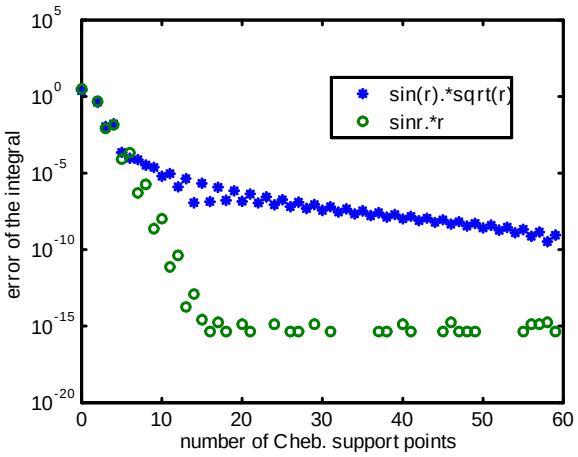

Figure 1: Convergence properties of the Gauss-Chebyshev integration procedure as a function of the number of Chebyshev support points, for both the integrals $I_1 = \int_0^\pi \sin(r)\ r^{1/2}\ dr$ and $I_2 = \int_0^\pi \sin(r)\ r\ dr$

Lecture 6:

In lecture 5 we presented examples of the rate of convergence of the Chebyshev expansion of two functions

$$f_1 = \sin(r)\ r^{1/2} \text{ and } f_2 = \sin(r)\ r \tag{1}$$

and also compared the result with Fourier series expansions. In both cases the expansion of f_1 was slower than that of f_2, because the first derivative of f_1 has a square root singularity, while f_2 has an infinite number of non-singular derivatives. As we will see in a future lecture, there are theorems that demonstrate these properties.

We also introduced the matrices S_L and S_R that give the Chebyshev expansion of the indefinite integrals $F(r) = \int_a^r f(r')dr'$ in terms of the Chebyshev expansions of the function f. By summing the expansion coefficients of the indefinite integral using S_L one also obtains the definite integral $I = \int_a^b f(r)dr$. We will make much use of these matrices. These properties are discussed extensively in Refs [1]-[4].

If the Chebyshev expansion of the function f converges slowly, then the error of the integral I also decreases slowly with the number of Chebyshev polynomials used to expand f. This will now be demonstrated numerically. The error of the two definite integrals

$$I_1 = \int_0^\pi \sin(r)\ r^{1/2} \text{ and } I_1 = \int_0^\pi \sin(r)\ r \tag{2}$$

is displayed in Fig. 1 A comparison of the error of the integrals I_1 and I_2 with

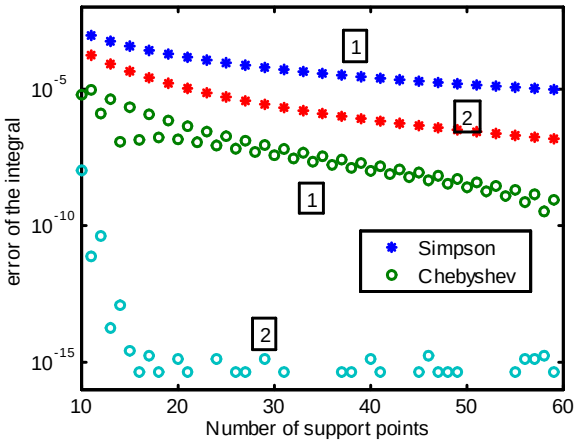

Figure 2: Comparison of the convergence properties of the Gauss-Chebyshev and the Simpson integration procedures as a function of the number of support points. The labels 1 or 2 denote the integrals $I_1 = \int_0^\pi \sin(r)\ r^{1/2}\ dr$ or $I_2 = \int_0^\pi \sin(r)\ r\ dr$, respectively.

the corresponding errors of the finite difference Simpson method is displayed in Fig. 2. The figure shows that for the same number of mesh-points, the accuracy of the Simpson method is less than that of the Chebyshev method. This difference is especially pronounced for the case of I_2

Another important property is the estimate of the error of a Chebyshev expansion. That error is the error of truncating the expansion at a certain value of N terms. The rule of thumb is that this error is proportional to the absolute value of the last expansion coefficient a_N, once the expansion begins to converge very rapidly. In order to demonstrate this property, we reconsider the expansion of the function

$$f(x) = e^x, \quad -1 \leq x \leq 1. \tag{3}$$

The Chebyshev expansion coefficients a_i are illustrated in Fig. 3 and the error ϵ_N of the expansion is defined in Eq. (4).

$$f(x) = \sum_{k=1}^{n} a_k T_{k-1}(x) + \epsilon_n. \tag{4}$$

In order to show that this error is proportional to the last expansion coefficient a_n, the ratio ϵ_n/a_n is displayed in Fig. 4.

This figure shows not only that the error is indeed proportional to the last expansion coefficient, but also that the error is uniform in the variable x, i.e., the upper limit of the absolute value of the error is independent of the value of x. This is one of the interesting properties of Chebyshev expansions, as will be discussed further in a future lecture.

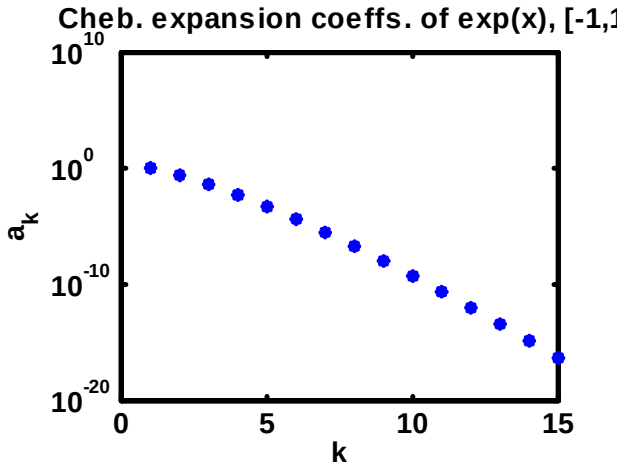

Figure 3: The Chebyshev expansion coefficients a_k of $\exp(x) = \sum_{k=1}^{n} a_k T_{k-1}(x)$ in the interval $[-1, 1]$

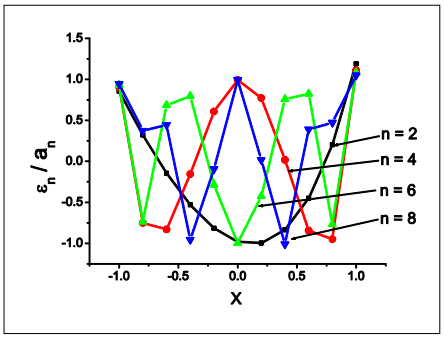

Figure 4: Error $\epsilon_n(x)$ of the expansion of $\exp(x)$, in the interval $[-1, 1]$, divided by the last. Chebyshev expansion coefficients a_n in the expansion $\exp(x) = \sum_{i=1}^{n} a_i T_{i-1}(x) + \epsilon_n$.

The integral equation corresponding to a differential equation

The Schrödinger second order differential equation in one dimension has the form

$$\left(\frac{d^2}{dr^2} + k^2\right)\psi(r) = V(r)\psi(r), \tag{5}$$

that normally is solved by a finite difference method, such as Runge-Kutta. Here $\psi(r)$ is the wave function to be obtained, r is the radial distance, k^2 is the energy in units of inverse length squared (assumed given), k is the wave number in units of inverse length, and $V(r)$ (assumed given) is the potential. V , also in units of inverse length squared, and ψ is dimensionless. The connection between the energy and the potential, both in energy units (joules) involves Plank's constant and the reduced mass of the two interacting objects, i.e., The energy and the potential, both in energy units, after being multiplied by $2m/\hbar^2$, are the quantities that appear in Eq. (5)

There exists the equivalent integral equation, denoted as Lippmann-Schwinger $(L-S)$, of the form

$$\psi(r) = \sin(kr) + \int_0^\infty \mathcal{G}_k(r,r')\ V(r')\ \psi(r')\ dr'. \tag{6}$$

The Greens function $\mathcal{G}_k(r,r')$ and the boundary conditions for ψ will be described below. Physicists prefer to solve the differential equation because of the simplicity of the numerical recurrence relation algorithm, and shy away from solving integral equations because the matrices are non-sparse and cumbersome to handle as well as memory intensive. However $\mathcal{G}_k(r,r')$ in configuration space is much simpler than in momentum space, where there occur no denominators with $i\varepsilon$, i.e., the singularity in configuration space is simpler to handle computationally and leads to higher accuracy.

In configuration space the Green's function $\mathcal{G}_k(r,r')$ is given by

$$\mathcal{G}_k(r,r') = -\frac{1}{k}F(r_<)G(r'_>) \tag{7}$$

$r_<$ and $r_>$ being the lesser and larger values of r and r', respectively, where

$$F(r) = \sin(kr), \qquad G(r) = \cos(kr) \tag{8}$$

and where k is the wave number defined in Eq. (5). Thus, the explicit form of Eq. (6) is

$$\begin{aligned}\psi(r) &= F(r) - \frac{1}{k}F(r)\int_r^\infty G(r')\ V(r')\ \psi(r')\ dr' \\ &\quad -\frac{1}{k}G(r)\int_0^r F(r')\ V(r')\ \psi(r')\ dr'.\end{aligned} \tag{9}$$

The functions F and G are solutions of $\left(d^2/dr^2 + k^2\right)F(r) = 0$, and $\left(d^2/dr^2 + k^2\right)G(r) = 0$. They are linearly independent of each other, and F approaches 0 as $r \rightarrow$

0, while G approaches a constant. If the differential operator includes the term$L(L+1)/r^2$,i.e., $\left(d^2/dr^2 + k^2\right)$ is replaced by $\left(d^2/dr^2 - L(L+1)/r^2 + k^2\right)$, then F and G are the regular and irregular spherical Bessel functions.

Please note (or show) that the solution of Eq. (9) also obeys Eq. (5), and further, that the derivative $\psi'(r) = d\psi(r)/dr$ is given by

$$\begin{aligned} \psi'(r) &= k\cos(kr) - \frac{1}{k}F'(r)\int_r^\infty G(r')\ V(r')\ \psi(r')\ dr' \\ &\quad -\frac{1}{k}G'(r)\int_0^r F(r')\ V(r')\ \psi(r')\ dr'. \end{aligned} \tag{10}$$

In the derivation of Eq. (10) the terms due to the derivatives of the integrals cancel each other. This equation is very useful because it contains the derivatives of known functions F and G, and the rest is done by integrals that in the spectral method do not lose accuracy.

The spectral expansion method (S-IEM).

The spectral representation of Eq. (9) proceeds as follows:

1. The upper limit of integration ∞ is replaced by $R_{\max}$, beyond which the potential V is sufficiently negligible, and the number N of Chebyshev expansion polynomials is chosen.

2. The unknown expansion coefficient a_k of ψ are written in a column form (a^ψ), and the corresponding column of the (unknown) function $\psi(\xi_k)$ at at the position of the support points ξ_k, $k = 1, 2, ..N$ is written as $(\psi) = C(a^\psi)$.

3. The functions F and V are written as diagonal matrices, with the values at the support points written at the diagonal of the matrices.

$$F_D = \begin{pmatrix} F(\xi_1) & & & \\ & F(\xi_2) & & \\ & & \ddots & \\ & & & F(\xi_N) \end{pmatrix}$$

The product $F_D V_D C(a^\psi)$ is a column vector containing as entries $F(\xi_k)V(\xi_k)\psi(\xi_k)$.

4. The expansion coefficients of this column vector are given by $C^{-1}F_D V_D C(a^\psi)$, and the expansion coefficients b_k of the integral $\int_r^{R_{\max}} FV\psi dr'$are given by $S_R C^{-1} F_D V_D C(a^\psi)$.

5. With the additional multiplication by C the column vector in step 4. is transformed back into a column vector of the corresponding function evaluated at the ξ_k's . That in turn is multiplied by $-(1/k)(R_{\max}/2)G_D$, and "voila'", one has the column vector of the functions representing the last term term of Eq. (9). That can again be transformed into the column vector of the respective expansion coefficients by an additional multiplication by C^{-1}. The factor $(R_{\max}/2)$ is due to the integral being over $dr\prime$ rather over dx.

In summary the last term of Eq. (9) is

$$-C^{-1}(1/k)(R_{\max}/2)G_D C S_L C^{-1} F_D V_D C(a^\psi)$$

The middle term of Eq. (9) is correspondingly

$$-C^{-1}(1/k)(R_{\max}/2)F_D C S_R C^{-1} G_D V_D C(a^{\psi})$$

and the sum of these two terms gives rise to the matrix

$$M = -C^{-1}(1/k)(R_{\max}/2)\left[F_D C S_R C^{-1} G_D + G_D C S_L C^{-1} F_D\right] V_D C \qquad (11)$$

The final equation for the expansion coefficients (a^{ψ}),according to Eq. (**??**) is

$$(1_D - M)(a^{\psi}) = (a^F). \qquad (12)$$

In order to solve for (a^{ψ}), the inverse of the matrix $(1_D - M)$ appears to be required. However in MATLAB there is a command "\",

$$(a^{\psi}) = (1_D - M)\backslash(a^F)$$

that instead solves a set of linear equations.

The above manipulations are at the heart of the S-IEM method to solve the one-dimensional radial Schrödinger equation. In practice however, additional details are needed in order to divide the whole radial domain $[0, R_{\max}]$ into partitions, as will be explained in a future lecture.

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[2] R. A. Gonzales, R.A., Kang, S.-Y., Koltracht, I. and Rawitscher G., "Integral Equation Method for Coupled Schrödinger Equations", *J. of Comput. Phys.,*1999, **153**, 160-202;

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[4] Rawitscher, George H. 2009 "Applications of a Numerical Spectral Expansion Method to Problems in Physics; a Retrospective" in Operator Theory: Advances and Applications 203 (2009, Birkhauser Verlag, Basel/Switzerland) 409-426