BG-NCSs for the ISQW representation $\langle z|N|z\rangle$. In other words the BG-NCSs for the ISQW have non-classical behavior (states with no classical analogue). Due to their non-classical behavior, these states have received considerable attention in many modern fields of physics (quantum optics, quantum information, quantum communication, nanotechnology and so on).

In the end of this section we examine some aspects of the BG-NCSs for the ISQW from the point of view of the, "generalized IWOP technique." The IWOP (Integration Within an Ordered Đroduct of Operators) technique was founded by Fan (see, e.g., Ref. [10] and the references therein, where we can see their main rules).

By using Eq. (9), we obtain $(K_+)^n|0> = n!|n>$ and, inserting this result in Eq. (14), we obtain:

$$\begin{aligned}|z> &= \frac{1}{\sqrt{I_0(2|z|)}} \sum_{n=0}^{\infty} \frac{(zK_+)^n}{(n!)^2}|0> \\ &= \frac{1}{\sqrt{I_0(2|z|)}} I_0(2\sqrt{zK_+})|0>\end{aligned} \tag{30}$$

which shows that the BG-NCSs for the ISQW can be obtained also as the normalized action of the operatorial modified Bessel function of the first kind $I_0(2\sqrt{z\,K_+})$ on the vacuum fundamental state $|0>$.

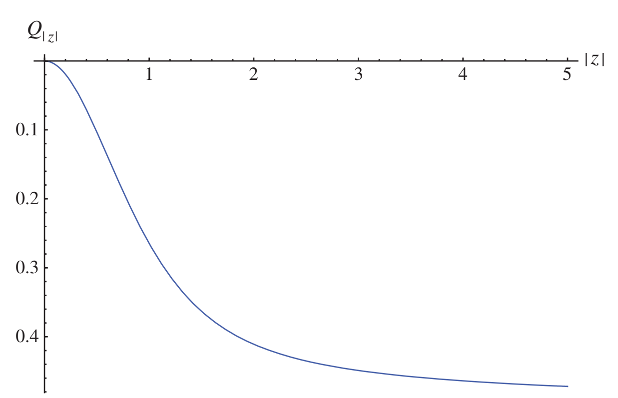

Fig. 1. The Mandel parameter $Q_{|z|}$ of BG-NCSs for the ISQW.

Their counterpart is, then obtained by the conjugation

$$< z| = \frac{1}{\sqrt{I_0(2|z|)}} < 0|I_0(2\sqrt{z^*K_-}) \quad (31)$$

The projector onto a BG-NCS for the ISQW is the written in an ordered operatorial manner (this was pointed out by using the normal ordered symbol : :), i.e.,

$$|z >< z| = \frac{1}{I_0(2|z|)} : I_0(2\sqrt{zK_+})|0 >< 0|I_0(2\sqrt{z^*K_-}) : \quad (32)$$

In order to deduce the expression of the projector on the vacuum state $|0 >< 0|$ for the case of the BG-NCSs for the ISQW we appeal to the resolution of the unity operator, Eq. (17) where we replace Eqs. (30) and (31):

$$\int d\mu(z)|z >< z| = 2\int_0^\infty d(|z|^2)K_0(2|z|)\int_0^{2\pi}\frac{d\varphi}{2\pi} : I_0(2\sqrt{zK_+}) \\ |\, 0 >< 0\, |\, I_0(2\sqrt{z^*K_-}) := 1 \quad (33)$$

The angular integral is solved by using the definition of $I_0(x)$:

$$\int_0^{2\pi}\frac{d\varphi}{2\pi} : I_0(2\sqrt{zK_+})|0 >< 0|I_0(2\sqrt{z^*K_-}) := \\ =: |0 >< 0| \sum_{n,m=0}^{\infty} \frac{(K_+)^n(K_-)^m}{(n!)^2(m!)^2} : \int_0^{2\pi}\frac{d\varphi}{2\pi} z^n\,(z^*)^m \\ =: |0 >< 0| \sum_{n,m=0}^{\infty}\frac{(K_+K_-)^n}{(n!)^4} : |z|^{2n} \quad (34)$$

$$: |\, 0 >< 0\, | \sum_{n,m=0}^{\infty}\frac{(K_+K_-)^n}{(n!)^4} : 2\int_0^\infty d(|z|^2)K_0(2|z|)|z|^{2n} = 1 \quad (35)$$

The last integral is $(n!)^2$,[6] so we obtain:

$$: |0 >< 0| \sum_{n,m=0}^{\infty}\frac{(K_+K_-)^n}{(n!)^4} :=: |0 >< 0|I_0(2\sqrt{K_+K_-}) := 1 \quad (36)$$

Finally, the projector on the vacuum state of the BG-NCSs for the ISQW is

$$|0 >< 0| =: \frac{1}{I_0(2\sqrt{K_+K_-})} : \quad (37)$$

and then the projector onto a BG-NCS for the ISQW becomes:

$$|z >< z| = \frac{1}{I_0(2|z|)} : \frac{I_0(2\sqrt{zK_+})I_0(2\sqrt{z^*K_-})}{I_0(2\sqrt{K_+K_-})} : \quad (38)$$

Consequently, using the rules of generalized IWOP technique, the expectation value of an operator built in the ordered operator manner $A = A(K_+, K_-)$ can be written as:

$$< z|A|z > = \frac{1}{I_0(2|z|)} < 0 \\ |: \frac{I_0(2\sqrt{zK_+})A(K_+, K_-)I_0(2\sqrt{z^*K_-})}{I_0(2\sqrt{K_+K_-})} : |0 > \quad (39)$$

5. STATISTICAL PROPERTIES

In order to examine the statistical properties of the BG-NCSs for the ISQW let we consider a mixed (thermal) state with the corresponding canonical normalized density operator:

$$\rho = \frac{1}{Z(\beta)}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n^2}|n >< n| \quad (40)$$

where $Z(\beta)$ is the partition function:

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n^2} = \frac{1}{2}[\theta_3(0; e^{-\beta\hbar\omega}) - 1] \quad (41)$$

Generally, we have been expressed the partition function through the Jakobi theta function θ_3^0, but the use of this expression is inconvenient. Therefore it is useful to fix our attention on the similarity between the expressions for the expected values of energy in two representations, $|n>$ and $|z>$:

$$E_n = \hbar\omega n^2 \Leftrightarrow E_{|z|^2} = \hbar\omega|z|^2 \quad (42)$$

i.e., to the similarity $n^2 \Leftrightarrow |z|^2$.

In addition, given that the value of $\hbar\omega$ is very small (see the values at the end of Section 2), we can calculate the partition function as integral over the variable $|z|$:

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n^2} \Leftrightarrow Z_c(\beta) \\ = \int_0^\infty e^{-\beta\hbar\omega|z|^2}d(|z|) = \frac{1}{2}\sqrt{\frac{\pi}{\hbar\omega}}\frac{1}{\sqrt{\beta}} \quad (43)$$

The internal energy of a particle "gas" of N_{tot} non- interacting particles "embedded" in the infinite quantum well, at the equilibrium temperature T, usually calculated as

$$U = N_{\mathrm{tot}}\langle H\rangle = N_{\mathrm{tot}}\mathrm{Tr}(\rho H) = N_{\mathrm{tot}}\frac{1}{Z(\beta)}\sum_{n=0}^{\infty}E_n e^{-\beta E_n} \\ = -\nu N_A\frac{\partial}{\partial\beta}\ln Z(\beta) \quad (44)$$

due to the above similarity can be calculated as follows:

$$U_c = -\nu N_A\frac{\partial}{\partial\beta}\ln Z_c(\beta) = -\nu N_A\frac{1}{2}\frac{1}{\beta} \quad (45)$$

Then the molar heat capacity at the constant volume is

$$C_V = \frac{1}{\nu}\frac{\partial U_c}{\partial T} = -\frac{1}{\nu}k_B\beta^2\frac{\partial U_c}{\partial\beta} = \frac{1}{2}R \quad (46)$$

This result is the same as for on degree of freedom in the motion of the ideal non-interacting monoatomic gas. This coincidence should not surprise us because for the particle trapped into an ISQW the confinement effect may appear only in the transverse direction while particles are free to move in one dimension (along the structure, the axis Ox in our example).

6. CONCLUDING REMARKS

In the paper we have examined some properties of the Barut-Girardello coherent states (BG-CSs) for a particle embedded in an infinite square quantum well (ISQW). We have used the fact that the quantum group associated with this physical model is SU(1,1) which allows building of these kind of states by choosing the Bargmann index $k = 1/2$. These coherent states have always the sub-Poissonian behaviour. We have also showed that is exists a certain similarity between the energy main quantum number n and the absolute value of the complex variable z which labels the coherent states. This similarity allows us to make an useful approximation in order to calculate the partition function and also some thermodynamic characteristics of a canonical non interacting particle gas embedded in the infinite square quantum well. Due to non-classical behavior of the BG-NCSs for the ISQW, these states have received an important role in many modern fields of physics (quantum optics, quantum information, quantum communication, nanotechnology and so on).

At this place we can say that it exists various approaches related to the construction of the CSs for infinite quantum well,[5, 11, 12–16] which demonstrate the practical interest on this subject. Even if the infinite quantum well model is usually far from the properties of real quantum systems, this simple model has several advantages in order to highlight some behaviors or effects in various simple nanostructure systems. Our approach only completes this image.

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