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The He-He dimer binding energy: A new computational method..
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An iterative method has been developed for calculating negative energy eigenvalues, based on the Lippmann-Schwinger integral equation [1]. A reliable method for finding approximate starting values for the iteration will be described. The He-He dimer is used to test the method, using the He-He TTY potential [2]. Due to the weak binding, the wave function extends out to large distances. For a distance of 3,000 a.u., 208 mesh points suffice to obtain an accuracy of three significant figures for the binding energy, while with 320 mesh points the accuracy is increased to six significant figures. [1] G. Rawitscher and I. Koltracht, "A new method to calculate Dimer binding energies with an economical number of mesh-points", submitted for publication. [2] K. T. Tang, J. P. Toennies, and C. L. Yiu, Phys. Rev. Lett. 74, 1546 (1995).

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