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Excitonic Coherent States: Symmetries and Thermalization

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Abstract In this paper we considered the theoretical treatment of a physical system of excitons and its behaviour under temperature by means of a new coherent state construction of bounded states in a quantum field theoretical context.

Keywords Excitons · Coherent states · Thermalization

1 Introduction

In previous work [1], new bounded coherent states construction, based on a Keldysh conjecture, was introduced. As was shown in [1] the particular group structure arising from the model leads to new symmetry transformations for the coherent states system. As was shown, the emergent new symmetry transformation is reminiscent of the Bogoliubov ones and was successfully applied to describe an excitonic system showing that it is intrinsically related to the stability and its general physical behaviour. The group theoretical structure of the model permits to analyse its thermal properties in theoretical frameworks that arise as a consequence of the definition of the squeezed coherent states as transformed vacua under the automorphism group of the commutation relations, as the thermofield dynamics case given by Umezawa and other similar developments [11]. On the other hand, the idea of a possible Bose–Einstein condensation (BEC) of excitons in semiconductors has attracted the attention of both experimentalists and theoreticians for more than three decades being one of the main questions what happens with the influence of non-zero temperature in the case that such condensation really exists [2,3]. In this paper we considered the theoretical

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treatment of the excitonic behaviour by means of a new coherent state construction of bounded states in a quantum field theoretical context. The possibility to introduce the coherent states in a physical system of excitons is mainly fundamented by the idea of "exciton state splitting" and "exciton wave function" introduced by Keldysh [4–7] earlier and developed by us in [1]. This paper is organized as follows: in Sect. 1 we make basically a short review of our earlier work [1] adding several new comments and concepts necessary to the clear understanding of this approach, and Sect. 2 is devoted to introduce the thermalization of excitonic coherent states by means of a specific unitary transformation described by a composed displacement operator.

2 Exciton Model: Review and New Concepts

2.1 General Description

As was shown before [1], our starting point is based in the following splitting of the fermionic state in the material to be considered

$$\psi_\alpha(\mathbf{x}) \equiv \psi_\alpha^{(e)}(\mathbf{x}) + \psi_\alpha^{\dagger(h)}(\mathbf{x}) \tag{1}$$

with $\psi_\alpha^{(e)}(\mathbf{x}) \equiv \sum_{j>j_0} a_j \chi_\alpha^j(\mathbf{x})$, $\psi_\alpha^{\dagger(h)}(\mathbf{x}) \equiv \sum_{j>j_0} a_j \chi_\alpha^j(\mathbf{x})$, where $\left[a_j^\dagger, a_{j'}\right]_+ = \delta_{jj'}$, $\left[a_j, a_{j'}\right]_+ = 0$ We have defined $\chi_\alpha^j(\mathbf{x})$ the basic functions of Hartree–Fock (HF) of the system and the indices $j > j_0$ and $j \leq j_0$ numerate the bounded states from the electronic zone and the free states, respectively.

Remark 1 Definition (1) describes correctly the excitonic operator being the same operator acting in the characteristic zones. Then, in sharp contrast with the traditionally accepted use of different operators for electron and hole, respectively, the construction (1) avoid all type of overcounting and spurious states that are clearly non-physical.

Let us consider, without losing generality and only to exemplify in concrete cases, the symmetries of a periodic system (e.g. crystal). In this case the functions of HF take the form of a Bloch state $\chi_{j\alpha}(\mathbf{x}) = \mathrm{e}^{i\mathbf{P}\cdot\mathbf{x}} u_{\mathbf{P}l\alpha}$, where P is the quasi-momentum and l is the number of zone, such that $j = \{\mathbf{P}, l\}$. If the case is for a non-metallic crystal, then the sum in $j \leq j_0$ corresponds to a sum over all $\mathbf{P}$ which live in the 1st Brillouin zone. The HF functions obey the HF equation

$$\int h_{\alpha\beta}\left(\mathbf{x}, \mathbf{x}'\right) \chi_j^\beta\left(\mathbf{x}'\right) \mathrm{d}^3\mathbf{x}' = \varepsilon_j \chi_{j\alpha}(\mathbf{x}) \tag{2}$$

with $h_{\alpha\beta}\left(\mathbf{x}, \mathbf{x}'\right) = \delta_{\alpha\beta}\delta\left(\mathbf{x}, \mathbf{x}'\right)\left\{\frac{-\hbar^2}{2m_0}\nabla^2 - \sum \frac{Z_k \mathrm{e}^2}{|\mathbf{R}_{n,k} - \mathbf{x}|} + \frac{\mathrm{e}^2}{2}\int \frac{g_{\beta\beta}(\mathbf{y},\mathbf{y})\mathrm{d}^3\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}\right\} - \mathrm{e}^2 \frac{g_{\alpha\beta}(\mathbf{x},\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$ being the HF operator, where we define $g_{\alpha\beta}\left(\mathbf{x}, \mathbf{x}'\right) \equiv \sum_{j\leq j_0} \chi_{j\alpha}(\mathbf{x}) \chi_\beta^j\left(\mathbf{x}'\right)$

Remark 2 The important observation here (in concordance with our remark about expression 1) is that the hamiltonian is not the sum of several terms involving electrons,

holes, etc. as separate entities, as is currently taken in the literature: only the state defined in expression (1) is involved into the Hamiltonian $h_{\alpha\beta}\left(\mathbf{x},\mathbf{x}'\right)$.

2.2 Exciton Wave Equation

Due to the composite characteristic of the excitonic state, firstly we have particular interest in the 2-particles 2-times Green functions

$$G^{(2)}_{\alpha\beta,\gamma\delta}\left(\mathbf{x},\mathbf{y},t;\mathbf{x}',\mathbf{y}',t'\right)=-\frac{i}{\hbar}\left\langle T\psi^{\dagger}_{\alpha}\left(\mathbf{x},t\right)\psi_{\beta}\left(\mathbf{y},t\right)\psi^{\dagger}_{\gamma}\left(\mathbf{x}',t'\right)\psi_{\delta}\left(\mathbf{y}',t'\right)\right\rangle_{0}, \quad (3)$$

where $\psi_{\beta}\left(\mathbf{y},t\right)$ is Heisenberg operators and $\langle T\cdots.\rangle_0$ chronological product. The second important point in the CS excitonic formulation is due to the observation pointed out in [2,3], that the $G^{(2)}_{\alpha\beta,\gamma\delta}\left(\mathbf{x},\mathbf{y},t;\mathbf{x}',\mathbf{y}',t'\right)$ can be written as

$$\begin{aligned} &i\hbar G^{(2)}_{\alpha\beta,\gamma\delta}\left(\mathbf{x},\mathbf{y},t;\mathbf{x}',\mathbf{y}',t'\right)\\ &=-\sum_{\mathbf{P}J}\begin{cases}\varphi^{J\mathbf{P}}_{\alpha\beta}\left(\mathbf{x},\mathbf{y}\right)\varphi^{J\mathbf{P}\star}_{\gamma\delta}\left(\mathbf{x}',\mathbf{y}'\right)\mathrm{e}^{\frac{i}{\hbar}\left(\frac{\mathbf{P}\cdot\left(\mathbf{x}+\mathbf{y}-\mathbf{x}'-\mathbf{y}'\right)}{2}-E_{J\mathbf{P}}(t-t')\right)}, & t>t'\\ \varphi^{J\mathbf{P}\star}_{\alpha\beta}\left(\mathbf{x},\mathbf{y}\right)\varphi^{J\mathbf{P}}_{\gamma\delta}\left(\mathbf{x}',\mathbf{y}'\right)\mathrm{e}^{\frac{-i}{\hbar}\left(\frac{\mathbf{P}\cdot\left(\mathbf{x}+\mathbf{y}-\mathbf{x}'-\mathbf{y}'\right)}{2}-E_{J\mathbf{P}}(t-t')\right)}, & t<t'\end{cases} \end{aligned} \quad (4)$$

here is easily seen that

$$\mathrm{e}^{\frac{i}{\hbar}\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}}\varphi^{J\mathbf{P}}_{\alpha\beta}\left(\mathbf{x},\mathbf{y}\right)=\left\langle 0\left|\psi^{\dagger}_{\alpha}\left(\mathbf{x}\right)\psi_{\beta}\left(\mathbf{y}\right)\right|J\mathbf{P}\right\rangle \quad (5)$$

Then, the above expression can be assumed as the basic wave function of the exciton[1] Taking account of the symmetries involved, the Von Karman periodic conditions are $\varphi^{J\mathbf{P}}_{\alpha\beta}\left(\mathbf{x}+\mathbf{R}_n,\mathbf{y}+\mathbf{R}_n\right)=\varphi^{J\mathbf{P}}_{\alpha\beta}\left(\mathbf{x},\mathbf{y}\right)$ with $\mathbf{R}_n$ a characteristic vector of the crystal lattice. Fourier transforming (4) in the time we obtain

$$G^{(2)}_{\alpha\beta,\gamma\delta}\left(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}';\mathbf{P}E\right)=\sum_{J,\delta\to+0}\frac{2E_{J\mathbf{P}}}{E^2-\left(E_{J\mathbf{P}}-i\delta\right)^2}\varphi^{J\mathbf{P}\star}_{\alpha\beta}\left(\mathbf{x},\mathbf{y}\right)\varphi^{J\mathbf{P}}_{\gamma\delta}\left(\mathbf{x}',\mathbf{y}'\right) \quad (6)$$

notice that, due the free field form, this formulas are independent of the specific form of the hamiltonian considered.

Remark 3 Due the composite and extended character of the exciton systems, the wave functions defined in (5) have a non-local behaviour in general

[1] Notice that form Eq. (8) the factorization in pairs of the two times/two field Green's functions is automatically assumed.

2.3 Excitonic Coherent State Construction

It is well known that CS provides naturally a close connection between classical and quantum formulations of a given system [8–10]. As is well known, the importance of coherent states in physics, and particularly in condensed matter physics, is huge. All the physical processes, where the quantum world is macroscopically manifested (as in BEC or laser physics) can be faithfully described by coherent states due the semiclassical behaviour, temporal stability and other mathematical requisites needed in the quantum field theoretical framework. There exist three standard definitions in the construction of coherent states. The most suitable for our proposes here is by means of a "displacing operator" acting over the vacuum (specific fiducial vector). The unitary operators

$$B_{J\mathbf{P}} = \frac{1}{V}\int \psi^{\alpha\dagger}(\mathbf{x})\,\varphi^{J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y})\,\mathrm{e}^{\frac{i}{\hbar}\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}}\psi^{\beta}(\mathbf{y})\,\mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}, \tag{7}$$
$$B^{\dagger}_{J\mathbf{P}} = \frac{1}{V}\int \mathrm{e}^{\frac{-i}{\hbar}\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}}\psi^{\alpha\dagger}(\mathbf{x})\,\varphi^{\dagger J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y})\,\psi^{\beta}(\mathbf{y})\,\mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y},$$

where $\varphi^{\dagger J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y}) = \left[\varphi^{J\mathbf{P}}_{\beta\alpha}(\mathbf{y},\mathbf{x})\right]^{\star}$, ($V =$ normalized volume) and the commutation relations take the following form

$$\begin{aligned}\left[B_{J\mathbf{P}}, B^{\dagger}_{J'\mathbf{P}'}\right] &= \delta_{JJ'}\delta_{\mathbf{P}\mathbf{P}'}\\ &-\left\{\frac{1}{V}\int \psi^{\alpha\dagger(e)}(\mathbf{x})\,\mathrm{e}^{\frac{i}{2\hbar}\mathbf{P}\cdot\mathbf{x}}\varphi^{J\mathbf{P}}_{\alpha\gamma}(\mathbf{x},\mathbf{z})\,\mathrm{e}^{\frac{-i}{2\hbar}(\mathbf{P}-\mathbf{P}')\cdot\mathbf{z}}\varphi^{\dagger J'\mathbf{P}'}_{\gamma\beta}(\mathbf{z},\mathbf{y})\,\mathrm{e}^{\frac{-i}{2\hbar}\mathbf{P}'\cdot\mathbf{y}}\psi^{\beta(e)}(\mathbf{y})\right.\\ &\left.+\frac{1}{V}\int \psi^{\alpha\dagger(h)}(\mathbf{x})\,\mathrm{e}^{\frac{-i}{2\hbar}\mathbf{P}'\cdot\mathbf{y}}\varphi^{\dagger J'\mathbf{P}'}_{\gamma\beta}(\mathbf{y},\mathbf{z})\,\mathrm{e}^{\frac{-i}{2\hbar}(\mathbf{P}-\mathbf{P}')\cdot\mathbf{z}}\varphi^{J\mathbf{P}}_{\alpha\gamma}(\mathbf{z},\mathbf{x})\,\mathrm{e}^{\frac{i}{2\hbar}\mathbf{P}\cdot\mathbf{x}}\psi^{\beta(h)}(\mathbf{y})\right\}\\ &\mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}\mathrm{d}^3\mathbf{z}\end{aligned} \tag{8}$$

indicating exactly the intricated interplay in the electron-hole system (notice the lack of canonicity). Although the complexity of expression (8), we take advantage of the unitarity of the $B_{J\mathbf{P}}$ (7) constructing the coherent states as

$$|\beta, J\mathbf{P}\rangle = \exp\left\{\beta B^{\dagger}_{J\mathbf{P}}\mathrm{e}^{iE_{J\mathbf{P}}t/\hbar} - \beta^{\star}B_{J\mathbf{P}}\mathrm{e}^{-iE_{J\mathbf{P}}t/\hbar}\right\}|0\rangle \equiv |\varphi\rangle \tag{9}$$

where, after the use of Eq. (1), the explicit form of the displacement operator is as follows:

$$\begin{aligned}D_{\varphi} = \exp\Bigg[\int &\psi^{\alpha\dagger(e)}(\mathbf{x})\,\varphi_{\alpha\beta}(\mathbf{x},\mathbf{y})\,\mathrm{e}^{\frac{-i}{\hbar}\left(\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}-mt\right)}\psi^{\beta\dagger(h)}(\mathbf{x})\\ &-\psi^{\alpha(h)}(\mathbf{x})\,\varphi^{\star}_{\alpha\beta}(\mathbf{x},\mathbf{y})\,\mathrm{e}^{\frac{-i}{\hbar}\left(\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}-mt\right)}\psi^{\beta(e)}(\mathbf{x})\Bigg]\mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}\end{aligned} \tag{10}$$

Remark 4 Expression (10) is the theoretical basis of our model being absolutely general and does not depend, in principle, on the hamiltonian under consideration.

3 Thermalization: New Symmetries and Emergent Transformations

To begin with and only in order to make a concise analysis of the construction given before in [1], let us consider a Wannier exciton system. As is well known, such system of excitons is characterized by the screening of the crystal structure being well described by the following Schrödinger equation $\left(i\hbar\frac{\partial}{\partial t} - h\right)|\varphi\rangle = 0$ that can be written using new displacement operators defined as $\widetilde{D} \equiv D_{th} D_{\varphi}$, where D_{th} is the thermal unitary operator that arises as a consequence of the definition of the squeezed coherent states as transformed vacua under the automorphism group of the commutation relations, as the thermofield dynamics case [11]. Then we have

$$\widetilde{D}^{\dagger}\left(i\hbar\frac{\partial}{\partial t} - h\right)\widetilde{D}\,|0\rangle = 0 \tag{11}$$

This transformation shows specifically the group structure, namely, the fundamental symmetries underlying the physics of the system. Clearly, a Bogoliubov-like transformation arises as in the pure excitonic case [1] or by definition in the pure thermal case [11]:

$$\begin{pmatrix} \widetilde{\psi}_{\alpha}^{(e)} \\ \widetilde{\psi}_{\alpha}^{\dagger(h)} \end{pmatrix} = \begin{pmatrix} \lambda\cos\varphi + \mu^{*}\frac{\varphi_{\alpha\beta}^{*}}{\varphi}\sin\varphi e^{-\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-mt)} & \mu\cos\varphi + \lambda^{*}\frac{\varphi_{\alpha\beta}^{*}}{\varphi}\sin\varphi e^{-\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-mt)} \\ -\lambda\frac{\varphi_{\alpha\beta}}{\varphi}\sin\varphi e^{\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-mt)} + \mu^{*}\cos\varphi & \lambda^{*}\cos\varphi - \mu\frac{\varphi_{\alpha\beta}}{\varphi}\sin\varphi e^{\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-mt)} \end{pmatrix} \times \begin{pmatrix} \psi_{\alpha}^{(e)} \\ \psi_{\alpha}^{\dagger(h)} \end{pmatrix} \tag{12}$$

$$|\lambda|^2 - |\mu|^2 = 1$$

The structure of above transformation is regulated by the same Green function that defines the exciton wave function plus the coefficients λ and μ that are related with the eigenvalues of the exciton and fermion number operators of the system (N_e, N_h) given precisely the specific form of the interaction hole electron in the thermal case [12]. Introducing the transformed fields via the displacement operator into the Schrödinger equation we obtain schematically

$$\left[\psi^{\dagger(e)}\widetilde{h}^{(e)}\psi^{(e)} + \psi^{\dagger(h)}\widetilde{h}^{(h)}\psi^{(h)} + \psi^{\dagger(e)}Q\psi^{\dagger(h)} + \psi^{(h)}Q^{\dagger}\psi^{(e)}\right]|0\rangle\,, \tag{13}$$

where

$$\widetilde{h}_{\alpha\beta}^{(e)} \equiv m\delta_{\alpha\beta}\left(|\lambda|^2\sin^2\varphi + |\mu|^2\cos^2\varphi\right) - h_{\alpha\beta}\left(|\lambda|^2 + |\mu|^2\right)\cos 2\varphi$$

and

$$Q^{th}_{\alpha\beta} \equiv -\left(|\lambda|^2 + |\mu|^2 + \mu\lambda\right) \mathrm{e}^{\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x} - mt)} \left(m\delta^{\gamma}_{\alpha} - 2h^{\gamma}_{\alpha}\right) \frac{\sin(2\varphi)}{\varphi} \varphi_{\gamma\beta} \tag{14}$$

(and analogically for $\widetilde{h}^{(h)}_{\alpha\beta}$ and $Q^{\dagger}_{\alpha\beta}$). We see that expression (14) must be zero if the number of particles is conserved. Is not difficult to see that one condition is $\frac{m}{2} = n_f h$: the chemical potential m is proportional to the energy times the fermionic number of the system (the total energy considering the binding). This is an equilibrium condition. The other one gives a condition over the specific strength of the interaction electron-hole, namely: $\sin(2\varphi) = 0$ with φ being the norm of the exciton wave function defined by expression (5). Notice that both conditions are independent of the thermal properties of the system. Other condition namely $\left(|\lambda|^2 + |\mu|^2 + \mu\lambda = 0\right)$ involves the thermal properties of the system [11]. And this fact is far from being trivial due to the behaviour of the transformations (12). The concrete explanation of these conditions from the physical and mathematical point of view will be part of a separate publications, and will not be discussed here [12]. But the main points arising from expressions (11–14) are

(i) Transformations (14) control the general behaviour of the physical system,
(ii) The group dependence of the transformation changes due to the basic wave function of the exciton expression (5) that contains intrinsically the electron-hole interaction. Notice that this interaction is precisely the building block of the Green function (4) and (6).
(iii) Facts (i) and (ii) reflect the conductance properties of the material under consideration and the thermal influence.

From points (i–iii) above, the model presented here can help to understand the metal-insulator transition in the thermal case. The transition from the excitonic phase of the electron-hole system to the conducting situation must be characterized by the breaking of the pair, then this fact is immediately reflected in the changing of the transformations (12). We believe that this effect is promising to be key to the interpretation and understanding of the metal-insulator transition even in the thermal case [12].

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