Satellite problem with application to exciton binding

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A particle may be trapped by a local potential due to the presence of a satellite particle that does not interact with the potential. A physical example is the trapping of an exciton by an isoelectronic impurity that is unable to bind the single electron.

In the present paper, we study a bound two-particle system, consisting of a negative and a positive charge, in which merely one of the particles is attracted by a local potential $V(\mathbf{r})$. An exciton, in the effective-mass description depicted as a bound hole-electron system, in which the electron, say, is attracted by the local potential, is such a system. The question we investigate is the following: Under the assumption that the potential $V(\mathbf{r})$ is unable to trap a single electron, can it nevertheless bind the electron plus its satellite, the hole? One might wonder whether the answer is trivially affirmative, by simply replacing the electron mass by the exciton mass. However, the problem is more subtle.

One physical motivation for studying this question comes from trapping of excitons by isoelectronic impurities, an impurity with the same valence electron configuration as that of the host atom it replaces.[1–5] The mechanism for binding has been described as follows: A primary particle (electron or hole) is trapped in the short-range potential of the isoelectronic impurity, and then the secondary particle (hole or electron) is bound by the Coulomb attraction from the primary particle.[2,3,5] However, Masselink and Chang[6] have suggested that this picture is too simple, and that systems may occur which display bound excitons even if the primary particle does not bind by itself. They studied exciton binding to the N impurity in gallium phosphide doped with nitrogen (GaP:N). The short-range isoelectronic potential $V(\mathbf{r})$ is attractive for electrons, and they find the electron to be barely bound with a binding energy less than 1 meV. On the other hand the bound exciton has a binding energy of 28 meV, considerably larger than the free-exciton binding energy of 20 meV. Although the electron is (weakly) bound in this system, their numerical results suggest that this is not necessary to obtain bound excitons. The theoretical calculations in Ref. 6 include the complications and approximations that a realistic detailed calculation must take into account. We want, on the contrary, to make a simple and transparent model study to demonstrate the effect.

Another physical scenario of relevance could be the question of binding of an exciton to a quantum dot in a limiting case in which the dielectric constant and the effective masses are material independent, and the conduction-band offset encourages the electron to be inside the dot, while the valence-band offset is negligible.

Thus motivated we investigate the Hamiltonian

$$H = -\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_h}\nabla_h^2 - \frac{e^2}{4\pi\varepsilon|\mathbf{r}_e - \mathbf{r}_h|} + V(\mathbf{r}_e). \quad (1)$$

Here m_e and m_h are the effective masses of the electron and hole, respectively. (The roles of the electron and hole could of course be interchanged.) As our local potential we choose for simplicity the square-well potential

$$V(\mathbf{r}) = \begin{cases} -V_0 & \text{if } r < R \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

(For application in a spherical quantum dot this would represent the conduction-band offset.) This defines our simple model system.

The binding of a single particle (electron) to the local potential (2) is a textbook problem. The electron is bound when

$$V_0 > \frac{\pi^2}{8}\frac{\hbar^2}{R^2 m_e}, \quad (3)$$

or

$$\tilde{V}_0 > \frac{\pi^2}{8} = 1.2337, \quad (4)$$

in terms of the dimensionless potential depth

$$\tilde{V}_0 = V_0\frac{R^2 m_e}{\hbar^2}. \quad (5)$$

We assume now that the binding condition (4) is *not* fulfilled.

Let us start by demonstrating that the answer to the question posed in the Introduction is affirmative: *The local potential can bind the electron plus the hole, even if the electron alone is not bound.*

This can be shown by a specific example. Assume $m_e = m_h, \tilde{R} = R/a_0 = 1$, and $\tilde{V}_0 = 1.2$, which by (4) implies that a single electron is not trapped by the potential. Here $a_0 = 4\pi\varepsilon\hbar^2/e^2 m_e$ is an effective Bohr radius. An upper bound on the energy of the two-particle problem can be provided by the Rayleigh-Ritz principle. We use the trial function

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = (e^{-|\mathbf{r}_h - \mathbf{r}_e|/a} + ce^{-r_h/b})g(r_e), \quad (6)$$

and integrate out the hole degree of freedom. This yields for the function $g(r_e)$ a one-dimensional Schrödinger equation that can be solved numerically exact. The first exponential term in the trial function is associated with the binding of the hole to the electron, the second with a possible localization of the hole near the local potential.

For a well-chosen set of the variational parameters a, b, and c we obtain

$$E_0 = -0.254 \frac{m_e}{\hbar^2} \left(\frac{e^2}{4\pi\varepsilon} \right)^2 . \tag{7}$$

This energy is *lower* than the energy E_0 of the free exciton (i.e., when the exciton is not in the neighborhood of the local potential), $E_0 = -0.25 m_e \hbar^{-2} \left(e^2/4\pi\varepsilon\right)^2$. Thus the exciton *is* trapped by the local potential, even if the electron alone could not be trapped. This verifies the Masselink-Chang conclusion.[6]

We can, moreover, estimate the *critical* potential strength V_0^c for binding the exciton in this equal-mass case. With a two-particle function of the form (6) we find the variational estimate

$$\tilde{V}_0^c \simeq 1.17 \qquad (m_h = m_e,\ \tilde{R} = 1). \tag{8}$$

This estimate is very far from what one would obtain by naively replacing the electron mass by the total exciton mass in the binding condition (3).

The problem can be analyzed accurately by the Born-Oppenheimer approach in the limit in which the satellite mass m_h is very large. With the hole at a fixed position $\mathbf{r}_h$ the eigenvalue problem for the electron is a one-particle problem in a potential consisting of the Coulomb attraction to the hole plus the local potential (2). When $m_h \gg m_e$ the *critical* local potential is very weak (to be verified *a posteriori*), and consequently we treat $V(r_e)$ by perturbation theory. To first order the ground-state energy for the electron problem equals

$$E_g(r_h; V_0) = -\frac{m_e}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon} \right)^2 - V_0 \int_{r_e < R} |\psi(|\mathbf{r}_e - \mathbf{r}_h|)|^2 d^3 r_e, \tag{9}$$

with $\psi(r) = e^{-r/a_0}/\sqrt{\pi a_0^3}$ the unperturbed ground-state Coulomb wave function. The integral can be evaluated analytically both for $r_h > R$ and $r_h < R$ by first performing the angular integration. We do not give the explicit expression here.

The function $E_g(r_h; V_0)$ acts as a potential for the hole degree of freedom. It is the difference between the lowest eigenvalues in the presence and in the absence of $V(r_e)$ that determines whether the exciton is trapped by the local potential or not. The critical value of V_0 corresponds to vanishing ground-state eigenvalue in the potential

$$v(r_h) = E_g(r_h; V_0) - E_g(r_h; 0) = -V_0 \frac{1}{\pi a_0^3} \int_{r_e < R} e^{-2|\mathbf{r}_e - \mathbf{r}_h|/a_0} d^3 r_e. \tag{10}$$

The potential, with a minimum

$$v(0) = -V_0[1 - (1 + 2\tilde{R} + 2\tilde{R}^2)e^{-2\tilde{R}}], \tag{11}$$

where $\tilde{R} = R/a_0$, is clearly shallower than the local potential (2), but may of course trap a sufficiently heavy particle. It is straightforward to obtain the complete analytic formula for $v(r_h)$, but we do not reproduce the explicit formula here. The Hamiltonian H_h for the heavy particle takes, in terms of the dimensionless variable $\mathbf{r} = \mathbf{r}_h/R$, the following form:

$$\frac{H_h}{\hbar^2/R^2 m_h} = -\frac{1}{2}\nabla^2 - \tilde{V}_0 \frac{m_h}{m_e} \frac{\tilde{R}^3}{\pi} \int_{r' < 1} e^{-2\tilde{R}|\mathbf{r}' - \mathbf{r}|} d^3 r'. \tag{12}$$

Consequently, the zero-eigenvalue condition must be of the form

$$\tilde{V}_0^c = A(\tilde{R}) \frac{m_e}{m_h} \qquad (m_h \gg m_e), \tag{13}$$

where A is a dimensionless function of $\tilde{R}$. It is easy to see from (10) that $A(\tilde{R})$ must be a decreasing function of $\tilde{R}$, and limiting cases can be evaluated. For small R the potential (10) is approximately

$$v(r_h) \simeq -\tfrac{4}{3} V_0 \tilde{R}^3 e^{-2r_h/a_0}, \tag{14}$$

and the s-state *zero-energy* Schrödinger equation with this potential is satisfied $J_0(\sqrt{8\tilde{V}_0 \tilde{R} m_h / 3 m_e e^{-r_h/a_0}})/r_h$, where J_0 is a Bessel function. The requirement that the wave function is finite at $r_h = 0$ selects the critical values of V_0. In our case $\tilde{V}_0^c = 3 j_0^2 m_e / 8\tilde{R} m_h$, in which $j_0 = 2.4048...$ is the first zero of $J_0(x)$. This corresponds to $A(\tilde{R}) = 2.17\tilde{R}^{-1}$. In addition to this small-$\tilde{R}$ behavior we have $A(\infty) = \pi^2/8$, and intermediate numerical values are easy to compute. We find, e.g., $A(0.10) = 21.73, A(0.25) = 8.8, A(0.50) = 4.5$, and $A(1) = 2.53$.

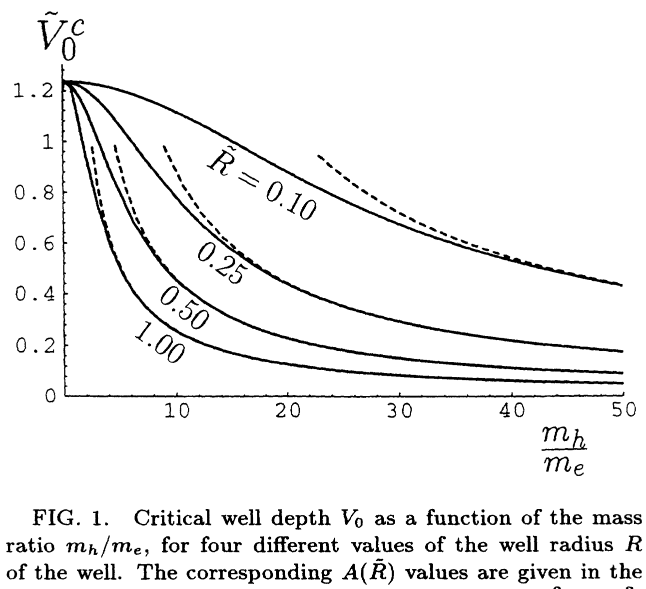

FIG. 1. Critical well depth V_0 as a function of the mass ratio m_h/m_e, for four different values of the well radius R of the well. The corresponding $A(\tilde{R})$ values are given in the main text. The well depth is measured in units of $\hbar^2/m_e R^2$, and the well radius is measured in units of the effective Bohr radius $a_0 = 4\pi\varepsilon\hbar^2/e^2 m_e$. The fully drawn curves represent the interpolation (16), and the dashed curves the asymptotic result (13).

By (13) the critical depth V_0^c falls off inversely proportional to the satellite mass m_h. Hence the perturbation treatment of the local potential is justified for large mass ratios.

In the opposite limit, when the satellite mass is very light, the critical trapping condition is clearly (4),

$$\lim_{m_h \to 0} \tilde{V}_0^c = \frac{\pi^2}{8}, \tag{15}$$

and a Born-Oppenheimer approach shows that the correction to first order in the mass ratio m_h/m_e vanishes.

A very simple interpolation formula that is consistent with both limiting cases is the following:

$$\tilde{V}_0^c = A \frac{m_e}{m_h} \tanh\left(\frac{\pi^2 m_h}{8A\, m_e} \right), \tag{16}$$

which is shown in Fig. 1, and compared with the corresponding asymptotic results (13). This sums up the situation qualitatively, as well as semiquantitatively. For the special case $m_h = m_e, \tilde{R} = 1$, Eq. (16) yields $\tilde{V}_0^c = 1.14$, close to, and on the correct side of, the variational result (8).

In conclusion, we have shown that a particle (an electron, say) may be trapped by a local potential, due to the presence of a satellite particle (a hole) that does not interact with the potential. The effect is less pronounced than a mass increase equal to the satellite mass would have brought about.

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