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The Pseudospectral Method: A Numerically Exact Partial Differential Equation Solver Applied to the Two-Electron Atom[1] PAUL GRABOWSKI, DAVID CHERNOFF, Cornell University — The pseudosprectral method can produce solutions to partial differential equations which converge exponentially fast towards the exact solution. We present how to use this method to solve the non-relativistic Schrödinger equation for helium and the negative hydrogen ion. We show how to properly treat the two-particle coalescence cusps and examine the effect of logarithmic terms in the exact solution. The only evidence of non-exponential convergence was for derivatives taken near the triple coalescence point. As developed and applied here the PS method has many virtues: no explicit assumptions need be made about the asymptotic behavior of the wavefunction near cusps or at large distances, the local energy ($\mathcal{H}\psi/\psi$) is exactly equal to the calculated global energy at all collocation points, local errors go down everywhere with increasing resolution, the effective basis using Chebyshev polynomials is complete and simple, and the method is easily extensible to other bound states. As the number of collocation points grows, the method achieves exponential convergence up to the resolution tested.

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