Solution of the Schroedinger Eq. in the presence of very long-range potentials

GEORGE RAWITSCHER, University of Connecticut — Conventional finite difference methods usually do not provide the required accuracy for the relative motion wave function of two colliding atoms or molecules for the large distances required in the presence of long range potentials at low temperatures. An alternative method is presented that obtains two independent solutions at large distances, that can be matched to the conventional solution at short distances. The method is akin to the Born approximation applied iteratively in the large distance domain, and hence by-passes the conventional methods of solving a differential equation. With this method, for a potential of the form $C_6/r^6$, 10 iterations suffice to achieve an accuracy of $10^{-10}$ in the radial domain $[100,1000]a_0$ for a wave number $k = 10^{-3}(a_0)^{-1}$. For the case $C_3/r^3$ convergence still takes place, but is not as fast, and requires a smaller radial domain. For example, an accuracy of $10^{-8}$ is obtained after 19 iterations in the domain $[2500,3000]a_0$, with $k = 10^{-3}(a_0)^{-1}$.

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