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# Solution of Wannier exciton for electron and hole spatially separated in perpendicular 1D quantum wires in terms of 2D exciton states.

By

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*Abstract.* We analyze a Wannier-Mott exciton in which the electron is constrained to move freely in a one-dimensional quantum wire (1DQW) and the hole moves freely in another perpendicular 1DQW. The resulting two-dimensional (2D) exciton Schrödinger equation in the laboratory frame of reference is solved in terms of the common 2D exciton equation in the center of mass frame when both electron and hole are in the same 2D quantum layer.

## 1 Introduction

Studies of excitons in confined systems are interesting due to the possibility of growing high-quality nanostructures with prescribed configurations. Within the spirit of studying Wannier-Mott excitons in novel systems that exhibit spatial separation between electron and hole (such as type II semiconductor heterostructures), we investigate here from a theoretical point of view Wannier-Mott excitons in which the electron is confined within a one dimensional quantum wire (1DQW) and the hole is confined in another perpendicular 1DQW as shown in Fig. 1 .To our knowledge, excitons in such configuration has not been investigated before. Analogous systems presenting spatial separation between electron and hole have been theoretically investigated in Refs. [1], [2] and [3]. Reyes and del Castillo-Mussot

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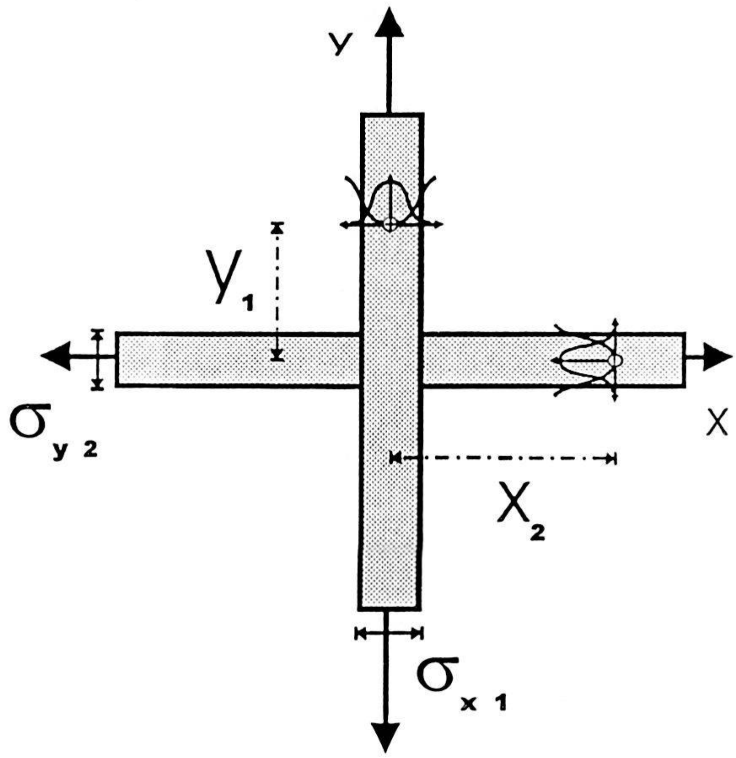


Figure 1: Diagram of the system formed by two infinite perpendicular 1D quantum wires (1DQWs) where both electron $e$ and hole $h$ experience transverse harmonic potential confinement in the $x$ and $y$ directions. Their dimensions are given in terms of the standard deviations $\sigma_{y1}$ and $\sigma_{x2}$ , which are inversely proportional to the stiffness of the corresponding harmonic potential. The transverse harmonic potential and the corresponding wavefunctions are indicated at the positions $y_1$ and $x_2$.

[1] analyzed a Wannier-Mott exciton in which the electron is confined in one 1DQW and the hole is confined in another parallel 1DQW. Lozovik and Nishanov [2] studied excitons in which the electron is confined within a two-dimensional quantum layer (2DQL) and the hole is confined in another parallel 2DQL assuming layers with vanishing widths. Bastard *et al.* [3] performed a variational calculation of the exciton binding energy of a type II semiconductor heterostructure consisting of a hole in InAs well confined between two semi-infinite GaSb layers where the electron lied.

## 2 2D exciton Schrödinger equation

Without loss of generality, we restrict our system of two perpendicular 1DQWs to be a 2D system, that is, the system lies in the $xy$ plane and has a vanishing width in the $z$-direction. The 2D system assumes that in the confinement direction ($x$-direction for the hole and $y$-direction for the electron) both charged particles are in their respective ground state of a harmonic potential, and each one of them is free to move in one of the two perpendicular 1DQW (Fig. 1). The widths of the 1DQWs are $\sigma_{x1}$ for the hole and $\sigma_{y2}$ for the electron. We neglect all possible variations and defects which could be present in the 1DQW walls, and we assume that in the region were both 1DQWs overlap ($|x| < \sigma_{x1}$ and $|y| < \sigma_{y2}$) there is no tunneling. For small $\sigma_{x1}$ and $\sigma_{y2}$ this latter assumption is reasonable from both the theoretical and experimental point of views since, in the first place, that region is small as compared with the spatial extension of the exciton, and a very thin layer could be positioned at the interface between the 1DQWs to avoid contact between them.

We proceed to solve the Schrödinger equation given by

$$\widehat{H}\Psi\left(x_1,y_1,x_2,y_2\right) = E_t\Psi\left(x_1,y_1,x_2,y_2\right), \tag{2.1}$$

where $E_t$ is the total energy of the system and we use the labels 1 and 2 for particles $p_1$ and $p_2$ (but later we will study the particular case of an electron and a hole). $\widehat{H}$ is defined as

$$\widehat{H} = \widehat{H}_1 + \widehat{H}_2 + \widehat{V}_{int}, \tag{2.2}$$

and the Hamiltonian of each particle is

$$\widehat{H}_1 = \frac{-\hbar^2}{2m_\nu}\nabla_\nu^2 + V_\nu\left(y_\nu\right), \tag{2.3}$$

with $\nu$ =1, 2, $m_\nu$ are the effective masses, $V_\nu\left(y_\nu\right)$ is the transverse confinement potential of each carrier and the Coulomb interaction potential is

$$\widehat{V}_{int}\left(\overrightarrow{r_1} - \overrightarrow{r_2}\right) = \frac{q_1q_2}{\epsilon\sqrt{\left(x_1-x_2\right)^2 + \left(y_1-y_2\right)^2}} \tag{2.4}$$

where $\epsilon$ is the appropriate dielectric screening of the semiconductor media.

The two-particle wave function can be separated as

$$\Psi\left(x_1,y_1,x_2,y_2\right) = \Psi_1^0(y_1)\Psi_2^0(x_2)S(x_1,y_2), \tag{2.5}$$

where $\Psi_1^0(y_1)$ , $\Psi_2^0(x_2)$ are the groundstate wave functions of the transverse confinement satisfying

$$\frac{-\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial y_1^2}\right)\Psi_1^0(y_1) + V_1\left(y_1\right)\Psi_1^0(y_1) = E_1^{0t}\Psi_1^0(y_1) \tag{2.6}$$

$$\frac{-\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2}\right)\Psi_2^0(x_2) + V_2\left(x_2\right)\Psi_2^0(x_2) = E_2^{0t}\Psi_2^0(x_2) \tag{2.7}$$

and $S(x_1,y_2)$ is the part of the wave function that contains the interparticle Coulomb potential

We calculate

$$\left\langle \Psi_1^0(y_1)\Psi_2^0(x_2)\left|\widehat{H}\right|\Psi\right\rangle = E_t S(x_1, y_2) \tag{2.8}$$

to obtain

$$\left[\frac{-\hbar^2}{2}\left(\frac{1}{m_1}\left(\frac{\partial^2}{\partial x_1^2}\right)+\frac{1}{m_2}\left(\frac{\partial^2}{\partial y_2^2}\right)\right)+E_1^{0t}+E_2^{0t}+V_{eff}\right] S\left(x_1, y_2\right) = E_t S\left(x_1, y_2\right) \tag{2.9}$$

where

$$V_{eff}\left(x_1, y_2\right) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\left|\Psi_1^0(y_1)\right|^2\left|\Psi_2^0(x_2)\right|^2 \widehat{V}_{int} dy_1 dx_2 \tag{2.10}$$

is the effective interparticle Coulomb potential and the excitonic energy $E$ is defined as

$$E = E_t - E_1^{0t} - E_2^{0t} \tag{2.11}$$

Eq. (2.9) is general for two particles $p_1$ and $p_2$ except for the fact that both particles are in their respective transverse groundstate. For the exciton problem they represent the hole and the electron respectively ($p_1 = h$ and $p_2 = e$), and in the case of $m_1 \neq m_2$ this equation is similar to the Schrödinger equation of an isotropic 2D exciton. For convenience we will choose for both particles harmonic potentials as transverse confined potentials, that is, $\hat{V}_1(y_1) = k_1 y_1^2/2$ and $\hat{V}_2(x_2) = k_2 x_2^2/2$. The choice of a harmonic confinement has the advantage over a hard-well confinement that it could physically represent either soft or hard possible confinements. In terms of standard deviations $\sigma_{y1} = \langle (y_1)^2\rangle_0$ and $\sigma_{x2} = \langle (x_2)^2\rangle_0$ (which are of the order of magnitude of the thickness of 1DQS and subindex 0 indicates groundstate) these potentials yield the normalized groundstate transverse wavefunctions

$$\left|\Psi_1^0(y_1)\right|^2 = \frac{e^{\frac{-y_1^2}{2\sigma_{y1}^2}}}{\sqrt{2\pi}\sigma_{y1}} \tag{2.12}$$

$$\left|\Psi_2^0(x_2)\right|^2 = \frac{e^{\frac{-x_2^2}{2\sigma_{x2}^2}}}{\sqrt{2\pi}\sigma_{x2}}$$

In Eq. (2.9) we choose $m_1 = m_2 = m$ to give

$$\left[\frac{-\hbar^2}{2m}\left(\left(\frac{\partial^2}{\partial x_1^2}\right)+\left(\frac{\partial^2}{\partial y_2^2}\right)\right)+E_1^{0t}+E_2^{0t}+V_{eff}\right] S\left(x_1, y_2\right) = E_t S\left(x_1, y_2\right) \tag{2.13}$$

which is similar to the isotropic 2D exciton equation for the relative radial coordinate with one particle is at position ($x_2$, $y_1$) and the other is fixed at the origin (see Fig. 2), namely,

$$\left[\frac{-\hbar^2}{2\mu}\left(\left(\frac{\partial^2}{\partial x_1^2}\right)+\left(\frac{\partial^2}{\partial y_2^2}\right)\right)-\frac{e^2}{\epsilon\sqrt{x_2^2+{y_1}^2}}\right] S\left(x_1, y_2\right) = E_{n,2D}^{(o)} S\left(x_1, y_2\right). \tag{2.14}$$

Eqs. (2.13) and (2.14) are similar except for the use of the reduced mass $\mu = m_1 m_2/(m_1+m_2)$ with $m_1$ and $m_2$ are the effective masses, a different $e$-$h$ potential, and the addition of a transverse energy constant. Notice that the distance $\rho = \sqrt{x_1^2 + y_2^2}$ between the expected value of the quantum particles $p_1$ and $p_2$ (dashed line), is the same as that of the electron e and the hole h at the origin (solid line) as indicated in Fig. 2.

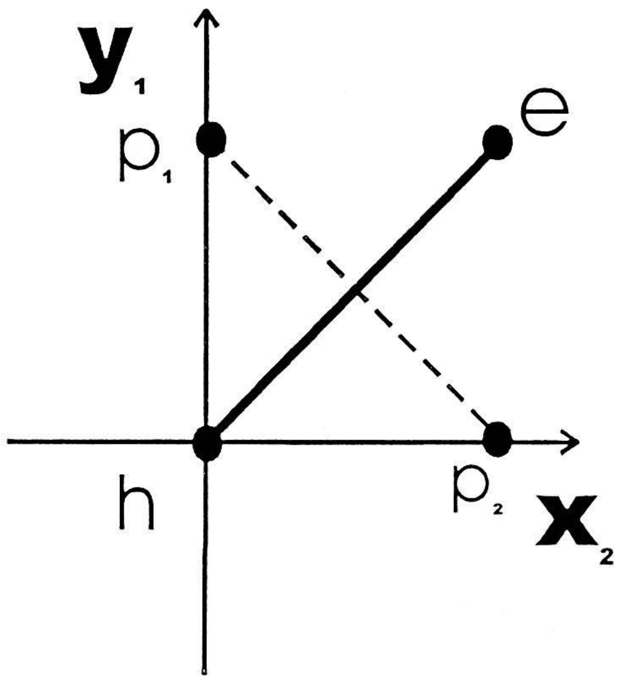


Figure 2: Equivalence of interaction distances for two different systems . A fictitious 2D exciton with a hole at the origin and our system.

# 3 Numerical results and discussion

Eq. (2.14) has as solutions the following eigenenergies and eigenfunctions [4]:

$$E_{n,2D} = -\left|E_o^{3D}\right| \frac{1}{\left(n+\frac{1}{2}\right)^2} \text{ with } n = 0, 1, ..., \tag{3.1}$$

$$\Phi_{n,l}(\rho,\phi) = \Xi_{n,l}(\rho)\exp(il\phi) = A_{n,l}\rho'^{|l|}\exp(-\frac{\rho'}{2})L^{2|l|}_{n+|l|}(\rho')\exp(il\phi) \text{ with } l = 0, \pm 1, \pm 2, ... \tag{3.2}$$

where $E_o^{3D} = -e^2/(2\epsilon a_o^{3D})$ is the 3D exciton ground state binding energy [6], $a_o^{3D} = \hbar^2\epsilon/(e^2\mu)$ is the 3D exciton Bohr radius, $|l| \leq n$, $\rho' = \frac{2\rho}{(n+1/2)a_o^{3D}}$, $L_q^p(\rho') = \sum_{\nu=0}^{p-q}(-1)^{\nu+p}\frac{(q!)^2}{(q-p-\nu)!(p+\nu)!\nu!}$ are the associate Laguerre polynomials [5] and $A_{n,l}$ is a normalization constant. Notice that $E_{o,2D} = 4E_o^{3D}$.

Using polar coordinates; $\rho^2 = x_1^2 + y_2^2$ and $\tan\phi = \frac{y_2}{x_1}$ yields

$$\widehat{V}_{int}(\overrightarrow{r_1} - \overrightarrow{r_2}) = -\frac{e^2}{\epsilon\sqrt{\rho^2 - 2\rho x_2\cos\phi + x_2^2 + y_1^2 - 2\rho y_1\sin\phi}} \tag{3.3}$$

and

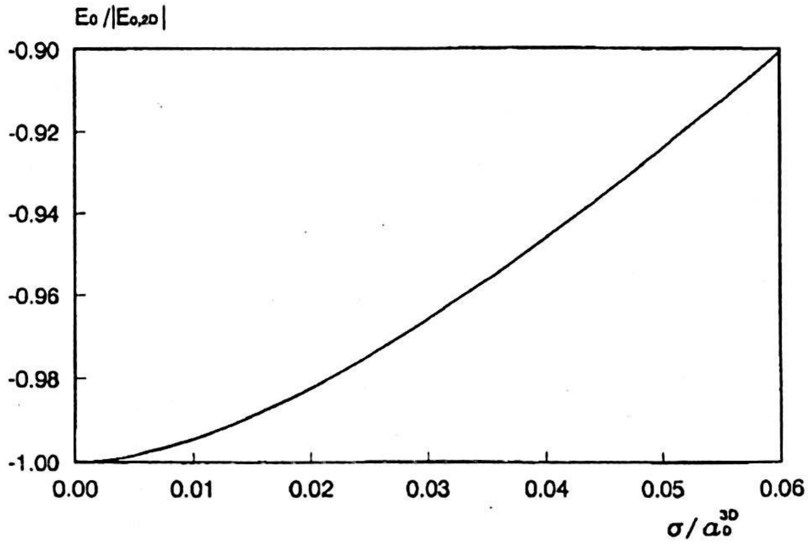


Figure 3: Normalized exciton groundstate energy of the two perpendicular 1DQWs. $E_0$ is plotted as function of $\sigma/a_o^{3D}$ when $m_1 = m_2 = m = 0.05\ m_e$ with $E_{o,2D} = 4E_o^{3D} = -2e^2/(\epsilon a_o^{3D})$ and $a_o^{3D} = \hbar^2\epsilon/(e^2 m)$.

$$\begin{aligned} V_{eff}(\rho,\phi) &= -\frac{e^2}{2\pi\epsilon\sigma^2}\int_0^{2\pi}\int_0^{\infty} e^{-\frac{1}{2\sigma^2}\left(\gamma^2+\rho^2-2\gamma\rho\cos(\eta-\phi)\right)}d\gamma d\eta \\ &= -\frac{e^2}{\epsilon\sigma^2}e^{\frac{1}{2}\frac{\rho^2}{\sigma^2}}\int_0^{\infty} I_0\left(\frac{\gamma\rho}{\sigma^2}\right)e^{-\frac{\gamma^2}{2\sigma^2}}d\gamma. \end{aligned} \tag{3.4}$$

where we have used $\gamma\cos\eta = x_2 - \rho\cos\phi$ and $\gamma\sin\eta = y_1 - \rho\sin\phi$ together with $\sigma_{y1} = \sigma_{x2}$. Last integral can be calculated exactly to yield

$$V_{eff} = -\frac{e^2\sqrt{\pi}}{\epsilon\sigma}Exp\left[-\frac{\rho^2}{4\sigma^2}\right]I_0\left(\frac{\rho^2}{4\sigma^2}\right) \tag{3.5}$$

where $I_0$ is the modified Bessel function of zero order.

Since $V_{eff}$ does not depend on $\phi$, Eq. (2.13) in polar coordinates

$$\begin{aligned} &\left[\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+V_{eff}\right]S(\rho,\phi) \\ &= ES(\rho,\phi), \end{aligned} \tag{3.6}$$

can be separated to yield

$$\frac{d^2\Theta(\phi)}{d\phi^2} = -l^2\Theta(\phi) \tag{3.7}$$

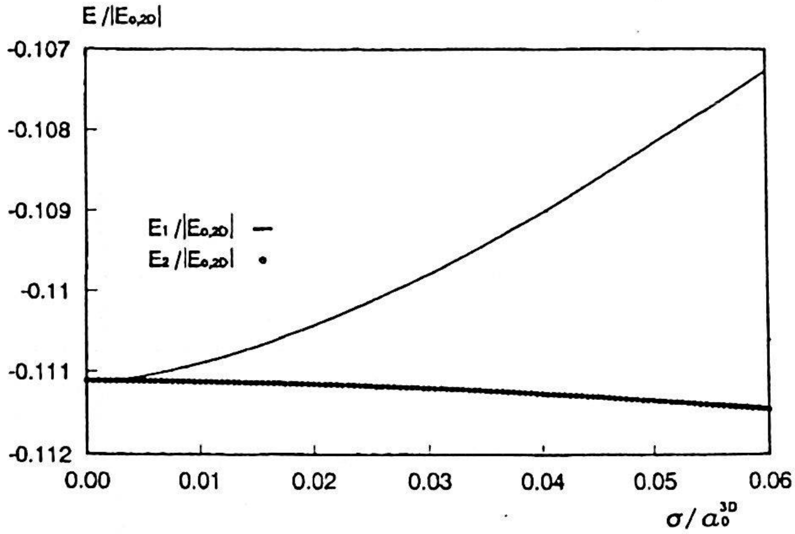


Figure 4: Same as Fig. 3 but for exciton first excited state energies $E_1$ and $E_2$ and with a different scale. Notice that $E_2$ is double degenerated.

and

$$\left[\frac{-\hbar^2}{2m}\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{l^2}{\rho^2}\right)+V_{eff}\right]Q(\rho)=EQ\left(\rho\right) \tag{3.8}$$

where $S\left(\rho,\phi\right)=Q(\rho)\Theta(\phi)$ and the angular quantum number $l$ must be an integer.

We can easily solve radial equation (3.8) perturbately by taking the behavior of $V_{eff}$ for $\rho << \sigma$ and the asymptotic behavior of $V_{eff}$ for $\rho >> \sigma$ :

$$V_{eff}=-\frac{e^2\sqrt{\pi}}{\epsilon\sigma}\left[1-\left(\frac{\rho}{\sigma}\right)^2+\frac{9}{2}\left(\frac{\rho}{\sigma}\right)^4+O\left(\left[\frac{\rho}{\sigma}\right]^6\right)\right],\quad \rho<<\sigma \tag{3.9}$$

$$V_{eff}=-\frac{e^2}{\epsilon\rho}+O\left(\left[\frac{\sigma}{\rho}\right]^3\right),\quad \rho>>\sigma \tag{3.10}$$

if we realize that Eq. (3.6) together with last equation is almost identical to the 2D exciton (Eq. (2.14)). If $\sigma$ is small as compared with the size of the 2D exciton, the region where $V_{eff}$ differs from the aforementioned 2D exciton behavior is small. Therefore we employ the 2D exciton states (Eqs. (3.1) and (3.2)) to solve Eq. (3.8) by common time-independent degenerate perturbation theory with a perturbing potential operator $V_p\left(\sigma\right)=V_{eff}-\left(-\frac{e^2}{\epsilon\rho}\right)$. Here the natural dimensionless perturbation parameter is $p_n=2\sigma/\left[\left(n+1/2\right)a_o^{3D}\right]$, which should be in fact a small number for typical values of $\sigma$.

For the anisotropic case when the values of $m_1$ and $m_2$ are close together, then also perturbation theory can be employed. In order to illustrate numerically our results, we present in Figs. 3 and 4 model calculations of $E_0\left(\sigma\right)=E_{o,2D}+<\Phi_{0,0}\left|V_p\right|\Phi_{0,0}>$ , $E_1\left(\sigma\right)=E_{1,2D}+<\Phi_{1,0}\left|V_p\right|\Phi_{1,0}>$ and $E_2\left(\sigma\right)=E_{1,2D}+<\Phi_{1,1}\left|V_p\right|\Phi_{1,1}>=E_{1,2D}+<\Phi_{1,-1}\left|V_p\right|\Phi_{1,-1}>$ with $\epsilon=10$ and $m=0.05\ m_e$ ($m_e$ is the electron mass) yielding for the 3D exciton the values

$E_o^{3D} = 0.0425$ meV and $a_o^{3D} = 150$ . As expected, the first order corrections of the ground-state exciton energy are larger than those of the first excited states since the probability density of the ground state wavefunction near the origin (where the perturbing potential effects are more important) is larger than those of the excited states. In turn, changes in $E_1(\sigma)$ are larger than in $E_2(\sigma)$ since $\Phi_{1,0}$ is finite at the origin while $\Phi_{1,\pm1}$ vanishes at the origin. Since $V_p$ does not depend on $\phi$, its corresponding matrix in the basis of the $n+1$ degenerate states $\Phi_{n,l}$ is diagonal, and degeneracy is only partially removed by $V_p$ because the states coming from the $\Phi_{n,l}$ and $\Phi_{n,-l}$ remain degenerate.

In summary, we found for our system a 2D exciton Schrödinger equation which for the case of vanishing thickness ($\sigma_1 = \sigma_2 = 0$) and $m_1 = m_2$ is mathematically identical to the well known 2D exciton equation but with the difference that in the former case the equation is set in the laboratory frame of reference whereas in the latter case the equation is set for the relative coordinates in the center of mass reference. We assumed that in the confinement directions both electron and hole were in their respective groundstate of a harmonic potential which yielded an analytical expression for the effective interparticle Coulomb potential for the case $\sigma_1 = \sigma_2$, and we solved our main equation perturbately by employing the eigenenergies and eigenfunctions of the 2D exciton when both electron and hole lie in the same 2D quantum layer in the $xy$ plane. Since our results for small $\sigma$ are not mathematically very different from the two dimensional exciton, we obtain the surprising outcome that the spatial separation between electron and hole is approximately the same as in the 2D exciton. This fact can be explained in terms of the same number of degrees of freedom of two different systems. As shown in Fig. 2, a two-particle system like ours with only one degree of freedom per particle is equivalent to a system where one particle is fixed at the origin and the other particle has the remaining two degrees of freedom. We hope that our efforts can stimulate further experimental and theoretical work on the study of novel heterostructure systems that exhibit spatial separation between the electron and the hole.

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