

## Quantum mechanics with 2 particles

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### Abstract

A change of co-ordinates can often be used to simplify the analytic solution of the few-particle Schrödinger equation. Examples are given for the case of 2 interacting particles.

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It is often difficult to solve the Schrödinger equation for more than one interacting particle. Typically, computationally intensive numerical methods must be used however, in a few cases, there are some tricks available to help develop analytical and semi-analytical solutions. One trick that is particularly easy to apply to 2 interacting particles involves a simple change of co-ordinates. For example, in 1D positronium, the Schrödinger equation is

$$\left\{ \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_p^2} + \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_e^2} + v(x_p - x_e) \right\} \Psi(x_p, x_e) = E\Psi(x_p, x_e), \quad (1)$$

where  $x_p$  is the position of the positron,  $x_e$  is the position of the electron,  $m$  is the electron mass and  $v(x_p - x_e)$  is the Coulomb interaction. This equation can be simplified by transforming into centre of mass (CM) and relative motion (RM) co-ordinates:  $x_{CM} = x_p + x_e$  and  $x_{RM} = x_p - x_e$ . Then,

$$\left\{ \frac{-\hbar^2}{2(m/2)} \frac{\partial^2}{\partial x_{CM}^2} + \frac{-\hbar^2}{2(m/2)} \frac{\partial^2}{\partial x_{RM}^2} + v(x_{RM}) \right\} \Psi(x_{CM}, x_{RM}) = E\Psi(x_{CM}, x_{RM}). \quad (2)$$

In this form the Schrödinger equation is clearly separable,  $\Psi(x_{CM}, x_{RM}) = \phi(x_{CM})\psi(x_{RM})$ , and is relatively easy to solve. This example is also easily generalised to 3 dimensions.

Another situation where CM and RM co-ordinates are useful is when two interacting particles are trapped within a parabolic potential. This situation is particularly common because, near a minimum, all potentials are approximately parabolic. For example, for two electrons confined in a one dimensional electrostatic potential on a carbon nanotube the Schrödinger equation is approximately

$$\left\{ \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} + \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 + v(x_1 - x_2) \right\} \Psi(x_1, x_2) = E\Psi(x_1, x_2). \quad (3)$$

Here,  $x_1$  and  $x_2$  are the co-ordinates of each of the 2 electrons and the Coulomb interaction is often approximated as  $v(x_1 - x_2) = e^2/[(4\pi\epsilon_0\epsilon_r)(|x_1 - x_2| + R)]$ . Experimentally, 1D nanotube quantum dots have been engineered, and typically  $\hbar\omega \sim 10$  meV,  $\epsilon_r \sim 4$  and  $R \sim 1$  nm. Again, by rewriting in CM and RM co-ordinates this equation can be shown to be separable. The CM part of the equation is easily solved and the RM part can be solved approximately after Taylor expanding the RM potential to second order about its minimum.