Two- and three particle complexes with logarithmic interaction: compact wave functions for two-dimensional excitons and trions

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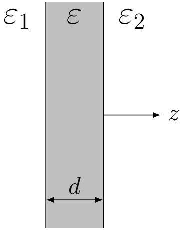

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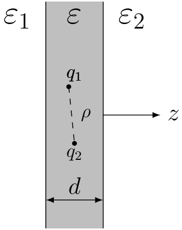

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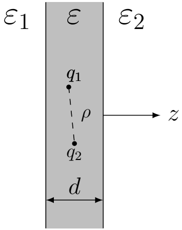

Interaction[1] ($d \ll 1$)

$$V(\rho) = \frac{\pi q_1 q_2}{(\varepsilon_1 + \varepsilon_2)\rho_0} W\left(\frac{\rho}{\rho_0}\right)$$

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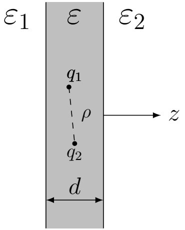

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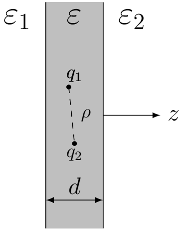

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When $a_0 \ll \rho_0$:

$$\boxed{V(\rho) \approx -\frac{q_1 q_2}{\rho_0} \ln\left(\frac{\rho}{\rho_0}\right)}$$

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How to study such complexes?

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d.o.f. = $2N - 3$ $\qquad N$: number of particles

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Variational Method + Orthogonalization Conditions
→ Optimal Configuration of Parameters

Results: Exciton

Variational energies provide 5 – 6 exact decimal digits

n_ρ \ $\|m\|$	0	1
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1	**1.314 677** 846 047 317	**1.662 90**1 190 508 306
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Our trial functions are **locally accurate** in the whole domain[2]

$$\left\| \frac{\psi_{exact}(\rho) - \psi^{approx}(\rho)}{\psi_{exact}(\rho)} \right\| \le 10^{-3} \ , \qquad \rho \in [0, \infty)$$

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→ They lead to accurate expectation values, not only energies.

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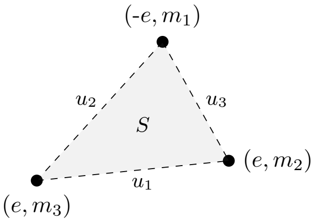

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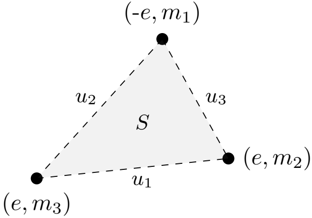

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For trions we may assume: $m_2 = m_3$

$$\sigma = \frac{m_1}{m_{2,3}}$$

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Schrödinger equation in *exciton units*[3]:

$$-\frac{1}{2}\Delta_\sigma\psi \; + \; \ln\left(\frac{u_2 u_3}{u_1}\right)\psi \; = \; \varepsilon(\sigma)\,\psi$$

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$$dV \;\propto\; u_1\,u_2\,u_3\,S^{-1}\,du_1\,du_2\,du_3$$

$$S \;=\; \frac{1}{4}\sqrt{(u_1+u_2+u_3)(u_1+u_2-u_3)(u_2+u_3-u_1)(u_1+u_3-u_2)}$$

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$$\psi^{(approx)}(u_1, u_2, u_3) = \frac{1}{2}(1 + P_{23})\left[\left(1 + \gamma\, u_1^2 \ln\left(u_1^2\right)\right) e^{-\Phi_{0,0}(\alpha^2 u_2) - \Phi_{0,0}(\beta^2 u_3)}\right]$$

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- $\Phi_{0,0}$: exciton phase with optimal parameters, and

$$e^{-\Phi_{0,0}(\alpha^2 u_2) - \Phi_{0,0}(\beta^2 u_3)}$$

Compact Wave Function

$$\psi^{(approx)}(u_1, u_2, u_3) = \frac{1}{2}(1 + P_{23})\left[\left(1 + \gamma\, u_1^2 \ln\left(u_1^2\right)\right) e^{-\Phi_{0,0}(\alpha^2 u_2) - \Phi_{0,0}(\beta^2 u_3)}\right]$$

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$\rightarrow$ Correlated functions

$$\boxed{\varepsilon_{fit}(\sigma) \;=\; a \;+\; b \ln(1 + c\,\sigma)}$$

$$a \;=\; 0.094\,, \qquad b \;=\; 0.472\,, \qquad c \;=\; 1.012$$

Results: Trions

Binding Energy

$$E_b = |E_{trion} - E_{exciton}|$$

[4]Taken from Szyniszewski, et al. Phys. Rev. 95, 2017

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Material	ρ_0 (Å)	σ	E_b (meV)	
			Present Results	Experiments/Theory[4]
MoS_2	39	0.81	40	34, 35
$MoSe_2$	40	0.86	38	30
WS_2	38	0.84	40	34, 36
WSe_2	45	0.85	34	30

(Results checked with an alternative trial function)

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Summary

- Excitons: benchmark variational calculations for energies and (locally accurate) wave functions.

- Trions: correlated wave function leads to binding energies in good agreement with experimental results.
- We find a simple formula for the binding energy as a function of the mass ratio of the constituent particles.

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Thanks for your attention!