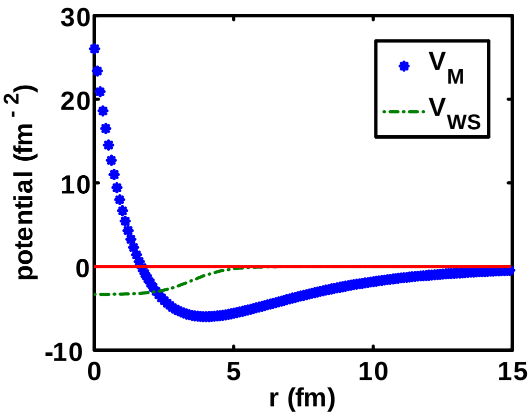

Figure 1: The Morse potential used in the calculations reported in the Table

Lecture 10

Program *wave.m* provided an example of the spectral Chebyshev solution of the Lippmann-Schwinger integral equation that corresponds to the radial Schrödinger Eq. with an exponential potential $V_0 \exp(-r/\alpha)$.In this example there was only one overall partition from $r = 0$ to $r_{\max}$ containing $N+1$ Chebyshev support points. Below a different and more complicated potential of the Morse-type is used that has a repulsive part near the origin, an attractive part further out, and decays exponentially with distance. The $S-IEM$ solution of the equivalent integral equation required, in this case, a partitioning of the radial domain, as described in Ref. [**?**]. Comparison with other methods of calculation is presented in the Table below, based on the study of a spectral finite element method presented in Ref. [2] . The potential, given in units of inverse length squared, defined in the radial range $[0 \leq r \leq 100]$, has the form

$$V_M(r) = 6\exp(z)[\exp(z) - 2]; \;\; z = -0.3r + 1.2, \tag{1}$$

and is illustrated in Fig. 1. The table below presents a comparison of the computational properties of three different methods: a) a S-IEM method [1], b) a Numerov method, and c) a finite element spectral method using Lagrange polynomials in each partition [2]. The computation used MATLAB on a desk PC using an Intel TM2 Quad, with a CPU Q 9950, a frequency of 2.83 GHz, and a RAM of 8 GB. As can be seen from the Table, the finite element method requires the shortest computing time, but accumulates errors at a faster rate than the S-IEM method, and will be described in detail in a future lecture.

$Method$	$\#points$	$phase\ shift\ error$	$time(s)$
$S-IEM$	425	5×10^{-11}	0.18
$S-IEM$	187	5×10^{-7}	0.16
$Numerov$	1600	6×10^{-7}	1.0
$FE-Lagr$	1300	10^{-8}	0.05

References

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