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Trions in first and second quantizations

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Abstract. We reconsider the semiconductor trions from scratch. We first determine the very many "reasonable" ways to write the trions in first quantization. We then select the forms which are easy to relate to physical pictures. In a second part, we derive the corresponding creation operators in second quantization. We pay particular attention to the expression of the X^- trion in terms of exciton and free-electron, as it is the one adapted to future works on many-body effects with trions.

PACS. 71.35.-y Excitons and related phenomena

In semiconductor physics, we call X^- trions [1-7] the bound states of two electrons and one hole, so that these X^- trions may be seen as the bound states of one exciton and one electron. In a similar way, the X^+ trions are the bound states of two holes and one electron, so that they can be seen as an exciton with a hole bound to it. Except for their effective masses and dielectric constant, these trions are essentially the same as the H^- or H_2^+ ions studied long ago in atomic physics. Due to the extremely high experimental accuracy usually reached in this field, various very elaborate numerical methods [8] have been developed to obtain the bound states energies of these H^- or H_2^+ ions with up to 10 digits, an amazing — and useless — precision in solid state physics.

Although their existence was predicted for a long time [1], clear experimental evidences of X^- or X^+ trions in semiconductors have been obtained recently only [9–12]: Due to their very small binding energies in bulk materials, the X^- trions are in fact dissociated into electron and exciton in usual experimental conditions. The development of good semiconductor quantum wells made however possible the observation of these trions, as the reduction of dimensionality enhances the absolute values of all binding energies. In more recent experiments, the interaction of these trions with carriers has been studied in highly doped materials [13–15], and the observed phenomenon has been associated to the excitonic Fermi edge singularities predicted long ago [16].

To our opinion, a clean treatment of this last problem is extremely difficult and the full answer not yet given. With this goal in mind, the present paper constitutes the first step towards a new approach to this problem, the trion being inserted in the more general framework of an exciton interacting with other carriers.

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In recent works [17–19], we have studied the simplest of these problems, namely the interaction of an exciton with an electron gas located in a distant metal. We predicted changes of the exciton absorption lines when this exciton is created close to a metal. These changes, which include shifts, asymmetric broadenings and splittings, have similarities with Fermi edge singularities. They come from the *sudden* Coulomb interactions between the electron and hole of the photocreated exciton and the various electrons of the metal, these electrons being distinguishable from the electron of the exciton as they are spacially separated.

The problem is much more complex when the electron of the photocreated exciton and the electrons already present are indistinguishable, which is what happens when we study the interactions between various excitons or between one exciton and a sea of electrons around it, as for a trion in doped materials. The major difficulty comes from the indistinguishability of the carriers, and its straightforward consequence that there are *a priori* various ways to choose the electron possibly bound to the hole to make the exciton. Up to now, it has been commonly accepted that, in order to include this indistinguishability, which is at the origin of the close-to-boson character of the excitons, it is enough to dress the Coulomb interaction by so-called exchange processes [20]. However this idea, at the origin of all bosonisation procedures [21] which tend to replace the exact semiconductor Hamiltonian by an effective Hamiltonian for boson-excitons, fails to produce purely fermionic contributions. These terms have to exist independently from any Coulomb process. A very intuitive way to grasp this point is to say that excitons interact because they "feel" each other. The existence of Coulomb forces is of course an obvious way for two excitons to feel each other. A less obvious one is Pauli exclusion: the two electrons of two excitons having to be in different states, this induces an "interaction" between excitons, which has to appear, even in the absence of any Coulomb force. This Pauli way for two excitons to "feel" each other is the extremely tricky part of all problems dealing with interacting excitons. In recent works [22,23], we have shown that the effective exciton-exciton scattering found 30 years ago and reported by everyone up to now [20], cannot be correct because it induces an effective boson-exciton Hamiltonian which is not hermitian. Very recently, we have even shown [24] that the concept of effective Hamiltonian itself has to be abandoned because, whatever the exciton-exciton scattering is, it cannot reproduce the X-X correlations correctly.

In the exciton-exciton interaction, Pauli exclusion between electrons and Pauli exclusion between holes both enter. In view of the complexity of the consequences of these Pauli exclusions, which are at the origin of all the incorrect results published in the literature on interacting excitons, it may appear as reasonable to study the simplest situation first, namely one exciton interacting with N other electrons, as only Pauli exclusion between electrons have then to play a rôle. Inside this type of problems, the case $N = 1$ is clearly the simplest one. This is just the trion problem: We only have three particles with Coulomb interactions between them. The problems linked to the indistinguishability of the two electrons nevertheless exist in the trion and have to be handled properly.

The purpose of this paper is not to find a new way to derive precise values of the trion binding energy: The wide literature of atomic physics already provides much more accuracy than needed in any precise semiconductor experiment. However, as most of these works have in mind a fast numerical convergence in the resolution of the trion Schrödinger equation, their approaches to the trion problem cannot be extended to the interactions of a trion with other carriers. As an example, in his pioneer work [1], Hylleraas uses an expansion in terms of the three parameters $u = |\mathbf{r}_e - \mathbf{r}_{e'}|$, $s = |\mathbf{r}_e| + |\mathbf{r}_{e'}|$ and $t = |\mathbf{r}_e| - |\mathbf{r}_{e'}|$; the two last ones are obviously hard to relate to any meaningful quantity and, far worse, to extend to problems with one hole plus three, four, five... electrons.

What we want to do here, is to provide tools for the extension of the trion problem to more complex situations. We have in fact in mind to do for trions something similar to what has been done for excitons: Beside the determination of the exciton eigenstates through the resolution of the hydrogen-like Schrödinger equation, which can be analytical in this case, as it reads in terms of hypergeometric functions [25], the excitons have been shown to be specific linear combinations of electrons and holes.This view of an exciton turns out to be the convenient one for many-body effects involving excitons, mostly when this linear combination is written in second quantization.

The trion is actually far more complex than the exciton. In addition to the fact that the trion eigenstates are not analytically known, the trion has an intrinsic difficulty which comes from the fact that there are very many possible ways to represent it as shown below. This leaves a certain freedom in choosing the "best" approaches to a given problem on trions. In order to settle future works with interacting trions on solid grounds, it appeared to us quite useful to reconsider the trion problem from scratch.

Section 1 deals with the X^- trion in first quantization. We show that there are *a priori* various "good" ways to choose the three spatial coordinates of the trion. Surprisingly enough, the most symmetrical one with respect to the two electrons turns out to be a very bad choice for physical understanding. We also pay particular attention to the consequences of the symmetry condition induced by Pauli exclusion between the two electrons, and we show that, depending on the chosen set of coordinates, some of them are physically totally obscure.

In Section 2, we derive the trion creation operators in second quantization. Here again, various creation operators are possible. We give two possible expressions for these trion operators in terms of two electrons and one hole, and two expressions of these operators in terms of one exciton and one electron. These last representations are in fact the convenient ones to study one trion in doped materials, as they relate this problem to the more general one of an exciton in the presence of other carriers, with Pauli exclusion between them (and all the complexities associated to it). We also show that the invariance conditions coming from the symmetry of the trion wave function, which appeared as totally obscure in first quantization, simply correspond to have the prefactors of these linear combinations invariant under the anticommutation of the two electron operators, as expected for fermions.

This paper is rather formal as its goal is to settle firm basis for future works on interacting trions. The space dimension remains undefined, the equations being valid for bulk semiconductors as well as quantum wells, the carrier or exciton momenta being 3D vectors for bulk and 2D vectors for quantum wells, while the exciton relative motion index ν is a 3-component index for bulk and a 2-component index for quantum wells.

The level of approximations used in this work on trions is the one which leads to write the exciton Hamiltonian as

$$H = \frac{\mathbf{p}_e^2}{2m_e} + \frac{\mathbf{p}_h^2}{2m_h} - \frac{e^2}{r_{eh}} \cdot \tag{1}$$

It in particular neglects all the complexities of the valence band by assuming one hole mass only. This is *a priori* valid for narrow quantum wells as the heavy and light hole bands are usually well separated in energy by the confinement. On the opposite, this is more questionable for bulk materials. However, the introduction of heavy and light holes goes with the introduction of a non-diagonal Coulomb interaction between them [26], which makes all many-body effects far more complex. The Hamiltonian (1) also neglects "electron-hole exchange", *i.e.*, the possible Coulomb scatterings between the valence and the conduction bands: The electrons and the holes are thus assumed to be unrelated species. This electron-hole exchange is known to have a small effect on excitons, as it induces a splitting of the degenerate exciton level, since it differentiates the exciton with spin such that this electron-hole exchange is possible from the other one. The introduction of electron-hole exchange in the trion problem is far beyond the scope of this preliminary work.

1 The X^- trion in first quantization

1.1 The various "reasonable" choices of carrier coordinates

In first quantization, the X^- trion wave function can be divided into an orbital part and a spin part. The orbital part is eigenfunction of the semiconductor Hamiltonian which depends on the positions of the two electrons and the hole. They can appear either as $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$ or as three linear combinations of these quantities. In terms of $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$, the equivalent of the exciton Hamiltonian given in equation (1) reads

$$H = \frac{\mathbf{p}^2_{\mathbf{r}_e}}{2m_e} + \frac{\mathbf{p}^2_{\mathbf{r}_{e'}}}{2m_e} + \frac{\mathbf{p}^2_{\mathbf{r}_h}}{2m_h} + \frac{e^2}{|\mathbf{r}_e - \mathbf{r}_{e'}|} - \frac{e^2}{|\mathbf{r}_e - \mathbf{r}_h|} - \frac{e^2}{|\mathbf{r}_{e'} - \mathbf{r}_h|}. \tag{2}$$

Being invariant under $(\mathbf{r}_e \leftrightarrow \mathbf{r}_{e'})$, the eigenfunctions of this Hamiltonian have a given parity with respect to the $(\mathbf{r}_e \leftrightarrow \mathbf{r}_{e'})$ interchange. However, as the electrons are fermions, the total trion wave functions must be antisymmetrical with respect to the $(e \leftrightarrow e')$ interchange. It is thus appropriate to have appearing in the spin part, the total electron spin $(S = 1, S_z = 0, \pm 1)$ or $(S = 0 = S_z)$ instead of the individual spins $(s_e = \pm 1/2, s_{e'} = \pm 1/2)$, as the triplet is symmetrical with respect to the $(e \leftrightarrow e')$ interchange while the singlet is antisymmetrical. Consequently we are led to write the trion wave function as

$$\Psi^{(i)}(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)|S_i, S_{iz}\rangle \otimes |m_i\rangle, \tag{3}$$

where m_i is the hole kinetic momentum. For quantum wells in which only the heavy band plays a role, $m_i = \pm 3/2$, while for bulk materials, $m_i = \pm 3/2, \pm 1/2$. The orbital part then verifies

$$H\Psi^{(i)} = \mathcal{E}_i \Psi^{(i)}, \tag{4}$$

the symmetry imposed by Pauli exclusion leading to

$$\Psi^{(i)}(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h) = (-1)^{S_i} \Psi^{(i)}(\mathbf{r}_{e'}, \mathbf{r}_e, \mathbf{r}_h). \tag{5}$$

a) **Carrier coordinates** $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$

In order to solve the Schrödinger equation (4), the most simple-minded idea is to expand the H eigenfunctions on the plane wave basis for $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$ functions, namely

$$\Psi^{(i)}(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h) = \sum_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h} \bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_e \cdot \mathbf{r}_e}}{\sqrt{\mathcal{V}}} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_{e'} \cdot \mathbf{r}_{e'}}}{\sqrt{\mathcal{V}}} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_h \cdot \mathbf{r}_h}}{\sqrt{\mathcal{V}}}, \tag{6}$$

where $\mathcal{V}$ is the sample volume. If we insert this expansion into equation (4), we find that the $\bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h}$'s verify

$$\begin{aligned} 0 = {} & [\epsilon_e(\mathbf{k}_e) + \epsilon_e(\mathbf{k}_{e'}) + \epsilon_h(\mathbf{k}_h) - \mathcal{E}_i] \bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h} \\ & + \sum_{\mathbf{q}} V_{\mathbf{q}} \Bigg(\bar{\Psi}^{(i)}_{\mathbf{k}_e + \mathbf{q}, \mathbf{k}_{e'} - \mathbf{q}, \mathbf{k}_h} \\ & - \bar{\Psi}^{(i)}_{\mathbf{k}_e + \mathbf{q}, \mathbf{k}_{e'}, \mathbf{k}_h - \mathbf{q}} - \bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'} + \mathbf{q}, \mathbf{k}_h - \mathbf{q}} \Bigg), \end{aligned} \tag{7}$$

where we have set $\epsilon_{e,h}(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m_{e,h}}$. The three terms of the sum over $\mathbf{q}$ correspond to the Coulomb interactions between the three carriers. The $\bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h}$'s which have the symmetry property imposed by Pauli exclusion (Eq. (5)), are such that

$$\bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h} = (-1)^{S_i} \bar{\Psi}^{(i)}_{\mathbf{k}_{e'}, \mathbf{k}_e, \mathbf{k}_h}, \tag{8}$$

while they should be such that

$$\sum_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h} \left| \bar{\Psi}^{(i)}_{\mathbf{k}_e, \mathbf{k}_{e'}, \mathbf{k}_h} \right|^2 = 1, \tag{9}$$

for the wave function $\Psi^{(i)}(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$ to be normalized.

b) **Introduction of the trion center of mass $\mathbf{R}_t$**

It is however physically obvious that the $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$ variables are not the good variables of the trion problem: The trion center of mass,

$$\mathbf{R}_t = \frac{m_e \mathbf{r}_e + m_e \mathbf{r}_{e'} + m_h \mathbf{r}_h}{2m_e + m_h}, \tag{10}$$

is surely playing an important rôle. In order to make this $\mathbf{R}_t$ coordinate appearing, we must replace the three coordinates $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$ of the trion carriers by three other coordinates $(\mathbf{R}_t, \mathbf{r}_1, \mathbf{r}_2)$ which have to fulfil certain relations, given below in equations (12, 14), in order to be "good" coordinates. Let us write these two new coordinates as

$$\begin{aligned} \mathbf{r}_1 &= a\mathbf{r}_e + a'\mathbf{r}_{e'} + a''\mathbf{r}_h \\ \mathbf{r}_2 &= b\mathbf{r}_e + b'\mathbf{r}_{e'} + b''\mathbf{r}_h . \end{aligned} \tag{11}$$

By enforcing the center of mass momentum operator,

$$\mathbf{P}_{\mathbf{R}_t} = (2m_e + m_h)\dot{\mathbf{R}}_t = \mathbf{p}_{\mathbf{r}_e} + \mathbf{p}_{\mathbf{r}_{e'}} + \mathbf{p}_{\mathbf{r}_h},$$

to commute with $\mathbf{r}_1$ and $\mathbf{r}_2$,

$$[\mathbf{r}_1, \mathbf{P}_{\mathbf{R}_t}] = [\mathbf{r}_2, \mathbf{P}_{\mathbf{R}_t}] = 0, \tag{12}$$

we get

$$a + a' + a'' = 0 = b + b' + b'' . \tag{13}$$

If, in addition, we enforce the momentum operators associated to $\mathbf{r}_1$ and $\mathbf{r}_2$, namely $\mathbf{p}_{\mathbf{r}_1} = \mu_1 \dot{\mathbf{r}}_1$ and $\mathbf{p}_{\mathbf{r}_2} = \mu_2 \dot{\mathbf{r}}_2$ (with the effective masses μ_1 and μ_2 yet undefined) to be such that

$$[\mathbf{r}_1, \mathbf{p}_{\mathbf{r}_2}] = [\mathbf{r}_2, \mathbf{p}_{\mathbf{r}_1}] = 0, \tag{14}$$

we get another relation

$$\frac{ab + a'b'}{m_e} + \frac{(a + a')(b + b')}{m_h} = 0\ . \qquad (15)$$

Note that this relation is independent of the masses μ_1 and μ_2 chosen to define $\mathbf{p}_{\mathbf{r}_1}$ and $\mathbf{p}_{\mathbf{r}_2}$. With equations (13) and (15), there are still very many ways to choose the two coordinates $(\mathbf{r}_1, \mathbf{r}_2)$.

c) **A choice of coordinates symmetrical with respect to** $(e \leftrightarrow e')$

In view of the symmetry property of the wave function, equation (5), we may think appropriate to use for the two new coordinates, quantities in which $(\mathbf{r}_e, \mathbf{r}_{e'})$ play similar rôles [27]. This leads to use $\mathbf{r}_\pm$ defined as

$$\mathbf{r}_\pm = \frac{1 \pm \eta}{2}(\mathbf{r}_e - \mathbf{r}_h) + \frac{1 \mp \eta}{2}(\mathbf{r}_{e'} - \mathbf{r}_h). \qquad (16)$$

In order to fulfil the conditions (13, 15) between the components of $(\mathbf{r}_+, \mathbf{r}_-)$, we find that the parameter η must be equal to $[(2m_e + m_h)/m_h]^{1/2}$.

Although this symmetrical choice may be appealing at first, it is hard to give any physical meaning to η. Moreover, these variables $\mathbf{r}_\pm$ are also hard to extend to the problem of a trion interacting with an electron gas (*i.e.* one hole and N electrons), problem we have in mind as a future extension of this work.

d) **Choice of coordinates appropriate to physical understanding**

On that respect, the coordinates which are easy to understand physically, and which turn out to be quite appropriate for the formulation of the interaction of a trion with other electrons, correspond to take $a' = 0$ (or $b' = 0$). By choosing $a = 1$, which is just a rescaling of $\mathbf{r}$, the coordinates $(\mathbf{r}_1, \mathbf{r}_2)$ which fulfil equations (13) and (15) are either $(\mathbf{r}, \mathbf{u}')$ or $(\mathbf{r}', \mathbf{u})$ with [28]

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_e - \mathbf{r}_h \\ \mathbf{u}' &= \mathbf{r}_{e'} - \frac{m_e \mathbf{r}_e + m_h \mathbf{r}_h}{m_e + m_h}, \end{aligned} \qquad (17)$$

$(\mathbf{r}', \mathbf{u})$ being obtained from equation (17) by interchanging $\mathbf{r}_e$ and $\mathbf{r}_{e'}$. Note that, by choosing $a = 1$, these new coordinates are such that $\mathrm{d}\mathbf{r}_e\, \mathrm{d}\mathbf{r}_{e'}\, \mathrm{d}\mathbf{r}_h = \mathrm{d}\mathbf{R}_t\, \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{u}'$.

For physical understanding, we can note that $\mathbf{r}$ is the distance between (e, h) while $\mathbf{u}'$ is the distance between e' and the center of mass of (e, h) (see Fig. 1). In terms of $(\mathbf{r}, \mathbf{u}')$, the two other distances between the X^- carriers are

$$\begin{aligned} \mathbf{r}_{e'} - \mathbf{r}_e &= \mathbf{u}' - \alpha_h \mathbf{r} \\ \mathbf{r}_{e'} - \mathbf{r}_h &= \mathbf{u}' + \alpha_e \mathbf{r} = \mathbf{r}'\ , \end{aligned} \qquad (18)$$

with $\alpha_{e,h} = m_{e,h}/(m_e + m_h)$. In the following, it will be useful to note that the two couples of coordinates $(\mathbf{r}, \mathbf{u}')$ and $(\mathbf{r}', \mathbf{u})$ are related by

$$\begin{aligned} \mathbf{r}' &= \mathbf{u}' + \alpha_e \mathbf{r} \\ \mathbf{u} &= \mathbf{r} - \alpha_e(\mathbf{u}' + \alpha_e \mathbf{r})\ , \end{aligned} \qquad (19)$$

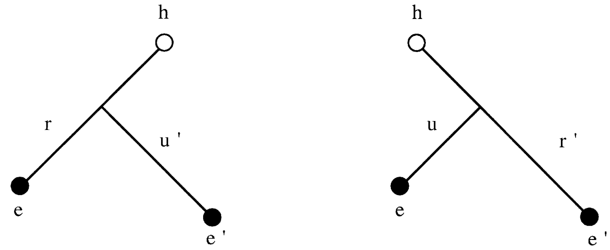

Fig. 1. The trion variables $(\mathbf{r}, \mathbf{u}')$ and $(\mathbf{r}', \mathbf{u})$ as defined in equation (17). $\mathbf{r}$ is the distance between e and h, while $\mathbf{u}'$ is the distance between e' and the center of mass of (e, h).

while $(\mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h)$ read in terms of $(\mathbf{R}_t, \mathbf{r}, \mathbf{u}')$ as

$$\begin{aligned} \mathbf{r}_e &= \mathbf{R}_t + \alpha_h \mathbf{r} - \beta_e \mathbf{u}' \\ \mathbf{r}_{e'} &= \mathbf{R}_t + \beta_x \mathbf{u}' \\ \mathbf{r}_h &= \mathbf{R}_t - \alpha_e \mathbf{r} - \beta_e \mathbf{u}'\ , \end{aligned} \qquad (20)$$

where $\beta_{e,h} = m_{e,h}/(2m_e + m_h)$ and $\beta_x = (m_e + m_h)/(2m_e + m_h)$. For physical understanding, we can note that, as α_e and α_h are the reduced electron and hole masses of the exciton, β_e and β_h are the reduced electron and hole masses of the trion, while β_x is the reduced exciton mass.

The masses associated to the $(\mathbf{r}, \mathbf{u}')$ coordinates, and which enter the definition of the momenta $\mathbf{p}_\mathbf{r}$ and $\mathbf{p}_{\mathbf{u}'}$, can be obtained by enforcing

$$[\mathbf{r}, \mathbf{p}_\mathbf{r}] = [\mathbf{u}', \mathbf{p}_{\mathbf{u}'}] = \mathrm{i}\hbar. \qquad (21)$$

This gives for the mass associated to $\mathbf{r}$, the mass of the (e, h) relative motion, namely

$$\frac{1}{\mu_x} = \frac{1}{m_e} + \frac{1}{m_h}\cdot \qquad (22)$$

It is just the exciton relative motion mass. In a similar way, the mass associated to $\mathbf{u}'$ is nothing but the mass for the relative motion of the electron e' and the center of mass of the (e, h) pair, namely

$$\frac{1}{\mu_t} = \frac{1}{m_e} + \frac{1}{m_e + m_h}\cdot \qquad (23)$$

It is thus the trion relative motion mas.

It is then easy to check that the H Hamiltonian given in equation (2) can be rewritten in terms of these new coordinates as

$$H = \frac{\mathbf{P}^2_{\mathbf{R}_t}}{2(2m_e + m_h)} + h_{\mathbf{r},\mathbf{u}'} = \frac{\mathbf{P}^2_{\mathbf{R}_t}}{2(2m_e + m_h)} + h_{\mathbf{r}',\mathbf{u}}\cdot \qquad (24)$$

The quantity $h_{\mathbf{r},\mathbf{u}'}$ appears as the Hamiltonian for the X^- trion relative motion. It precisely reads

$$h_{\mathbf{r},\mathbf{u}'} = h_\mathbf{r} + \frac{\mathbf{p}^2_{\mathbf{u}'}}{2\mu_t} + v(\mathbf{r}, \mathbf{u}'), \qquad (25)$$

where $h_\mathbf{r}$ is the relative motion Hamiltonian of the (e, h) exciton,

$$h_\mathbf{r} = \frac{\mathbf{p}^2_\mathbf{r}}{2\mu_x} - \frac{e^2}{r}, \qquad (26)$$

while $v(\mathbf{r},\mathbf{u}')$ is nothing but the Coulomb interaction between the e' electron and the (e,h) pair (see Eq. (18)),

$$v(\mathbf{r},\mathbf{u}')=\frac{e^2}{|\mathbf{u}'-\alpha_h\mathbf{r}|}-\frac{e^2}{|\mathbf{u}'+\alpha_e\mathbf{r}|}\cdot \tag{27}$$

Note that, by enforcing "good" coordinates, through the commutation rules given in equations (12, 14), we have no crossed kinetic terms in $\mathbf{p}.\mathbf{p}'$, as found in some papers on trions.

1.2 Trion relative motion

In view of the X^- trion Hamiltonian given in equation (24), we are led to isolate the center of mass motion and write the trion wave function as

$$\Psi^{(i)}(\mathbf{r}_e,\mathbf{r}_{e'},\mathbf{r}_h)=\frac{\mathrm{e}^{\mathrm{i}\mathbf{K}_i\cdot\mathbf{R}_t}}{\sqrt{\mathcal{V}}}\,\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}'), \tag{28}$$

with $\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')$ solution of

$$(h_{\mathbf{r},\mathbf{u}'}-\varepsilon_{\eta_i})\,\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')=0, \tag{29}$$

the energy ε_{η_i} being the trion relative motion energy,

$$\mathcal{E}_i=\varepsilon_{\eta_i}+\frac{\hbar^2\mathbf{K}_i^2}{2(2m_e+m_h)}\cdot \tag{30}$$

In the following, the trion index (i) will stand for $(\eta_i,\mathbf{K}_i)$. Within these variables, the symmetry of the wave function with respect to $(\mathbf{r}_e\leftrightarrow\mathbf{r}_{e'})$ imposes

$$\begin{aligned}\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')&=(-1)^{S_i}\Phi^{(\eta_i)}(\mathbf{r}',\mathbf{u})\\&=(-1)^{S_i}\Phi^{(\eta_i)}(\mathbf{u}'+\alpha_e\mathbf{r},\mathbf{r}-\alpha_e(\mathbf{u}'+\alpha_e\mathbf{r})),\end{aligned} \tag{31}$$

which follows from equation (19). While easy to derive, the above invariance would be hard to guess!

a) **The most naïve trion relative motion wave function**

In order to determine the $\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')$'s solutions of equation (29), the first idea can be to expand them on a plane wave basis for $(\mathbf{r},\mathbf{u}')$ functions. This leads to write $\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')$ as

$$\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')=\sum_{\mathbf{k},\mathbf{p}}\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}\,\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\mathcal{V}}}\,\frac{\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{u}'}}{\sqrt{\mathcal{V}}}, \tag{32}$$

see Figure 2b. By inserting this expansion into the Schrödinger equation (29), we find that the $\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}$'s must verify

$$\begin{aligned}0=&\left(\frac{\hbar^2\mathbf{k}^2}{2\mu_x}+\frac{\hbar^2\mathbf{p}^2}{2\mu_t}-\varepsilon_{\eta_i}\right)\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}\\&+\sum_{\mathbf{q}}V_{\mathbf{q}}\left(\bar{\Phi}^{(\eta_i)}_{\mathbf{k}-\alpha_h\mathbf{q},\mathbf{p}+\mathbf{q}}-\bar{\Phi}^{(\eta_i)}_{\mathbf{k}+\alpha_e\mathbf{q},\mathbf{p}+\mathbf{q}}-\bar{\Phi}^{(\eta_i)}_{\mathbf{k}+\mathbf{q},\mathbf{p}}\right),\end{aligned} \tag{33}$$

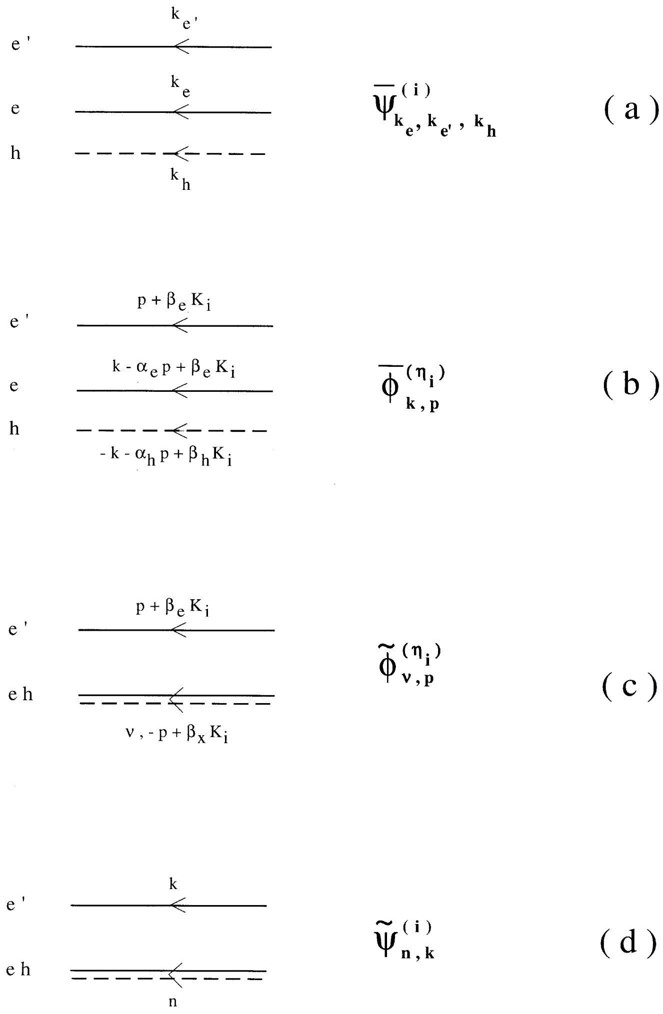

Fig. 2. Some possible representations of the trions in terms of two electrons and one hole ((a) and (b)), or in terms of one electron and one exciton ((c) and (d)).

the three terms of the sum over $\mathbf{q}$ coming from the (e,e'), (e,h) and (e',h) Coulomb interactions.

Due to equation (19), we have

$$\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}\,\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{u}}=\mathrm{e}^{\mathrm{i}(\mathbf{p}+\alpha_e(\mathbf{k}-\alpha_e\mathbf{p}))\cdot\mathbf{r}}\,\mathrm{e}^{\mathrm{i}(\mathbf{k}-\alpha_e\mathbf{p})\cdot\mathbf{u}'}, \tag{34}$$

so that the symmetry condition on $(\mathbf{r},\mathbf{u}')\leftrightarrow(\mathbf{r}',\mathbf{u})$ resulting from Pauli exclusion, as given in equation (31), imposes

$$\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}=(-1)^{S_i}\bar{\Phi}^{(\eta_i)}_{\mathbf{p}+\alpha_e(\mathbf{k}-\alpha_e\mathbf{p}),\mathbf{k}-\alpha_e\mathbf{p}}\,. \tag{35}$$

By comparing equation (6) with equation (28, 32), we can relate $\bar{\Phi}^{(\eta_i)}$ to $\bar{\Psi}^{(i)}$ through

$$\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}=\bar{\Psi}^{(i)}_{\mathbf{k}-\alpha_e\mathbf{p}+\beta_e\mathbf{K}_i,\mathbf{p}+\beta_e\mathbf{K}_i,-\mathbf{k}-\alpha_h\mathbf{p}+\beta_h\mathbf{K}_i}\,, \tag{36}$$

see Figures (2a, b). From the above equation and equation (35), it is indeed possible to recover the $(e\leftrightarrow e')$ symmetry condition (8). However except from their pedestrian derivations, the two above equations would be hard to trust.

b) **Our best choice**

In view of the precise form of the Hamiltonian $h_{\mathbf{r},\mathbf{u}'}$ given in equation (25), it may appear as a better idea to use the $\varphi_\nu(\mathbf{r}) = \langle \mathbf{r}|x_\nu\rangle$ eigenstates of $h_\mathbf{r}$ as a basis for the $\mathbf{r}$ part of the $\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}')$ functions. This leads to write these functions as

$$\Phi^{(\eta_i)}(\mathbf{r},\mathbf{u}') = \sum_{\nu,\mathbf{p}} \tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}\, \varphi_\nu(\mathbf{r})\, \frac{\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{u}'}}{\sqrt{\mathcal{V}}}, \tag{37}$$

(see Fig. 2c). By inserting this expansion into equation (29), we find that the $\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}$'s must verify

$$\left[\epsilon_\nu + \frac{\hbar^2\mathbf{p}^2}{2\mu_t} - \varepsilon_{\eta_i}\right] \tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}} + \sum_{\nu',\mathbf{q}} V_\mathbf{q}\gamma_{\nu\nu'}(\mathbf{q})\, \tilde{\Phi}^{(\eta_i)}_{\nu',\mathbf{p}+\mathbf{q}} = 0, \tag{38}$$

where we have set

$$\gamma_{\nu\nu'}(\mathbf{q}) = \langle x_\nu|\mathrm{e}^{\mathrm{i}\alpha_h\mathbf{q}\cdot\mathbf{r}} - \mathrm{e}^{-\mathrm{i}\alpha_e\mathbf{q}\cdot\mathbf{r}}|x_{\nu'}\rangle. \tag{39}$$

The equation verified by $\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}$ has now one coupling term only, instead of three as in the previous procedures, $V_\mathbf{q}\gamma_{\nu\nu'}(\mathbf{q})$ being the Fourier transform of the potential

$$v_{\nu\nu'}(\mathbf{u}') = \langle x_\nu|v(\mathbf{r},\mathbf{u}')|x_{\nu'}\rangle, \tag{40}$$

which scatters the ν' exciton to a ν state, while a $\mathbf{p}+\mathbf{q}$ electron is scattered into a $\mathbf{p}$ state.

The quantity $\gamma_{\nu\nu'}(\mathbf{q})$ already appeared in our commutation technique for interacting close-to-boson excitons [22,23]. It was associated to the scattering of a ν' exciton into a ν state under a $\mathbf{q}$ Coulomb excitation, making the exciton center of mass momentum going from $\mathbf{Q}$ to $\mathbf{Q}+\mathbf{q}$. In the trion problem, the exciton-electron state $(\nu',\mathbf{p}+\mathbf{q})$ is scattered into the $(\nu,\mathbf{p})$ state due to the Coulomb interaction $v(\mathbf{r},\mathbf{u}')$ between the e' electron and the (e,h) exciton. As the trion *total* momentum $\mathbf{K}_i$ stays constant under this coupling, when the e' electron changes its momentum from $\mathbf{p}+\mathbf{q}$ to $\mathbf{p}$, the (e,h) exciton has to change its center of mass momentum from $\mathbf{Q}$ to $\mathbf{Q}+\mathbf{q}$, while its relative motion goes from ν' to ν. Consequently, the $\gamma_{\nu\nu'}(\mathbf{q})$ scattering has indeed to appear in the scattering of the $(\nu',\mathbf{p}+\mathbf{q})$ state into the $(\nu,\mathbf{p})$ state.

If we expand $\varphi_\nu(\mathbf{r}')$ on plane waves and use equation (34), we find

$$\begin{aligned}\varphi_\nu(\mathbf{r}')\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{u}} &= \sum_\mathbf{k} \langle \mathbf{r}'|\mathbf{k}\rangle\, \langle \mathbf{k}|x_\nu\rangle\, \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{u}} \\ &= \sum_{\mathbf{p}'} \langle \mathbf{r}|\mathbf{p}+\alpha_e\mathbf{p}'\rangle\, \langle \mathbf{p}'+\alpha_e\mathbf{p}|x_\nu\rangle\, \mathrm{e}^{\mathrm{i}\mathbf{p}'\cdot\mathbf{u}'},\end{aligned} \tag{41}$$

so that

$$\varphi_\nu(\mathbf{r}')\, \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{u}} = \sum_{\nu',\mathbf{p}'} \langle x_{\nu'}|\mathbf{p}+\alpha_e\mathbf{p}'\rangle\, \langle \mathbf{p}'+\alpha_e\mathbf{p}|x_\nu\rangle\, \varphi_{\nu'}(\mathbf{r})\, \mathrm{e}^{\mathrm{i}\mathbf{p}'\cdot\mathbf{u}'}. \tag{42}$$

From this equation, it is then easy to show that the symmetry condition (Eq. (31)) on the $(\mathbf{r}_e,\mathbf{r}_{e'})$ coordinates imposed by Pauli exclusion leads to

$$\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}} = (-1)^{S_i} \sum_{\nu',\mathbf{p}'} \langle x_\nu|\mathbf{p}'+\alpha_e\mathbf{p}\rangle\, \langle \mathbf{p}+\alpha_e\mathbf{p}'|x_{\nu'}\rangle\, \tilde{\Phi}^{(\eta_i)}_{\nu',\mathbf{p}'}. \tag{43}$$

If we compare equation (32) to equation (37), we find that $\bar{\Phi}^{(\eta_i)}$ and $\tilde{\Phi}^{(\eta_i)}$ are related by

$$\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}} = \sum_\mathbf{k} \langle x_\nu|\mathbf{k}\rangle\, \bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}} \tag{44}$$

$$\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}} = \sum_\nu \langle \mathbf{k}|x_\nu\rangle\, \tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}\ . \tag{45}$$

By using the above equations, it is possible to recover equation (43) directly from equation (35).

1.3 Trions in terms of exciton and free electron

For further works on interacting trions, it will be useful to note that equations (28, 37) lead to

$$\Psi^{(i)}(\mathbf{r}_e,\mathbf{r}_{e'},\mathbf{r}_h) = \sum_{\nu,\mathbf{p},\mathbf{K}_i} \tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}\, \frac{\mathrm{e}^{\mathrm{i}(\mathbf{p}+\beta_e\mathbf{K}_i)\cdot\mathbf{r}_{e'}}}{\sqrt{\mathcal{V}}} \times \varphi_\nu(\mathbf{r}_e-\mathbf{r}_h)\, \frac{\mathrm{e}^{\mathrm{i}(-\mathbf{p}+\beta_x\mathbf{K}_i)(\alpha_e\mathbf{r}_e+\alpha_h\mathbf{r}_h)}}{\sqrt{\mathcal{V}}}, \tag{46}$$

so that it is possible to write the trion wave function as a product of an exciton and a free electron wave functions through

$$\Psi^{(i)}(\mathbf{r}_e,\mathbf{r}_{e'},\mathbf{r}_h) = \sum_{n,\mathbf{k}} \tilde{\Psi}^{(i)}_{n,\mathbf{k}}\, \phi_n(\mathbf{r}_e,\mathbf{r}_h)\, \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{e'}}}{\sqrt{\mathcal{V}}}, \tag{47}$$

(see Fig. 2d), where $\phi_n(\mathbf{r}_e,\mathbf{r}_h)$ is the n exciton total wave function, n standing for $(\nu_n,\mathbf{Q}_n)$. Due to equation (46), the prefactors $\tilde{\Psi}$ are equal to

$$\tilde{\Psi}^{(i)}_{n,\mathbf{k}} = \tilde{\Phi}^{(\eta_i)}_{\nu_n,\mathbf{k}-\beta_e\mathbf{K}_i}\, \delta_{\mathbf{K}_i,\mathbf{k}+\mathbf{Q}_n}\ . \tag{48}$$

From the Schrödinger equation (38) verified by $\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}$, we can deduce the Schrödinger equation verified by $\tilde{\Psi}^{(i)}_{n,\mathbf{k}}$. It reads

$$(E_n + \epsilon_e(\mathbf{k}) - \mathcal{E}_i)\, \tilde{\Psi}^{(i)}_{n,\mathbf{k}} + \sum_{n',\mathbf{k}'} \delta_{\mathbf{Q}_{n'}+\mathbf{k}',\mathbf{Q}_n+\mathbf{k}}\, V_{\mathbf{Q}_n-\mathbf{Q}_{n'}}\, \gamma_{\nu_n\nu_{n'}}(\mathbf{Q}_n-\mathbf{Q}_{n'})\, \tilde{\Psi}^{(i)}_{n',\mathbf{k}'} = 0, \tag{49}$$

where $E_n = \epsilon_{\nu_n} + \hbar^2\mathbf{Q}_n^2/2(m_e+m_h)$ is the n exciton energy, and $\mathcal{E}_i = \varepsilon_{\eta_i} + \hbar^2\mathbf{K}_i^2/2(2m_e+m_h)$ is the i trion energy [29].

Using equations (43, 48), the ($\mathbf{r}_e \leftrightarrow \mathbf{r}_{e'}$) symmetry imposed by Pauli exclusion now leads to

$$\tilde{\Psi}^{(i)}_{n,\mathbf{k}} = (-1)^{S_i} \times \sum_{n',\mathbf{k}'} \delta_{\mathbf{k}+\mathbf{Q}_n,\mathbf{k}'+\mathbf{Q}_{n'}} \langle x_{\nu_n}|\mathbf{k}'-\alpha_e \mathbf{Q}_n\rangle \langle \mathbf{k}-\alpha_e \mathbf{Q}_{n'}|x_{\nu_{n'}}\rangle \tilde{\Psi}^{(i)}_{n',\mathbf{k}'}. \tag{50}$$

While the consequences of Pauli exclusion on the ($e \leftrightarrow e'$) symmetry are rather simple on the $\bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h}$'s (see Eq. (8)), they are less clear on the $\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}$'s (see Eq. (35)), and completely obscure on the $\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}$'s and $\tilde{\Psi}^{(i)}_{n,\mathbf{k}}$'s (see Eqs. (43, 50)). In the next paragraph, we are going to show, using the second quantization, how these conditions can in fact appear in a quite transparent way. This understanding is in fact of importance, as the representation of the trion in terms of exciton and electron is the good one for future works on many-body effects with trions.

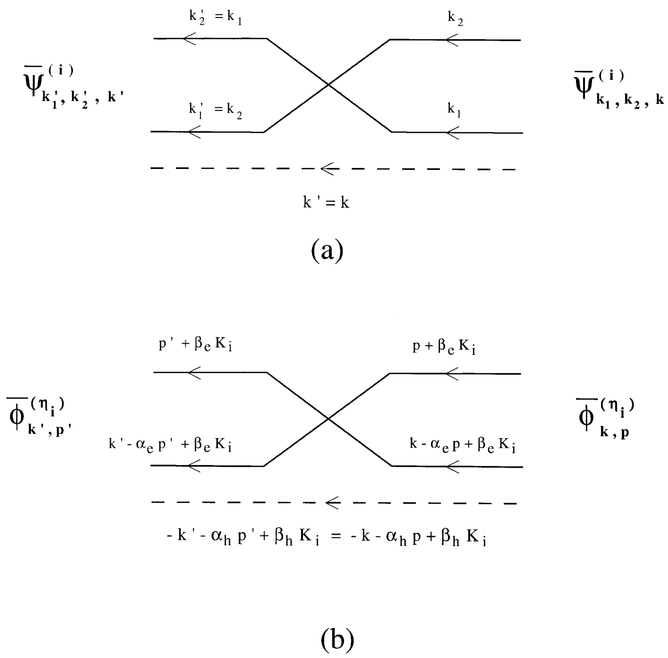

Fig. 3. The invariance relations (8) and (35) come from the possible exchange of the two electrons.

2 The X⁻ trion in second quantization

In second quantization, the trions appear through trion creation operators $T_i^\dagger$. They are such that

$$\left\langle \mathbf{r}_e, \mathbf{r}_{e'}, \mathbf{r}_h | T_i^\dagger | v \right\rangle \tag{51}$$

corresponds to the X⁻ trion wave function given in equation (3), $|v>$ being the electron-hole vacuum state. We are now going to derive the four formulations of these trion operators which correspond to the four forms of the orbital wave functions given in equation (6), equations (28, 32), equations (28, 37) and equation (47).

2.1 First formulation of the X⁻ trion operator in terms of two electrons and one hole

Let us first consider the X⁻ trion operators which correspond to an electron total spin ($S_i = 1, S_{iz} = \pm 1$) so that its two electrons have the same spin $\pm 1/2$. In this case, the X⁻ trion operator simply reads (see Fig. 2a),

$$T^\dagger_{i;S_i=1,S_{iz}=\pm 1,m_i} = \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h} \bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h} a^\dagger_{\mathbf{k}_e,\pm} a^\dagger_{\mathbf{k}_{e'},\pm}, b^\dagger_{\mathbf{k}_h,m_i}. \tag{52}$$

Indeed using the symmetry condition (Eq. (8)) for the $\bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h}$'s of $S_i = 1$ trions, and the relation

$$\left\langle \mathbf{r}_e, \mathbf{r}_{e'} | a^\dagger_{\mathbf{k}_e,s} a^\dagger_{\mathbf{k}_{e'},s'} | v \right\rangle = \frac{1}{\sqrt{2}} \left[\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_e \cdot \mathbf{r}_e}}{\sqrt{\mathcal{V}}} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_{e'} \cdot \mathbf{r}_{e'}}}{\sqrt{\mathcal{V}}} |s, s'\rangle - \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_{e'} \cdot \mathbf{r}_e}}{\sqrt{\mathcal{V}}} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_e \cdot \mathbf{r}_{e'}}}{\sqrt{\mathcal{V}}} |s', s\rangle \right], \tag{53}$$

it is straightforward to check that this $T_i^\dagger$ operator inserted in equation (51) just gives the orbital part of the wave function appearing in equation (6). In a similar way, we can check that when the electron total spin of the trion S_{iz} is zero, the X⁻ trion operator is given by

$$T^\dagger_{i;S_i=(0,1),S_{iz}=0,m_i} = \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h} \bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h} \times \left(\frac{(a^\dagger_{\mathbf{k}_e,+} a^\dagger_{\mathbf{k}_{e'},-} - (-1)^{S_i} a^\dagger_{\mathbf{k}_e,-} a^\dagger_{\mathbf{k}_{e'},+}}{\sqrt{2}} \right) b^\dagger_{\mathbf{k}_h,m_i}. \tag{54}$$

Let us note that the Pauli exclusion condition (5), enforced on the $\bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h}$'s through equation (8), just corresponds to have the prefactors of equation (52) or (54) unchanged with respect to the possible anticommutation of the two $a^\dagger$ operators (see Fig. 3a). Indeed, equation (52) gives

$$T^\dagger_{i;S_i=1,S_{iz}=\pm 1,m_i} = -\frac{1}{\sqrt{2}} \sum_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h} \bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h} a^\dagger_{\mathbf{k}_{e'},\pm} a^\dagger_{\mathbf{k}_e,\pm} b^\dagger_{\mathbf{k}_h,m_i}, \tag{55}$$

which is identical to equation (52) provided that the $\bar{\Psi}^{(i)}_{\mathbf{k}_e,\mathbf{k}_{e'},\mathbf{k}_h}$'s verify equation (8). This is also true for $S_{iz} = 0$ trions.

2.2 Second formulation of the X⁻ trion operator in terms of two electrons and one hole

We now turn to the X⁻ trion operators which generate the trion wave functions given in equations (28, 32), with the trion center of mass momentum $\mathbf{K}_i$ appearing explicitly. Let us first give their expressions (see Fig. 2b),

$$T^\dagger_{\eta_i,\mathbf{K}_i;S_i=1,S_{iz}=\pm1,m_i} = \frac{1}{\sqrt{2}}\sum_{\mathbf{k},\mathbf{p}} \bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}\, a^\dagger_{\mathbf{p}+\beta_e\mathbf{K}_i,\pm}\, a^\dagger_{\mathbf{k}-\alpha_e\mathbf{p}+\beta_e\mathbf{K}_i,\pm}\, b^\dagger_{-\mathbf{k}-\alpha_h\mathbf{p}+\beta_h\mathbf{K}_i,m_i}, \tag{56}$$

with expresssions similar to equation (54) for $S_{iz}=0$ trions. These expressions can be checked by a brute force calculation relying on equation (53). Although the carrier momenta have some similarity with the ones appearing in equation (36), these forms may appear as far from obvious at first. Let us briefly outline how we can derive them from scratch. We will only consider $S_i = 1 = S_{iz}$ trions, for simplicity.

The expression of the trion wave function given in equation (28) makes the trion center of mass appearing as one of the three coordinates of the trion. Associated to it, is the trion total momentum $\mathbf{K}_i$. We are thus led to look for the trion operator as a linear combination of $a^\dagger_{\mathbf{k}_e}\, a^\dagger_{\mathbf{k}_{e'}}\, b^\dagger_{\mathbf{k}_h}$ with $\mathbf{k}_e+\mathbf{k}_{e'}+\mathbf{k}_h=\mathbf{K}_i$. Along with $\mathbf{K}_i$, we have to introduce two other momenta $\mathbf{k}$ and $\mathbf{p}$. Let us write the carrier momenta $\mathbf{k}_e$, $\mathbf{k}_{e'}$, $\mathbf{k}_h$ in terms of these three new momenta as

$$\begin{aligned}
\mathbf{k}_e &= b_e\mathbf{K}_i + c_e\mathbf{k} + d_e\mathbf{p}\ ,\\
\mathbf{k}_{e'} &= b_{e'}\mathbf{K}_i + c_{e'}\mathbf{k} + d_{e'}\mathbf{p},\\
\mathbf{k}_h &= (1-b_e-b_{e'})\mathbf{K}_i - (c_e+c_{e'})\mathbf{k} - (d_e+d_{e'})\mathbf{p}.
\end{aligned} \tag{57}$$

The above equations already contain the fact that $\mathbf{k}_e + \mathbf{k}_{e'} + \mathbf{k}_h = \mathbf{K}_i$. If in addition, we enforce the $\mathbf{k}.\mathbf{K}_i$ and $\mathbf{p}.\mathbf{K}_i$ terms to disappear from $\epsilon_e(\mathbf{k}_e)+\epsilon_e(\mathbf{k}_{e'})+\epsilon_h(\mathbf{k}_h)$, we get $b_e = b_{e'} = \beta_e$ so that $1-b_e-b_{e'}=\beta_h$. If we also enforce the $\mathbf{k}.\mathbf{p}$ term to disappear from this sum, we get

$$\frac{c_e d_e + c_{e'} d_{e'}}{m_e} + \frac{(c_e+c_{e'})(d_e+d_{e'})}{m_h} = 0, \tag{58}$$

which is basically similar to equation (15). As for the determination of the two spatial coordinates $(\mathbf{r}_1,\mathbf{r}_2)$ which go along with $\mathbf{R}_t$, we have here again to make an additional choice in order to determine the two momenta $(\mathbf{k},\mathbf{p})$ we want to associate to $\mathbf{K}_i$. The $a'=0$ choice we made, in fact corresponds in momentum space to take $c_e=0$. By setting $c_{e'}=1=d_e$ (which just rescales $\mathbf{k}$ and $\mathbf{p}$), we then find

$$\begin{aligned}
\mathbf{k}_e &= \beta_e\mathbf{K}_i + \mathbf{p}\ ,\\
\mathbf{k}_{e'} &= \beta_e\mathbf{K}_i - \alpha_e\mathbf{p} + \mathbf{k}\ ,\\
\mathbf{k}_h &= \beta_h\mathbf{K}_i - \alpha_h\mathbf{p} - \mathbf{k}.
\end{aligned} \tag{59}$$

These momenta are exactly those appearing in equation (56).

We have shown that, within this formulation of the orbital part of the wave function as given in equations (28, 32), Pauli exclusion imposes the $\bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}$'s to verify equation (35). This equation just follows from the anticommutation of the two $a^\dagger$'s in equation (56) (see Fig. 3b). Indeed the anticommutation gives

$$T^\dagger_{\eta_i,\mathbf{K}_i;S_i=1,S_{iz}=+1,m_i} = -\frac{1}{\sqrt{2}}\sum_{\mathbf{k},\mathbf{p}} \bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}\, a^\dagger_{\mathbf{k}-\alpha_e\mathbf{p}+\beta_e\mathbf{K}_i,+}\, a^\dagger_{\mathbf{p}+\beta_e\mathbf{K}_i,+}\, b^\dagger_{-\mathbf{k}-\alpha_h\mathbf{p}+\beta_h\mathbf{K}_i,m_i}. \tag{60}$$

So that, if we call $a^\dagger_{\mathbf{p}'+\beta_e\mathbf{K}_i}$ the first $a^\dagger$ and $a^\dagger_{\mathbf{k}'-\alpha_e\mathbf{p}'+\beta_e\mathbf{K}_i}$ the second $a^\dagger$, the prefactor becomes $\bar{\Phi}^{(\eta_i)}_{\mathbf{p}'+\alpha_e(\mathbf{k}'-\alpha_e\mathbf{p}'),\mathbf{k}'-\alpha_e\mathbf{p}'}$. We thus see that equation (35) just enforces this prefactor to stay unchanged under the $a^\dagger$ anticommutation. Condition (35) then becomes much clearer.

2.3 Third formulation of the X^- trion operator in terms of one exciton and one electron

A brute force calculation using once more equation (53) shows that the trion orbital wave function given in equations (28, 37) can be recovered from the trion operators (see Fig. 2c),

$$T^\dagger_{\eta_i,\mathbf{K}_i;S_i=1,S_{iz}=\pm1,m_i} = \frac{1}{\sqrt{2}}\sum_{\nu,\mathbf{p}} \tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}\, a^\dagger_{\mathbf{p}+\beta_e\mathbf{K}_i,\pm}\, B^\dagger_{\nu,-\mathbf{p}+\beta_x\mathbf{K}_i;\pm,m_i}, \tag{61}$$

$$\begin{aligned}
T^\dagger_{\eta_i,\mathbf{K}_i;S_i=(1,0),S_{iz}=0,m_i} = \frac{1}{2}\sum_{\nu,\mathbf{p}} \tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}} \Big[& a^\dagger_{\mathbf{p}+\beta_e\mathbf{K}_i,-}\, B^\dagger_{\nu,-\mathbf{p}+\beta_x\mathbf{K}_i;+,m_i} \\
& - (-1)^{S_i}\, a^\dagger_{\mathbf{p}+\beta_e\mathbf{K}_i,+}\, B^\dagger_{\nu,-\mathbf{p}+\beta_x\mathbf{K}_i;-,m_i}\Big],
\end{aligned} \tag{62}$$

where the operator $B^\dagger_{\nu,\mathbf{Q};s,m}$ is the usual creation operator of an exciton with total momentum $\mathbf{Q}$ and exciton relative motion wave function $|x_\nu\rangle$,

$$B^\dagger_{\nu,\mathbf{Q};s,m} = \sum_{\mathbf{p}} \langle\mathbf{p}|x_\nu\rangle\, a^\dagger_{\mathbf{p}+\alpha_e\mathbf{Q},s}\, b^\dagger_{-\mathbf{p}+\alpha_h\mathbf{Q},m}. \tag{63}$$

Before going further, let us note the similarity between the exciton creation operator (63) and the trion creation operator (61): The total momentum $\mathbf{Q}$ or $\mathbf{K}_i$ is in both cases split between the electron and the hole or the electron and the exciton according to their masses, namely $\alpha_e = m_e/(m_e+m_h)$ and $\alpha_h = m_h/(m_e+m_h)$ for the exciton, while $\beta_e = m_e/(2m_e+m_h)$ and $\beta_x = (m_e+m_h)/(2m_e+m_h)$ for the trion. For the trion operator, there is however an additional ν index in equation (61) when compared to equation (63), as the excitons are characterized by $(\nu,\mathbf{Q})$, while the holes are characterized by $\mathbf{p}$ only.

It is in fact possible to transform equation (56) into equation (61) by using

$$a^\dagger_{\mathbf{k}_e,s} b^\dagger_{\mathbf{k}_h,m} = \sum_\nu \langle x_\nu | \alpha_h \mathbf{k}_e - \alpha_e \mathbf{k}_h \rangle \, B^\dagger_{\nu,\mathbf{k}_e+\mathbf{k}_h;s,m}, \quad (64)$$

which is easy to check from equation (63). If we take for $a^\dagger_{\mathbf{k}_e,s}$ the second $a^\dagger$ of equation (56), we then get

$$T^\dagger_{\eta_i,\mathbf{K}_i;S_i=S_{iz}=1,m_i} = \frac{1}{\sqrt{2}} \sum_{\nu,\mathbf{p}} a^\dagger_{\mathbf{p}+\beta_e\mathbf{K}_i,+} \, B^\dagger_{\nu,-\mathbf{p}+\beta_x\mathbf{K}_i;+,m} \sum_{\mathbf{k}} \langle x_\nu | \mathbf{k} \rangle \, \bar{\Phi}^{(\eta_i)}_{\mathbf{k},\mathbf{p}}, \quad (65)$$

which is nothing but equation (61), if we use the relation (44) between the $\bar{\Phi}$'s and the $\tilde{\Phi}$'s. A similar transformation can be done for the other (S_i, S_{iz})'s.

We can note that equation (61) also reads (see Fig. 2d),

$$T^\dagger_{i;S_i=1,S_{iz}=\pm1} = \frac{1}{\sqrt{2}} \sum_{n,\mathbf{k}} \tilde{\Psi}^{(i)}_{n,\mathbf{k}} \, a^\dagger_{\mathbf{k},\pm} \, B^\dagger_{n;\pm,m}, \quad (66)$$

where the trion index i stands for $(\eta_i, \mathbf{K}_i)$ and the exciton index n stands for $(\nu_n, \mathbf{Q}_n)$; the prefactor $\tilde{\Psi}^{(i)}_{n,\mathbf{k}}$ deduced from equation (61) is equal to

$$\begin{aligned} \tilde{\Psi}^{(i)}_{n,\mathbf{k}} &= \delta_{\mathbf{K}_i,\mathbf{k}+\mathbf{Q}_n} \sum_{\mathbf{k}'} \langle x_{\nu_n} | \mathbf{k}' \rangle \, \bar{\Phi}^{(\eta_i)}_{\mathbf{k}',\mathbf{k}-\beta_e\mathbf{K}_i} \\ &= \delta_{\mathbf{K}_i,\mathbf{k}+\mathbf{Q}_n} \tilde{\Phi}^{(\eta_i)}_{\nu_n,\mathbf{k}-\beta_e\mathbf{K}_i}, \end{aligned} \quad (67)$$

which is nothing but equation (48), due to equation (44).

We can also recover the $(\mathbf{r}_e \leftrightarrow \mathbf{r}_{e'})$ symmetry condition imposed by Pauli exclusion on the $\tilde{\Psi}^{(i)}_{n,\mathbf{k}}$'s, as given in equation (50) (see Fig. 4a): Indeed, by "opening" the exciton of equation (66) into (e, h) pairs according to equation (63), we get

$$T^\dagger_{i;S_i=1=S_{iz}} = \frac{1}{\sqrt{2}} \sum_{\mathbf{p},\mathbf{k},\nu_n,\mathbf{Q}_n} \tilde{\Psi}^{(i)}_{n,\mathbf{k}} \langle \mathbf{p} | x_{\nu_n} \rangle \, a^\dagger_{\mathbf{k},+} \, a^\dagger_{\mathbf{p}+\alpha_e\mathbf{Q}_n,+} \, b^\dagger_{-\mathbf{p}+\alpha_h\mathbf{Q}_n,m}. \quad (68)$$

If we now anticommute the two $a^\dagger$ and form the exciton with $a^\dagger_{\mathbf{k},+} \, b^\dagger_{-\mathbf{p}+\alpha_h\mathbf{Q}_n,m}$ according to equation (64), we find

$$\begin{aligned} T^\dagger_{i;S_i=1=S_{iz}} = &-\frac{1}{\sqrt{2}} \sum_{\mathbf{p},\mathbf{k},\nu_{n'},\nu_n,\mathbf{Q}_n} a^\dagger_{\mathbf{p}+\alpha_e\mathbf{Q}_n,+} \, B^\dagger_{\nu_{n'},\mathbf{k}-\mathbf{p}+\alpha_h\mathbf{Q}_n;+,m} \\ &\times \langle x_{\nu_{n'}} | \alpha_h\mathbf{k} - \alpha_e(-\mathbf{p}+\alpha_h\mathbf{Q}_n) \rangle \, \langle \mathbf{p} | x_{\nu_n} \rangle \, \tilde{\Psi}^{(i)}_{n,\mathbf{k}}, \end{aligned} \quad (69)$$

which also reads

$$T^\dagger_{i;S_i=1=S_{iz}} = \frac{1}{\sqrt{2}} \sum_{n',\mathbf{k}'} \tilde{\Psi}^{(i)}_{n',\mathbf{k}'} \, a^\dagger_{\mathbf{k}',+} \, B^\dagger_{n';+,m}, \quad (70)$$

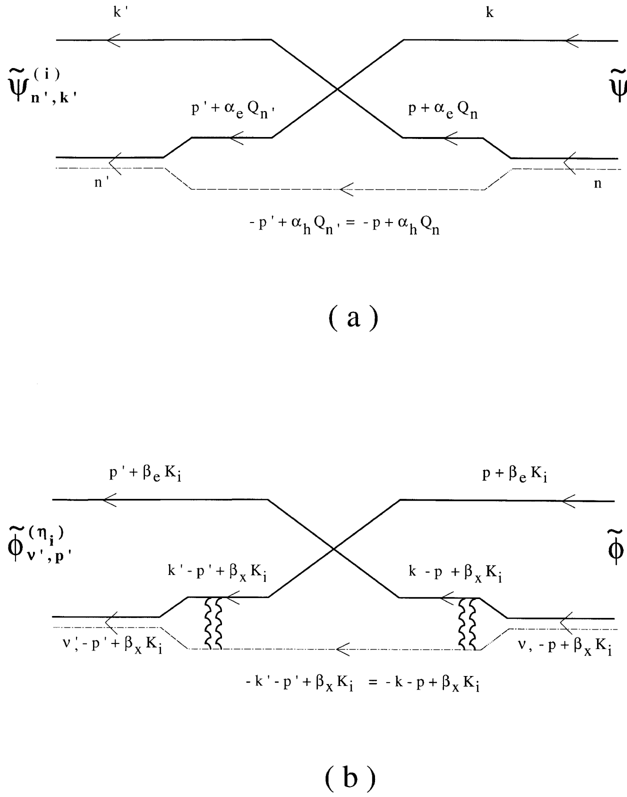

Fig. 4. The invariance relations (43) and (50) come from the possible change of electron when making the exciton.

if we set

$$\tilde{\Psi}^{(i)}_{n',\mathbf{k}'} = -\sum_{n,\mathbf{k}} \delta_{\mathbf{k}+\mathbf{Q}_n,\mathbf{k}'+\mathbf{Q}_{n'}} \langle x_{\nu_{n'}} | \mathbf{k} - \alpha_e \mathbf{Q}_{n'} \rangle \, \langle \mathbf{k}' - \alpha_e \mathbf{Q}_n | x_{\nu_n} \rangle \, \tilde{\Psi}^{(i)}_{n,\mathbf{k}}, \quad (71)$$

which is nothing but equation (50) (with $(n, \mathbf{k}) \leftrightarrow (n', \mathbf{k}')$). A similar procedure allows to get the invariance relation (43) between the $\tilde{\Phi}^{(\eta_i)}_{\nu,\mathbf{p}}$ (see Fig. 4b). We thus see that, in all cases, the conditions imposed by the $(\mathbf{r}_e \leftrightarrow \mathbf{r}_{e'})$ symmetry which results from Pauli exclusion is nothing but the invariance of the prefactors of the trion creation operators under the possible anticommutation of the two electron operators.

3 Conclusion

We have reconsidered the X^- trion in first quantization from scratch, paying particular attention to the various possible "good" choices of coordinates which make them independent, and to the resulting symmetry conditions imposed by Pauli exclusion between the two electrons.

In a second part, we have written various possible trion creation operators. The last formulation (Eq. (66)) in terms of exciton and electron is the most convenient one for future works on interacting trions: It allows to put the problems on trions into the general framework of interacting excitons for which we have recently developed a "commutation technique" [22,23] which allows to take exactly into account the close-to-boson character of the excitons induced by Pauli exclusion between their carriers.

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25. While the energies and wave functions in 3D and 2D are of course correct, the usual resolution of the Schrödinger equation, as found for example in Landau-Lifshitz, *Quantum mechanics*, is mathematically inconsistent as it relies on two hypergeometric functions which are accidentally proportional for the parameters of physical interest. As a dramatic consequence, the proposed resolution cannot be extended to 1D excitons. See M. Combescot, submitted to Solid State Com.
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27. Stébé *et al.* (ref (3, 4)) also use coordinates $\mathbf{r}_1 = \mathbf{r}_e - \mathbf{r}_{e'}$, $\mathbf{r}_2 = (\mathbf{r}_e + \mathbf{r}_{e'})/2 - \mathbf{r}_h$, in which $\mathbf{r}_e$ and $\mathbf{r}_{e'}$ play similar rôles and which fulfil equations (12, 14). They are however less convenient than our $(\mathbf{r}, \mathbf{u}')$ for the extension of this work to one hole plus 3,4,5... electrons
28. The variables $(\mathbf{R}, \mathbf{r})$ used by Thiligam (Ref. (6)) are nothing but our variables $(\mathbf{r}, \mathbf{u}')$. We however do not see why his $\mathbf{r}$ and $\mathbf{R}$ have to be colinear, as stated in his equation (13), even for 2D trions
29. In this paper, we have dropped all band gaps Δ. The exciton energy as well as the free electron energy should have an additional Δ, while the trion energy should have an additional 2Δ. This in fact implies to add a 2Δ to the RHS of the Hamiltonian given in equation (1). In equation (49) however, these Δ are unimportant since they cancel