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ФИЗИКА ТВЕРДОГО ТЕЛА И КОНДЕНСИРОВАННЫХ СРЕД

# BOUNDED COHERENT STATES AND EXCITONIC SYSTEMS

*D. J. Cirilo-Lombardo*

Joint Institute for Nuclear Research, Dubna

New bounded coherent states construction, based on a Keldysh conjecture, is presented. The particular group structure arising from the model leads to new symmetry transformations for the coherent states system. The emergent new symmetry transformation is reminiscent of the Bogoliubov one. This construction is applied to describe an excitonic system. We discuss how the symmetry of these transformations is intrinsically related to the stability and the behavior of the physical systems as in the excitonic case.

Представлена конструкция новых связанных когерентных состояний, основанная на гипотезе Келдыша. Особенная групповая структура, возникающая в модели, ведет к новым преобразованиям симметрии для когерентных состояний системы. Возникшая новая симметрия является аналогом симметрии Боголюбова. Найденная конструкция применена к системе экситонов. Обсуждается, каким образом эти преобразования связаны со стабильностью и поведением физических систем для случая экситонов.

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## INTRODUCTION

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 [1]. At different stages of this long history, the results of their efforts have been described and discussed in several papers and review articles. As is usually very well explained: if bosonic particles are cooled down below the temperature of quantum degeneracy, they can spontaneously form a coherent state in which individual matter waves synchronize and combine. Spontaneous coherence of matter waves forms the basis of a number of fundamental phenomena in physics, including superconductivity, superfluidity and Bose–Einstein condensation. Spontaneous coherence is the key characteristic of condensation in momentum space. Excitons — bound pairs of electrons and holes — form a model system to explore the quantum physics of cold bosons in solids. Cold exciton gases can be realized in a system of indirect excitons, which can cool down below the temperature of quantum degeneracy owing to their long lifetimes. Recently in [2] measurements of spontaneous coherence in a gas of indirect excitons were reported and it was found that spontaneous coherence of excitons emerges in the region of the macroscopically ordered exciton state and in the region of vortices of linear polarization. The coherence length in these regions is much larger than in a classical gas, indicating a coherent state with a much narrower than classical exciton distribution in momentum space, characteristic of a condensate. A pattern of extended spontaneous coherence is correlated with a pattern of spontaneous polarization, revealing the properties of a multicomponent coherent state. In this paper, we consider the theoretical treatment of the excitonic behavior by means of a new bounded coherent states construction in a quantum field theoretical context. The possibility to introduce the coherent states in a physical system of excitons is mainly based on the idea of «exciton state splitting» and «exciton wave function» introduced by L. V. Keldysh [3] earlier and will be the scope of Introduction and Sec. 1. Section 2 is devoted to introduction of the new coherent states by means of a specific displacement operator. In Sec. 3, we show how new symmetry transformations arise and how they are intrinsically related to the stability and general behavior of the physical systems as in the excitonic case. Finally, in Sec. 4 the concluding remarks and some comments on the metal-insulator transition in this new context are given.

## 1. THE EXCITON MODEL

Our starting point is based on the following splitting of the fermionic state in the material to be considered:

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

$$\psi_\alpha^{(e)}(\mathbf{x}) \equiv \sum_{j>j_0} a_j \chi_\alpha^j(\mathbf{x}), \quad \psi_\alpha^{\dagger(h)}(\mathbf{x}) \equiv \sum_{j\leqslant j_0} a_j \chi_\alpha^j(\mathbf{x}), \tag{2}$$

however

$$[a_j^\dagger, a_{j'}]_+ = \delta_{jj'}, \quad [a_j, a_{j'}]_+ = 0. \tag{3}$$

Above 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 $j \leqslant j_0$ numerate the bounded states from the electronic zone and the free states, respectively. Notice, that the above fermionic state considers effectively the real situation where the holes and electrons are one entity: they are not independent; this construction is far away to be trivial and will be one of the main cornerstones in the physical phenomena arising of this coherent-exciton model.

It is very important to remark here, that definition (1), presented for the first time by Keldysh [1], is not the standard one given traditionally in the literature: 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, construction (1) avoids all types of overcounting and spurious states that are clearly nonphysical.

Let us consider, without loose generality and only to exemplify in concrete cases, the symmetries of a periodic system (e.g., crystal) as the functions of Hartree–Fock (HF) take the form of a Bloch state

$$\chi_{j\alpha}(\mathbf{x}) = \mathrm{e}^{i\mathbf{P}\cdot\mathbf{x}} u_{\mathbf{P}l\alpha}, \tag{4}$$

where $\mathbf{P}$ is the quasi-impulse and $l$ is the number of zones, such that: $j = \{\mathbf{P}, l\}$. If the case is for a nonmetallic crystal, then the sum in $j \leqslant j_0$ corresponds to the sum over all $\mathbf{P}$ that live in the 1st Brillouin zone. The HF functions (4) obey the HF equation

$$\int h_{\alpha\beta}\left(\mathbf{x}, \mathbf{x}'\right) \chi_j^\beta(\mathbf{x}')\, d^3\mathbf{x}' = \varepsilon_j \chi_{j\alpha}(\mathbf{x}) \tag{5}$$

with

$$h_{\alpha\beta}(\mathbf{x},\mathbf{x}') = \delta_{\alpha\beta}\delta(\mathbf{x},\mathbf{x}')\left\{\frac{-\hbar^2}{2m_0}\nabla^2 - \sum \frac{Z_k e^2}{|\mathbf{R}_{n,k}-\mathbf{x}|} + \frac{e^2}{2}\int \frac{g_{\beta\beta}(\mathbf{y},\mathbf{y})\,d^3\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}\right\} - - e^2\frac{g_{\alpha\beta}(\mathbf{x},\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \qquad (6)$$

being the HF operator, where we define

$$g_{\alpha\beta}(\mathbf{x},\mathbf{x}') \equiv \sum_{j\leqslant j_0} \chi_{j\alpha}(\mathbf{x})\chi^j_\beta(\mathbf{x}'). \qquad (7)$$

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 Hamiltonian (6).

## 2. THE EXCITON WAVE EQUATION

Due to the composite characteristic of the excitonic state, firstly, we have particular interest in the two-time two-particle Green functions

$$G^{(2)}_{\alpha\beta,\gamma\delta}(\mathbf{x},\mathbf{y},t;\mathbf{x}',\mathbf{y}',t') = -\frac{i}{\hbar}\left\langle T\psi^\dagger_\alpha(\mathbf{x},t)\psi_\beta(\mathbf{y},t)\psi^\dagger_\gamma(\mathbf{x}',t')\psi_\delta(\mathbf{y}',t')\right\rangle_0, \qquad (8)$$

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

$$i\hbar G^{(2)}_{\alpha\beta,\gamma\delta}(\mathbf{x},\mathbf{y},t;\mathbf{x}',\mathbf{y}',t') = = -\sum_{\mathbf{P}J}\begin{cases}\varphi^{J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y})\varphi^{J\mathbf{P}\star}_{\gamma\delta}(\mathbf{x}',\mathbf{y}')\exp\left[\frac{i}{\hbar}\left(\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y}-\mathbf{x}'-\mathbf{y}')}{2} - E_{J\mathbf{P}}(t-t')\right)\right], & t>t',\\ \varphi^{J\mathbf{P}\star}_{\alpha\beta}(\mathbf{x},\mathbf{y})\varphi^{J\mathbf{P}}_{\gamma\delta}(\mathbf{x}',\mathbf{y}')\exp\left[\frac{-i}{\hbar}\left(\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y}-\mathbf{x}'-\mathbf{y}')}{2} - E_{J\mathbf{P}}(t-t')\right)\right], & t<t'.\end{cases} \qquad (9)$$

Here it is easily seen that

$$\exp\left[\frac{i}{\hbar}\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}\right]\varphi^{J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y}) = \left\langle 0\left|\psi^\dagger_\alpha(\mathbf{x})\psi_\beta(\mathbf{y})\right|J\mathbf{P}\right\rangle. \qquad (10)$$

Then, the above expression can be assumed as the basic wave function of the exciton[1]. Taking into account the symmetries involved, the von Karman periodic conditions are

$$\varphi^{J\mathbf{P}}_{\alpha\beta}(\mathbf{x}+\mathbf{R}_n,\mathbf{y}+\mathbf{R}_n) = \varphi^{J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y}), \qquad (11)$$

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

with $\mathbf{R}_n$ being a characteristic vector of the crystal lattice. Applying the Fourier transform to (9) in the time, we obtain

$$G^{(2)}_{\alpha\beta,\gamma\delta}(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}';\mathbf{P}E)=\sum_J \frac{2E_{J\mathbf{P}}}{E^2-(E_{J\mathbf{P}}-i\delta)^2}\varphi^{J\mathbf{P}\star}_{\alpha\beta}(\mathbf{x},\mathbf{y})\,\varphi^{J\mathbf{P}}_{\gamma\delta}(\mathbf{x}',\mathbf{y}'),\quad \delta\to+0. \tag{12}$$

Notice, that due to the free field form, these formulas are independent of the specific form of the Hamiltonian considered.

## 3. EXCITONIC COHERENT STATES CONSTRUCTION

It is well known that CS provide naturally a close connection between classical and quantum formulations of a given system [6]. 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 to the semiclassical behavior, 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 us is proposed here by means of a «displacing operator» acting over the vacuum (specific fiducial vector). The unitary operators

$$\begin{gathered}B_{J\mathbf{P}}=\frac{1}{V}\int\psi^{\alpha\dagger}(\mathbf{x})\,\varphi^{J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y})\exp\left[\frac{i}{\hbar}\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}\right]\psi^{\beta}(\mathbf{y})\,d^3\mathbf{x}\,d^3\mathbf{y},\\ B^{\dagger}_{J\mathbf{P}}=\frac{1}{V}\int\exp\left[\frac{-i}{\hbar}\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}\right]\psi^{\alpha\dagger}(\mathbf{x})\,\varphi^{\dagger J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y})\psi^{\beta}(\mathbf{y})\,d^3\mathbf{x}\,d^3\mathbf{y},\end{gathered} \tag{13}$$

where

$$\varphi^{\dagger J\mathbf{P}}_{\alpha\beta}(\mathbf{x},\mathbf{y})=\left[\varphi^{J\mathbf{P}}_{\beta\alpha}(\mathbf{y},\mathbf{x})\right]^{\star}\quad (V=\text{ normalized volume}), \tag{14}$$

and the commutation relations take the following form:

$$\begin{aligned}&[B_{J\mathbf{P}},B^{\dagger}_{J'\mathbf{P}'}]=\delta_{JJ'}\delta_{\mathbf{P}\mathbf{P}'}-\\ &-\left\{\frac{1}{V}\int\psi^{\alpha\dagger(e)}(\mathbf{x})\exp\left(\frac{i}{2\hbar}\mathbf{P}\cdot\mathbf{x}\right)\varphi^{J\mathbf{P}}_{\alpha\gamma}(\mathbf{x},\mathbf{z})\exp\left[\frac{-i}{2\hbar}(\mathbf{P}-\mathbf{P}')\cdot\mathbf{z}\right]\times\right.\\ &\times\varphi^{\dagger J'\mathbf{P}'}_{\gamma\beta}(\mathbf{z},\mathbf{y})\exp\left(\frac{-i}{2\hbar}\mathbf{P}'\cdot\mathbf{y}\right)\psi^{\beta(e)}(\mathbf{y})+\frac{1}{V}\int\psi^{\alpha\dagger(h)}(\mathbf{x})\exp\left(\frac{-i}{2\hbar}\mathbf{P}'\cdot\mathbf{y}\right)\times\\ &\left.\times\varphi^{\dagger J'\mathbf{P}'}_{\gamma\beta}(\mathbf{y},\mathbf{z})\exp\left[\frac{-i}{2\hbar}(\mathbf{P}-\mathbf{P}')\cdot\mathbf{z}\right]\varphi^{J\mathbf{P}}_{\alpha\gamma}(\mathbf{z},\mathbf{x})\exp\left(\frac{i}{2\hbar}\mathbf{P}\cdot\mathbf{x}\right)\psi^{\beta(h)}(\mathbf{y})\right\}d^3\mathbf{x}\,d^3\mathbf{y}\,d^3\mathbf{z},\end{aligned} \tag{15}$$

indicating exactly the intrincated interplay in the electron–hole system (notice the lack of canonicity). In spite of the complexity of expression (15), we take advantage of the unitarity of $B_{J\mathbf{P}}$ (13) constructing the coherent states as

$$|\beta,J\mathbf{P}\rangle=\exp\left\{\beta B^{\dagger}_{J\mathbf{P}}\,\mathrm{e}^{iE_{J\mathbf{P}}t/\hbar}-\beta^{\star}B_{J\mathbf{P}}\,\mathrm{e}^{-iE_{J\mathbf{P}}t/\hbar}\right\}|0\rangle\equiv|\varphi\rangle\,, \tag{16}$$

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

$$D_\varphi = \exp\left[\int \psi^{\alpha\dagger(e)}(\mathbf{x})\,\varphi_{\alpha\beta}(\mathbf{x},\mathbf{y})\exp\left[\frac{-i}{\hbar}\left(\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}-\mu t\right)\right]\psi^{\beta\dagger(h)}(\mathbf{x}) - \right.$$
$$\left. -\psi^{\alpha(h)}(\mathbf{x})\varphi^\star_{\alpha\beta}(\mathbf{x},\mathbf{y})\exp\left[\frac{-i}{\hbar}\left(\frac{\mathbf{P}\cdot(\mathbf{x}+\mathbf{y})}{2}-\mu t\right)\right]\psi^{\beta(e)}(\mathbf{x})\right] d^3\mathbf{x}\,d^3\mathbf{y}. \quad (17)$$

Expression (17) is the theoretical basis of our model and will be specifically proved and compared with other approaches in future works. As before, we remark that this construction is absolutely general and does not depend, in principle, on the Hamiltonian under consideration. This fact is very important because the model presented here is not restricted to a specific physical system or physical problem [5].

## 4. COHERENT STATES IN ACTION: NEW SYMMETRIES AND EMERGENT BOGOLIUBOV-LIKE TRANSFORMATIONS

To begin with and only in order to make a concise analysis of the construction given before, let us consider a Wannier excitonic system. As is well known, such a system of excitons is characterized by the screening of the crystal structure being well described by the following Schroedinger equation:

$$\left(i\hbar\frac{\partial}{\partial t}-h\right)|\varphi\rangle = 0. \quad (18)$$

Expression (18) can be written (using operators $D$) as

$$D_{\varphi^\dagger}\left(i\hbar\frac{\partial}{\partial t}-h\right)D_\varphi\,|0\rangle = 0. \quad (19)$$

The next, and very important step, is to see the action of the displacement operator over the states:

$$\psi_\alpha(\mathbf{x}) \equiv \psi_\alpha^{(e)}(\mathbf{x}) + \psi_\alpha^{\dagger(h)}(\mathbf{x}) \Rightarrow \widetilde{\psi}_\alpha(\mathbf{x}) \equiv \widetilde{\psi}_\alpha^{(e)}(\mathbf{x}) + \widetilde{\psi}_\alpha^{\dagger(h)}(\mathbf{x}), \quad (20)$$

$$D_\varphi^\dagger\psi_\alpha^{(e)}(\mathbf{x})D_\varphi \to \widetilde{\psi}_\alpha^{(e)}(\mathbf{x}) \equiv \psi_\alpha^{(e)}(\mathbf{x})\cos\varphi + \varphi_{\alpha\beta}\psi^{\dagger\beta(h)}(\mathbf{x})\frac{\sin\varphi}{\varphi}\exp\left[\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-\mu t)\right],$$
$$D_\varphi^\dagger\psi_\alpha^{\dagger(h)}(\mathbf{x})D_\varphi \to \widetilde{\psi}_\alpha^{\dagger(h)}(\mathbf{x}) \equiv \psi_\alpha^{\dagger(h)}(\mathbf{x})\cos\varphi - \psi^{\beta(e)}(\mathbf{x})\,\varphi_{\alpha\beta}\psi^{\dagger\beta(h)}(\mathbf{x})\frac{\sin\varphi}{\varphi}\times$$
$$\times\exp\left[\frac{-i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-\mu t)\right]. \quad (21)$$

This transformation shows specifically the group structure, namely, the fundamental symmetries underlying the physics of the system. Clearly a Bogoliubov-like transformation arises

$$\begin{pmatrix} \widetilde{\psi}_{\alpha}^{(e)}(\mathbf{x}) \\ \widetilde{\psi}_{\alpha}^{\dagger(h)}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \cos\varphi & \dfrac{\varphi_{\alpha\beta}}{\varphi}\sin\varphi\exp\left[\dfrac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-\mu t)\right] \\ -\dfrac{\varphi_{\alpha\beta}}{\varphi}\sin\varphi\exp\left[\dfrac{-i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-\mu t)\right] & \cos\varphi \end{pmatrix} \times \\ \times \begin{pmatrix} \psi_{\alpha}^{(e)}(\mathbf{x}) \\ \psi_{\alpha}^{\dagger(h)}(\mathbf{x}) \end{pmatrix}. \quad (22)$$

The structure of the above transformation is regulated (see expression (10)) by the same Green function that defines the exciton wave function, given precisely in the specific form of the electron–hole interaction. Introducing the transformed fields via the displacement operator into the Schroedinger equation, we obtain schematically

$$\left[\psi^{\dagger(e)}\widetilde{h}^{(e)}\psi^{(e)} + \psi^{\dagger(h)}\widetilde{h}^{(h)}\psi^{(h)} + \psi^{\dagger(e)}Q\psi^{\dagger(h)} + \psi^{(h)}Q^{\dagger}\psi^{(e)}\right]|0\rangle\,, \quad (23)$$

where

$$\widetilde{h}_{\alpha\beta}^{(e)} \equiv \mu\delta_{\alpha\beta}\sin^2\varphi - h_{\alpha\beta}\cos 2\varphi$$

and

$$Q_{\alpha\beta} \equiv \exp\left[\frac{i}{\hbar}(\mathbf{P}\cdot\mathbf{x}-\mu t)\right](\mu\delta_{\alpha}^{\gamma} - 2h_{\alpha}^{\gamma})\frac{\sin(2\varphi)}{\varphi}\varphi_{\gamma\beta} \quad (24)$$

(and analogically for $\widetilde{h}_{\alpha\beta}^{(h)}$ and $Q_{\alpha\beta}^{\dagger}$). We see that expression (24) must be zero if the number of particles is conserved. It is not difficult to see that one condition is $\mu/2 = n_f h$: the chemical potential is proportional to the energy times of 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 electron–hole interaction, namely: $\sin(2\varphi) = 0$ with $\varphi$ being the norm of the exciton wave function defined by expression (10). And this fact is far to be trivial due to the behavior of transformations (21). The concrete explanation of these conditions from the physical and mathematical points of view will be a part of separate publications, and will not be discussed here [4, 5]. But the main points arising from expressions (20)–(22) are:

i) transformations (22) control the general behavior of the physical system;

ii) the group dependence of the transformation changes due to the basic wave function of exciton expression (11), that contains intrinsically the electron–hole interaction. Notice, that this interaction is precisely the building block of the Green function (9) and (12);

iii) facts i) and ii) reflect the conductance properties of the material under consideration.

From points i–iii) above, the model presented here can help to understand the metal insulator transition. 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 transformations (22). We believe that this effect is promising to be the key to the interpretation and understanding of the metal-insulator transition.

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