Iterative Solution of the Schroedinger Equation

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There are cases where the potentials present in the Schrödinger equation are of long range and have measurable effects, as for instance for the interaction between atoms or molecules at low temperatures, or for the calculation of atomic three-body collisions. In these cases the solution of the Schrödinger equation for the wave functions by finite difference or finite element techniques may not achieve the desired accuracy. An iterative method is presented, based on the Lippmann-Schwinger integral equation in coordinate space, that is similar in spirit to the Born approximation, but is applied only in the region of the potential tails. This procedure extends the numerical solution obtained for short distances to large distances without loss of accuracy, by iteratively obtaining two linearly independent solutions $Y(r)$ and $Z(r)$ in the long-range region. Numerical examples are presented, for atomic van der Waals potentials C_n/r^n. For $V_6 = C_6/r^6$. the size of the radial interval for which an accuracy of 10^{-10} is achieved is $\simeq [100, 1000]$ atomic units a_0. An example of the convergence of $Y(r)$ is given in the fgure below. The wave numbers k chosen for these examples correspond to atomic collision energies in the micro-Kelvin range, and the limit $k \to 0$ is also investigated. A criterion is given for determining whether the iterations will converge in that limit, as is detailed in Ref. [1]. An application to the nonlinear Gross-Pitaevskii case will be presented, if time permits.

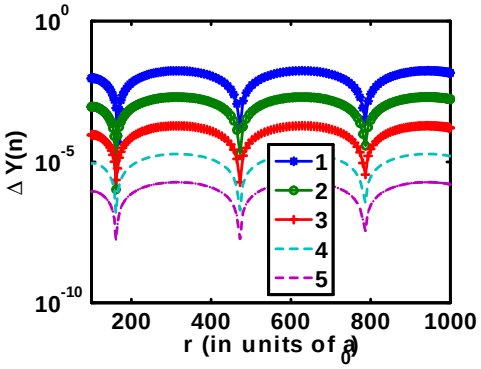
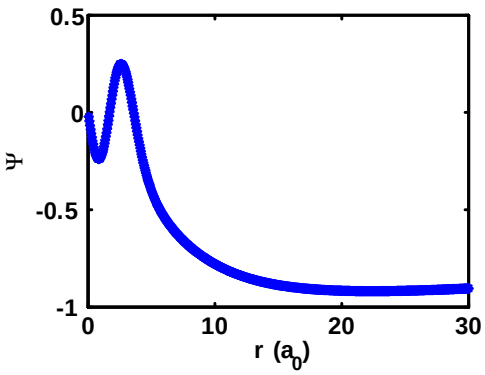


Fig. 1: The error of the function Y after 5 iterations The potential is V_6, the wave number is $k = 0.01\ a_0^{-1}$, $L = 0$, and the radial partition is $100 \le r \le 1000\ a_0$.



The wave function at small distances calculated non-iteratively, for potential V_6, $L = 0$, and $k = 0.01\ a_0^{-1}$

[1] G. Rawitscher, Phys. Rev. **A** (2013) 032708

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