

# **Solution of Quantum Mechanical Initial-Value Problems Using Finite Elements in Time**

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A new method for solving Quantum Mechanical initial-value problems is presented which avoids the time-propagator and uses spectral elements in time with a spectral spatial basis.[1] This results in a set of coupled simultaneous equations and is thus an implicit stable procedure. A description of how this algorithm can be used to solve the time-dependent Schrödinger equation in both the Schrödinger and the Dirac representations for both bound-state and scattering problems with and without external time-dependent fields, will be given. As a corollary, a “black-box” algorithm will be presented[2] for evaluating the exponential of an arbitrary square matrix, even when the matrix is singular.

[1] C.A. Weatherford, E. Red, and A. Wynn III, *J. Mol. Structure (Theochem)* 592, 47 (2002).

[2] D.H. Gebremedhin, C.A. Weatherford, X. Zhang, A. Wynn III, and G. Tanaka, arXiv:0811.2612v1 [math-ph] 17 Nov 2008.

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