

Space-Time Basis Functions For The Time-Dependent Schrödinger Equation

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The use of a basis set in space-time to solve the time-dependent Schrödinger equation is the subject of the presentation. The Schrödinger operator (SO) $[\hat{A}(x,t) - i\frac{\partial}{\partial t} - \hat{H}(x,t)]$ will thus be discretized using a basis in space and time. The spatial and spin coordinates are collectively represented by x . The objective is thus to solve the equation $\hat{A}(x,t) \psi(x,t) = 0$ using a space-time basis. The time axis will be discretized into time elements. Within each time-element, a decomposition will be made such that $\psi(x,t) = F(x,t) + \psi(x,t_0)$ where $F(x,t_0) = 0$. This presentation will discuss the use of various space-time basis sets in 1D and 3D for Coulomb potentials.