Bound states of two particles confined to parallel two-dimensional layers and interacting via dipole-dipole or dipole-charge laws

V. I. Yudson
Abteilung Theoretische Physik, Universität Ulm, 89069 Ulm, Germany
and Institute of Spectroscopy, Russian Academy of Science, Troitzk 142092, Moscow reg., Russia

M. G. Rozman
Institute of Physics, Riia 142, EE2400 Tartu, Estonia

P. Reineker
Abteilung Theoretische Physik, Universität Ulm, 89069 Ulm, Germany

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The problem of a bound state of two particles confined to parallel two-dimensional layers and interacting via dipole-dipole or dipole-charge laws arises in connection with the study of bound states of charge-transfer excitons at parallel interfaces or biexcitons and charged exciton complexes in double quantum wells. Binding energies of the dipole-charge and the dipole-dipole complexes are calculated as functions of the corresponding coupling constants. It is shown that for the dipole-charge interaction the bound state exists at an arbitrary small coupling constant, though the binding energy decreases dramatically when the coupling constant falls below some critical value. On the contrary, it is shown for the dipole-dipole interaction that the bound state exists only when the coupling constant exceeds a critical value. [S0163-1829(97)05408-8]

I. INTRODUCTION

The study of exciton-exciton and exciton-charge interactions in organic and semiconductor nanostructures is one of the hot topics of contemporary research.1 There is considerable interest in a bound complex of an exciton and an extra charge, as well as in a biexciton state, i.e., a bound state of two excitons (or exciton and a charge carrier) located in neighboring layers may lead to a bound exciton-exciton (or exciton-charge) state. In a somewhat idealized treatment this puts forward a problem of a bound state of two particles confined to two parallel two-dimensional (2D) layers and interacting via dipole-dipole or dipole-charge laws. This quantum-mechanical problem is the subject of the present paper. More extended physical applications of the obtained results will be considered in a separate publication.5

Below we calculate the binding energies of the dipole-dipole and dipole-charge complexes as functions of the corresponding coupling constants. We show that for the dipole-charge interaction the bound state exists at an arbitrary small coupling constant, though the binding energy decreases dramatically when the coupling constant falls below some critical value. On the contrary, for the dipole-dipole interaction the bound state exists only when the coupling constant exceeds a critical value. This seems contradictory with respect to the common opinion that a bound state may exist in an arbitrary shallow 2D potential well. We analyze the reason of this contradiction.

The present paper is organized as follows. In Sec. II we introduce the model. The cases of the dipole-charge and the dipole-dipole interactions are treated in the Secs. III and IV, respectively. The summary and discussion of the results are offered in Sec. V.

II. THE MODEL

We consider two particles, and each of them is confined to one of two parallel 2D layers separated by the distance \( l \). The dipole moment of each particle (if nonzero) is assumed to be oriented along the \( \hat{z} \) axis perpendicular to the layer plane. We study two cases: (1) one of the particles bears a charge \( e \) while the other is neutral and possesses a nonzero dipole moment \( \mu_1 \) such that the particle interaction is attractive; (2) both particles are neutral and have dipole moments \( \mu_1 \) and \( \mu_2 \), respectively. The interaction potential has the form

\[
V(p) = -\frac{e \mu}{\varepsilon} \frac{l}{(\rho^2 + l^2)^{3/2}} \tag{1}
\]

for the dipole-charge interaction and

\[
V(p) = \frac{\mu_1 \mu_2}{\varepsilon} \left[ \frac{1}{(\rho^2 + l^2)^{3/2}} - \frac{3l^2}{(\rho^2 + l^2)^{5/2}} \right] \tag{2}
\]

for the dipole-dipole interaction. Here \( \rho \) is the distance between the particles along the planes, and \( \varepsilon \) is the dielectric constant of the surrounding medium. The sign in Eq. (2) corresponds to the case of equally oriented dipoles (normal
to the layer planes). The opposite sign would correspond to the case of antiparallel dipoles, which we will discuss briefly in Sec. IV E. The interaction potentials (1) and (2) are presented in Fig. 1.

The radial wave function $\psi(\rho)$ of the relative motion of two particles with zero angular momentum obeys the Schrödinger equation

$$\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} \psi(\rho) = \left[ \frac{2mV(\rho)}{\hbar^2} + k^2 \right] \psi(\rho),$$

(3)

where $m$ is the reduced mass of the particles and $-\hbar^2k^2/(2m) = E$ is the bound state energy.

We are not aware of an exact solution of Eq. (3) for the potential given by Eqs. (1) and (2), so that in the following analysis we will use various approximate approaches whose choice will be determined by the value of a dimensionless coupling constant

$$\alpha = \frac{me\mu}{\hbar^2},$$

(4)

for the dipole-charge interaction, and

$$\alpha = \frac{m\mu_1\mu_2}{\hbar^2l}$$

(5)

for the dipole-dipole interaction.

III. DIPOLE-CHARGE INTERACTION

A. Large coupling constant

First, we consider the case of a large coupling constant $\alpha$ (4). In this case, we expect that the in-plane radius $\rho_0$ of the ground state is small as compared to the interlayer distance $l$. Expanding the potential energy Eq. (1) in powers of the small ratio $\rho/l$ we have approximately

$$V(\rho) = -\frac{e\mu}{\ell l} + \frac{3e\mu}{2\ell^2}\rho^2,$$

(6)

which corresponds to the potential of an isotropic 2D harmonic oscillator with frequency

$$\omega_0 = \sqrt{\frac{3e\mu}{em\ell^2}}.$$  

(7)

The wave function of the ground state is given by the expression

$$\psi(\rho) = \sqrt{\frac{\pi}{\rho_0}} e^{-\rho^2/\rho_0^2},$$

(8)

where

$$\rho_0 = \frac{\hbar}{m\omega_0} = \frac{l}{3\alpha}^{1/4}$$

(9)

is the characteristic radius of the bound state. As follows from Eq. (9), at large $\alpha$ the assumption $\rho_0 \ll l$ is justified, indeed. In this approximation, the ground-state energy of the bound particles is given by

$$E \approx E^{(0)} = -\frac{e\mu}{\ell l} + \hbar \omega_0$$

(10)

where the second (quantum) term is smaller than the first (classical) one by the factor $\sim 1/\sqrt{\alpha}$.

The next term of the expansion of the potential $V(\rho)$ Eq. (1) is

$$\delta V(\rho) = -\frac{15e\mu\rho^4}{8\ell^6}.$$  

The corresponding correction to the ground-state energy Eq. (10) can be calculated in the first-order perturbation theory with respect to $\delta V$:

$$\delta E = \langle \delta V \rangle_0,$$

where the matrix element $\langle \ldots \rangle_0$ is calculated using the ground state of the 2D harmonic oscillator (8). We arrive at the following expression for the bound state energy

$$E \approx \frac{\hbar^2}{2ml^2}\left(-2\alpha + 2\sqrt{3\alpha} - \frac{5}{2}\right),$$

(11)

which is arranged according to decreasing powers of $\sqrt{\alpha}$.

B. Small coupling constant

Now we consider the opposite case of a small coupling constant $\alpha \ll 1$. At $\rho = 0$ the potential Eq. (1) equals

$$V(0) = -\frac{e\mu}{\ell l} = -2\alpha \left(\frac{\hbar^2}{2ml^2}\right),$$

and $|V(\rho)|$ decays $\sim 1/\rho^3$ for $\rho \gg l$. A bound state at this shallow 2D potential well may be found using a known approach. The latter, introduced formally for potential wells of finite radii, should be modified to take into account a relatively slow power decay of $V(\rho)$ at large $\rho$. 

FIG. 1. Dimensionless potential $\tilde{V} = V(\rho)/|V(0)|$ of the dipole-charge (dc) and the dipole-dipole (dd) interactions.
For small $\alpha$, we are looking for a solution to Eq. (3) that corresponds to a weakly bound state with $k \ll 1/l$. Introducing the parameter $\tilde{\rho}$ by the equality $2m|V(\tilde{\rho})|\hbar^2 = k^2$, we find

$$\tilde{\rho} = \left( \frac{2me\mu l}{e\hbar^2k^2} \right)^{1/3} = \left( \frac{2al}{k^2} \right)^{1/3}. \tag{12}$$

Here we have assumed that

$$l \ll \tilde{\rho} \ll 1/k \tag{13}$$

and used the asymptotic expression for $V(\rho)$ at large $\rho$. At $\rho \ll \tilde{\rho}$ or at $\rho \simeq \tilde{\rho}$ one may neglect, respectively, the term $k^2$ or $2mV(\rho)/\hbar^2$ in the right-hand side (rhs) of Eq. (3). Multiplying both parts of Eq. (3) by $\rho$ and integrating from 0 to $\rho_1$ ($l \ll \rho_1 \ll \tilde{\rho}$), we obtain the following relation:

$$\left( \frac{d}{d\rho} \psi(\rho) \right)_{\rho_1} + \frac{2m}{\hbar^2} \int_0^{\rho_1} V(\rho)\psi(\rho)d\rho = \frac{2m}{\hbar^2} \psi(\rho_1) \int_0^\infty V(\rho)d\rho. \tag{14}$$

On the rhs of Eq. (14) we have neglected the change of the wave function at $\rho \ll 1/k$ and set its argument equal to $\rho_1$. Because of the fast convergence, the upper limit of the integral has been extended to infinity.

At $\rho \simeq \tilde{\rho}$ the function $\psi(\rho)$ is given by the solution of the Schrödinger equation for a free particle:

$$\psi(\rho) \sim K_0(k\rho),$$

where $K_0(x)$ is the zero-order Hankel function of the first kind. At small $x$ $K_0(x) \sim -\ln x$. Therefore, for an arbitrary $\rho_2$ in the interval $\rho_1 < \rho_2 \ll 1/k$ we obtain for the derivative of $\ln[\psi(\rho)]$:

$$\left( \frac{d}{d\rho} \ln[\psi(\rho)] \right)_{\rho_2} \approx \frac{1}{\ln(k\rho_2)}. \tag{15}$$

Now we extrapolate Eq. (14) and Eq. (15) to the case $\rho_1 \rightarrow \tilde{\rho} \rightarrow \rho_2$ and obtain the relation

$$\frac{2m}{\hbar^2} \int_0^\infty V(\rho)d\rho = \frac{1}{\ln(k\rho_2)}. \tag{16}$$

Using Eqs. (12) and (16) we find

$$k = \frac{\hbar^2}{2me\mu l}\exp\left( -\frac{3}{2m} \int_0^\infty |V(\rho)|\rho d\rho \right)^{-1} \tag{17}$$

with $\alpha$ given by Eq. (4). It is easy to check that this value of $k$ justifies the assumption Eq. (13). Thus, at small coupling constant $\alpha$, the binding energy $E = -\hbar^2k^2/(2m)$ is exponentially small,

$$|E| = \frac{\hbar^2}{2ml^2} \frac{1}{4\alpha} \exp\left( -\frac{3}{\alpha} \right), \tag{18}$$

which is typical for bound states in a weak 2D potential.\(^6\)

C. Intermediate values of coupling constant: Variational approach

For intermediate values of the coupling constant Eq. (4) we use the variational approach with a simple one-parameter probe wave function

$$\psi(\rho) = \sqrt{\frac{2}{\pi l}} e^{-\kappa \rho l}. \tag{19}$$

Evaluating the kinetic and potential energies with this probe function we obtain the averaged Hamiltonian as a function of the dimensionless variational parameter $\kappa$:

$$H(\kappa) = \frac{\hbar^2}{2ml^2} f(\kappa, \alpha), \tag{20}$$

where

$$f(\kappa, \alpha) = \kappa^2 - 2\alpha \int_0^\infty \exp(-x)d\rho. \tag{21}$$

The ground-state binding energy is determined as the minimum value of the function $H(\kappa)$:

$$E(\alpha) = \frac{\hbar^2}{2ml^2} f(\alpha). \tag{22}$$

Here

$$f(\alpha) = \min f(\kappa, \alpha) = f(\kappa(\alpha), \alpha), \tag{23}$$

where $\kappa(\alpha)$ is a root of the equation:

$$1 = \frac{3\alpha}{4\kappa^2} \int_0^\infty \frac{x^3 \exp(-x)}{[1 + x^2/(2\kappa^2)]^{3/2}} = \frac{3\alpha}{4} \int_0^\infty \frac{x^3 \exp(-\kappa x)}{[1 + x^2/4]^{3/2}}. \tag{24}$$

Equation (24) makes obvious that the solution $\kappa(\alpha)$ exists only at $\alpha$ exceeding some critical value $\alpha_c$:

$$\alpha \geq \alpha_c = \frac{4}{3} \left( \int_0^\infty \frac{x^3 dx}{[1 + x^2/4]^{3/2}} \right)^{-1} \frac{1}{8}. \tag{25}$$

This condition contradicts the above conclusion about the existence of the bound state at an arbitrary small $\alpha$ and demonstrates clearly the restricted validity of the variational approach for the range of small coupling constants. However, this formal restriction may be of no practical significance: estimating the factor $(2\alpha)^{-2} \exp(-3\alpha)$ in the rhs of Eq. (18) at $\alpha = 1/8$, we find the negligible value $6 \times 10^{-10}$.

D. Comparison of analytical results with numerical calculations

To conclude this section, we have found the bound-state energies Eq. (11) and Eq. (18) for large and small values of the coupling constant Eq. (4), respectively. For intermediate coupling we found the variational expression Eq. (22). These results are plotted in Fig. (2) as functions of the coupling constant $\alpha$. In order to check the accuracy of the analytical approximations we present in the same figure results of direct numerical solution of Eq. (3) for the potential (1). We see that the variational approach gives quite satisfactory re-
results for values $\alpha$ less than 5–6, while at larger $\alpha$ the harmonic oscillator approach is more adequate.

IV. DIPOLE-DIPOLE INTERACTION

In contrast to the dipole-charge interaction potential Eq. (1), the potential of the dipole-dipole interaction Eq. (2) is not a monotonic function of $\rho$ (see Fig. 1). It has a minimum at $\rho=0$ and a maximum at $\rho=2l$.

A. Large coupling constant

As in the previous section, we begin with the case of large values of the coupling constant Eq. (5) (a discussion about physical realizations of this case is postponed for the concluding section). We expect the bound state to be well localized in the vicinity of the minimum of $V(\rho)$ at $\rho=0$, so that the in-plane radius $\rho_0$ of the state is small as compared to the width $\sim l$ of the potential well. Expanding the potential energy Eq. (2) in $\rho/l$ we have

$$V(\rho) \approx -\frac{2\mu_1\mu_2}{\epsilon l^3} + \frac{6\mu_1\mu_2}{\epsilon l^3} \rho^2,$$

which corresponds to the potential of a harmonic oscillator with the frequency

$$\omega_0 = \sqrt{\frac{12\mu_1\mu_2}{\epsilon ml^5}} .$$

The ground-state wave function is given by Eq. (8) where the characteristic size

$$\rho_0 = \frac{l}{(12\alpha)^{1/4}}$$

of the ground state is, indeed, smaller than $l$ at large $\alpha$. The ground-state energy of the bound particles is given by

$$E = E^{(0)} = -\frac{2\mu_1\mu_2}{\epsilon l^3} + \hbar \omega_0 .$$

where the second (quantum) term is smaller than the first (classical) one by the factor $-1/\sqrt{\alpha}$. Just as for the case of the dipole-charge interaction, one may find the correction to the harmonic approximation Eq. (29). As a result, we obtain the following expression for the bound-state energy:

$$E = \frac{\hbar^2}{2m l^2} \left( -4\alpha + 4\sqrt{\alpha} - \frac{15}{4} \right),$$

which is arranged according to decreasing powers of $\sqrt{\alpha}$. We see that in the strong coupling limit the dipole-dipole and dipole-charge interactions result in similar qualitative features of the bound states.

B. Small coupling constant

On the contrary, in the small coupling limit there is a drastic difference for the two interactions: no bound state exists in the potential Eq. (2) at $\alpha \ll 1$. The standard method\(^6\) of finding a bound-state energy for a shallow 2D well does not apply straightforwardly to the potential Eq. (2) because the quantity

$$\left[ \int_0^\infty V(\rho) \rho d\rho \right]^{-1}$$

that enters the expression for the binding energy does not exist: the integral equals zero. The reason is that the potential $V(\rho)$ Eq. (2) has a repulsive part and its contribution to the integral cancels exactly the contribution of the attractive part. Below we carry out a more careful analysis of this case.

Similar to the approach of the previous section we introduce the parameter $\bar{\rho}$ determined by the equality $2m V(\bar{\rho})/\hbar^2 = k^2$. Being expressed via the dimensionless coupling constant, the parameter $\bar{\rho}$ is given formally by the same expression $\bar{\rho} = (2\alpha l/k^2)^{1/3}$ as in the case of the dipole-charge interaction with $\alpha$ defined by Eq. (5). Here we have again assumed that $l \leq \bar{\rho} \leq 1/k$ and used the asymptotic expression for $V(\rho)$ at large $\rho$. At $\rho \ll \bar{\rho}$ (or $\rho \gg \bar{\rho}$) one may neglect the term $k^2$ [or $2m V(\rho)/\hbar^2$] in the rhs of Eq. (3). The following derivation is similar to the one in the previous section. However, now we keep finite the upper limits $\rho_1$ and $\bar{\rho}$ of the integrals in Eqs. (14) and (16), respectively (otherwise these integrals would equal zero). So, for the integral on the left-hand side of Eq. (16) we obtain

$$\int_0^{\bar{\rho}} V(\rho) \rho d\rho = - \int_{\rho}^\infty V(\rho) \rho d\rho \approx - \frac{\mu_1\mu_2 l^2}{\epsilon} \frac{1}{\bar{\rho}} .$$

As a result, we have instead of Eq. (16) the following relation:
The modified interaction potential has a minimum at $\rho = 2l$. In the strong coupling limit there exists a bound state localized in the vicinity of this minimum with the binding energy

$$E = E^{(0)} = -\frac{2\sqrt{5}\mu_1\mu_2}{125\varepsilon l^3} + \frac{\hbar \omega_0}{2}$$

$$= \frac{\hbar^2}{2ml^2} \left[ -\frac{4\sqrt{5}\alpha}{125} + \left( \frac{24\sqrt{5}\alpha}{625} \right)^{1/2} \right].$$

Here the frequency is

$$\omega_0 = \left( \frac{24\sqrt{5}\mu_1\mu_2}{625\varepsilon ml^5} \right)^{1/2}.$$ 

Note that in this case we deal not with an isotropic 2D harmonic oscillator (as in the case of parallel dipoles) but with a 1D oscillator (for the radial degree of freedom), while the second degree of freedom corresponds to the free angular rotation. This difference explains the origin of the factor $1/2$ in the last term on the rhs of Eq. (37). Another remark concerns the difference between Eq. (3) and a standard 1D Schrödinger equation with the kinetic energy term $[\sim d^2/dx^2 \psi(x)]$. The substitution $\psi(x) = \tilde{\psi}(x)/\sqrt{\rho}$ transforms Eq. (3) to a 1D Schrödinger equation with the standard kinetic energy operator and a new potential

$$V_{\text{eff}}(\rho) = V(\rho) + \frac{\hbar^2}{8m\rho^2}.$$ 

In the considered case of large $\alpha$ the corrections to the ground-state energy caused by the additional term in the effective potential are of zero order in $\alpha$. These corrections are small as compared to the terms ($\sim \alpha$ and $\sim \sqrt{\alpha}$) retained in Eq. (37).

Similar to the previous case of parallel dipoles, there are no bound states in the weak coupling limit. However, the range of intermediate values of the coupling constant Eq. (5) requires a more delicate approach: the simplest choice of the probe function $\psi(\rho) \sim \exp(-\kappa \rho l)$ does not yield a minimum of the averaged Hamiltonian. This is because such a wave function overestimates the contribution of the region $\rho < \sqrt{2l}$ where the potential energy is positive. A more appropriate probe function should model the decrease of the true wave function in that region. Actually it would force one to go beyond the simple one-parameter variational approach and here we will not pursue this aim.

V. CONCLUSION

Here we make some comments concerning physical realizations of different regimes for excitons in a double quantum well. The weak coupling regime corresponds to the case of a weak external static electric field applied perpendicular to the QW plane, so that the induced static dipole moments of the excitons are small. The realization of the strong coupling case is more complicated. Assuming that the dipole moment of the particles is due to an electron displacement by a distance $d$, so that $\mu = ed$, the coupling constants Eqs. (4) and (5) may be rewritten as $\alpha = d/a$ for the dipole-charge coupling.
interactions and $\alpha = d^2/(a \ell)$ for the dipole-dipole interactions; $a = e\hbar^2/(me^2)$ is the effective Bohr radius. The case $\alpha \gg 1$ together with the validity condition $d \ll \ell$ of the dipole approximation result in the following range of parameters: $a \ll d \ll \ell$ and $\sqrt{a\ell} \ll d \ll \ell$, respectively. Thus, the realization of the strong coupling case would require a considerable electron-hole separation within “excitons.” This could be provided by a strong electric field. The possibility of physical realizations of various regimes and applications to excitons in double quantum wells will be considered in a separate publication\(^5\) using the above results.

To conclude, we have studied a bound-state problem for two particles confined to parallel two-dimensional (2D) layers and interacting via dipole-charge Eq. (1) or dipole-dipole Eq. (2) laws. The existence and the energy of the bound-state are determined by the corresponding coupling constant Eqs. (4) and (5). At $\alpha \gg 1$ the bound-state energy is given by Eqs. (11) and (30), respectively. At intermediate values of $\alpha, \alpha_c \ll \alpha$, the variational estimate for the binding energy is given by Eq. (22) with the function $f(\alpha)$ Eq. (23) determined correspondingly via Eqs. (21) and (34). The critical values $\alpha_c, \alpha_c'$ obtained within the framework of the variational approach are given by Eqs. (25) and (36). It has been demonstrated that no bound state exists for the dipole-dipole interaction at $\alpha \ll 1$, while for the dipole-charge interaction there may exist a weakly bound state with an exponentially small binding energy.

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