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Coulomb correlations of a few body system of spatially separated charges

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Abstract. A Hartree-Fock and Hartree-Fock-Bogoliubov study of a few body system of spatially separated charge carriers was carried out. Using these variational states, we compute an approximation to the correlation energy of a finite system of electron-hole pairs. This energy is shown as a function of the Coulomb coupling and the interplane distance. We discuss how the correlation energy can be used to theoretically determine the formation of indirect excitons in semiconductors which is relevant for collective phenomena such as Bose-Einstein condensation (BEC).

1. Introduction

The physical properties displayed by charge carriers in spatially confining settings could have a diverse range of potential applications relevant to technological developments in the near future. Systems with confined charge carriers such as semiconductor quantum wells, quantum wires and quantum dots, will likely have an important impact in the development of quantum computation and quantum information [1] and in producing new technological devices in electronics, spintronics and optoelectronics [2]. In order to take advantage of this important practical potential, it is necessary to have a thorough theoretical understanding of the physics of such systems.

In particular, it is well known that the physics of electron-hole pairs in quantum systems, such as quantum wells and quantum dots, is fundamentally affected by Coulomb correlations (see, for example, [3] and [4]). As a consequence, a complete theoretical study of the physical properties of charge carriers in confining settings must take into account the very important long-ranged Coulomb interaction.

With this in sight, we focus our study on a few-body system of electron-hole pairs confined to vertically stacked parabolic quantum dots. This type of system has been studied recently in the theory of quantum dot molecules (e.g. [5], [6]). Our calculations will involve twelve particles: six electrons and six holes, for a total of six electron-hole pairs. It is clear that such a system is a long way from the $O(10^2)$ pairs of real systems. However, the correlations that arise here should give us a first reasonable insight into the real physical system.

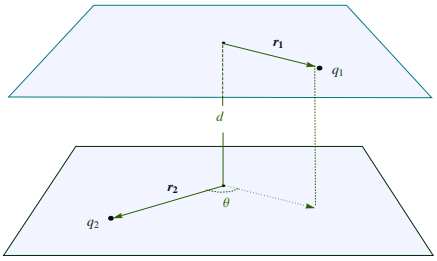

Fig 1: Schematic of our system with two charge carriers q_1 and q_2. They are in two different planes, spatially separated by a vertical distance d. The angle θ is the angle between the position vectors $\mathbf{r_1}$ and $\mathbf{r_2}$.

2. Theoretical framework

We compute the ground state energy of the system of electron-hole pairs using two variational approximations used in finite system studies: the Hartree-Fock (HF) state and a Hartree-Fock-Bogoliubov-type (HFB) state. These states differ in that the HF state fails to provide the so-called correlation energy of the few-body system, whereas the HFB state is able to yield a first approximation this energy. With this information, we will be able to assess under which conditions the correlation energy due to electron-hole pair formation is the greatest i.e. to assess when the formation of spatially indirect excitons is favoured.

To achive our goal, it is necessary to have an efficient way of computing the representation of the Coulomb interaction in the $2D$ harmonic oscillator basis. The Coulomb matrix elements read: $\langle ij|\hat{V}(d)|kl\rangle = \langle ij|\frac{1}{\sqrt{\mathbf{r}_{12}^2+d^2}}|kl\rangle$, where d denotes the separation distance (see Fig.(1)) and the indices in the bras and kets label the 2D harmonic oscillator eigenstates . We have been able to compute the matrix elements [7] by expanding the integrals in terms of a single infinite series followed by a series acceleration algorithm to achieve rapid convergence.

The hamiltonian of the electron-hole pairs in this system is given by

$$\begin{aligned} H &= \sum_i \{\epsilon_i^{(e)} e_i^\dagger e_i + \epsilon_i^{(h)} h_i^\dagger h_i\} + \beta_{ee} \sum_{ijkl} \langle ij|V(0)|kl\rangle e_i^\dagger e_j^\dagger e_l e_k + \\ &\quad + \beta_{hh} \sum_{ijkl} \langle ij|V(0)|kl\rangle h_i^\dagger h_j^\dagger h_l h_k - \beta_{eh} \sum_{i\bar{j}k\bar{l}} \langle ij|V(d)|kl\rangle e_i^\dagger h_{\bar{j}}^\dagger h_{\bar{l}} e_k. \end{aligned} \quad (1)$$

The β_{ee}, β_{hh} and β_{eh} parameters are dimensionless quantities that measure the relative strength of the Coulomb interaction and the harmonic potential: $\beta_{xx} = \left(\frac{me^4}{\epsilon_{xx}^2\hbar^2}/(\hbar\omega_o)\right)^{1/2}$. In this work, we take $\beta_{ee} = \beta_{hh} = \beta_{eh} = \beta$, because we only seek to understand the immediate physical effect of having spatial separation between the charge carriers. A more realistic calculation will need to take into account the fact that the β factor dependends on the dielectric constant of the materials involved in the semiconductor and, thus, their values are going to be different in general. Through out this work, we take the energy scale to be the harmonic potential energy $\hbar\omega$ and the length scale to be the harmonic oscillator length $l = \sqrt{\frac{\hbar}{m\omega}}$.

2.1. The Hartree-Fock ground state

In the first step of our calculation, we minimized the average energy using a slater determinant in order to compute the ground state energy of the few body system. The HF state is given by: $|\phi_{HF}\rangle = \prod_{\mu=1} e_{\alpha_\mu}^\dagger \prod_{\nu=1} h_{\beta_\nu}^\dagger |0\rangle$. As is well known, the Hartree-Fock energy provides the best energy for uncorrelated single particle wave functions. Deviations from this result will yield information of the correlations beyond a single particle picture of the system. This transition to a correlated state will involve, in a first approach, two-particle correlations between electrons and holes, thus generating a picture of bound electron-hole pairs.

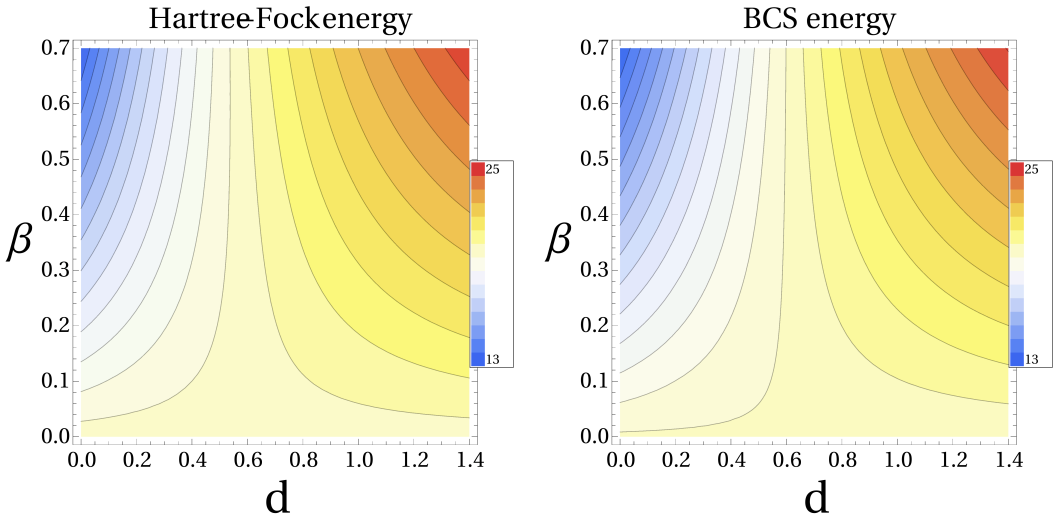

Figure 1. Contour plots of the HF and the BCS ground states in the (β, d) parameter space.

2.2. The BCS ground state

In order to include correlation effects, in the second step of our calculations we made use of the BCS (Bardeen-Cooper-Schrieffer) state, given by: $|\phi_{BCS}\rangle = \prod_i (u_i + v_i e_i^\dagger h_{\bar{i}}^\dagger)|0\rangle$ which is one of a various types of Hartree-Fock-Bogoliubov correlated variational ground state approximations. Such a state introduces pair correlations between electrons and holes from the outset. The coefficients v_i are the variational parameters in the system and are a measure of the likelihood for an i^{th} correlated pair to appear in the system.

3. Results and discussion

In Fig.(1), we show the HF and BCS energies in the parameter space (β, d). Both of these plots tell us how, by a suitable combination of the Coulomb coupling β and the interplane distance, we can go from energies below the energy of the noninteracting particles to energies well above this value. The appearance of the blue region shows that the attractive interaction between electrons and holes is dominant over that of the repulsive electron-electron and hole-hole ones, when β increases or when d decreases. However, as we separate the planes, the electron-hole energy gradually loses its predominance until we achieve a state in which the contribution from repulsive and attractive interactions cancels out, and we are left with the energy value of the noninteracting system.

Note that the contour level corresponding to the particular situation of equal contributions from attractive and repulsive energies is given approximately by a small region of constant distances, *independent of the Coulomb coupling*. This region is shifted to the right in the BCS plot, with respect to that in the Hartree-Fock plot.

The correlation energy, which is approximately given by $E_C(d,\beta) \approx E_{BCS}(d,\beta) - E_{HF}(d,\beta)$, is shown in Fig.(2); both plots in this figure provide different views of the correlation energy. We arrive at two important conclusions from the behaviour of $E_C(d,\beta)$.

First, the system electron-hole pairs show the strongest excitonic behaviour at a non-trivial value of interplane distance. This can be understood as follows: when $d = 0$, the interactions between the particles are effectively screened since they all exist in the same space i.e. in

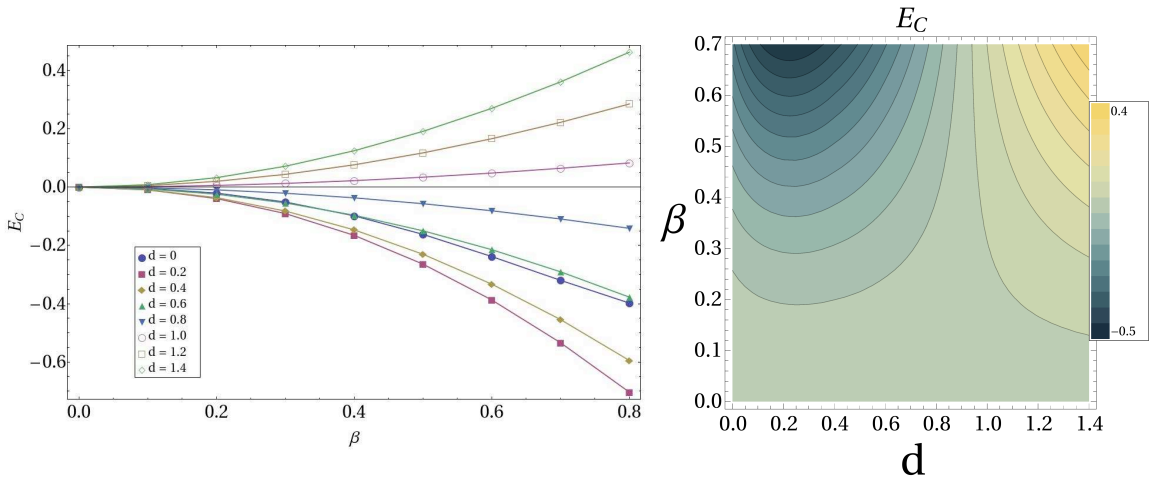

Figure 2. (**Left**) Correlation energy E_C for various values of the distance d. (**Right**) Contour plot of the correlation energy in the (d,β) plane.

the two-dimensional plane. However, when there is a finite distance between the planes, the screening between electrons and holes is reduced and, thus, the electron-hole attractive Coulomb interaction is reinforced. This enhanced attraction effect competes with the electron-electron and hole-hole repulsive interactions and with the suppression of the Coulomb interaction due to the finite distance between the electrons and holes. The attractive interactions eventually lose this competition when the repulsive interaction dominates the ground state of the system, which happens at a critical distance, as can be noted in the plot of the correlation energy.

This last physical turning point brings us to the second important feature of the correlation energy: at the aforementioned critical distance, the energy of the BCS state looses its superiority over the Hartree-Fock energy, since the BCS state energy becomes larger than that of the Hartree-Fock state. This means that the system is no longer suitably described through correlated pairs i.e. the system has suffered a structural change of quantum state, which is reminiscent of the quantum phase transitions that occur in large many-body systems. This transition point, together with the minimum of the correlation energy for finite d, are important pieces of information for understanding the BEC state of indirect excitons in semiconductors.

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