993SM - Laboratory of Computational Physics
II week
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The Numerov's method for the 1D Schroedinger equation

codes & notes from:

prof. Paolo Giannozzi (UniUD)

"Numerical methods in Quantum Mechanics"

https://www.fisica.uniud.it/~giannozz/Corsi/MQ/LectureNotes/mq.pdf

https://www.fisica.uniud.it/~giannozz/Corsi/MQ/Software/F90/harmonic0.f90

https://www.fisica.uniud.it/~giannozz/Corsi/MQ/Software/F90/harmonic1.f90

Note:
we choose a problem that can be solved exactly
(analytically)
to check the reliability of the code
and the possible problems

the harmonic oscillator

harmonic oscillator:
classical

Force $F = -Kx$

$$m\frac{d^2x}{dt^2} = -Kx$$

Potential $V(x) = V(-x) = \frac{1}{2}Kx^2$

A solution $x(t) = x_0 \sin(\omega t)$ with $\omega = \sqrt{\frac{K}{m}}$

probability $\rho(x)dx$ to find the mass between x and $x + dx$:

$$\rho(x)dx \propto \frac{dx}{v(x)}$$

Since $v(t) = x_0\omega\cos(\omega t) = \omega\sqrt{x_0^2 - x_0^2\sin^2(\omega t)}$, we have

$$\rho(x) \propto \frac{1}{\sqrt{x_0^2 - x^2}}$$

for $|x| < x_0$; 0 elsewhere

harmonic oscillator:
1D Schroedinger eq.

In standard notation:

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - \frac{1}{2}Kx^2\right)\psi(x) \qquad \text{with} \qquad \omega = \sqrt{\frac{K}{m}}$$

Note the symmetry of the potential: $V(-x) = V(x)$

Defining:

$$\xi = \left(\frac{m\omega}{\hbar}\right)^{1/2} x = \left(\frac{mK}{\hbar^2}\right)^{1/4} x = \frac{x}{\lambda} \quad \text{and} \quad \varepsilon = \frac{E}{\hbar\omega}$$

we rewrite the eq. in adimensional units:

$$\frac{d^2\psi}{d\xi^2} = -2\left(\varepsilon - \frac{\xi^2}{2}\right)\psi(\xi)$$

harmonic oscillator:
1D Schroedinger eq.

Exact solution (analytical):

$$\psi_n(\xi) = H_n(\xi)\mathrm{e}^{-\xi^2/2}$$

odd or even functions

n nodes and the same parity as n

Hermite polynomials. $H_n(\xi)$

The lowest-order Hermite polynomials are

$$H_0(\xi) = 1, \quad H_1(\xi) = 2\xi, \quad H_2(\xi) = 4\xi^2 - 2, \quad H_3(\xi) = 8\xi^3 - 12\xi.$$

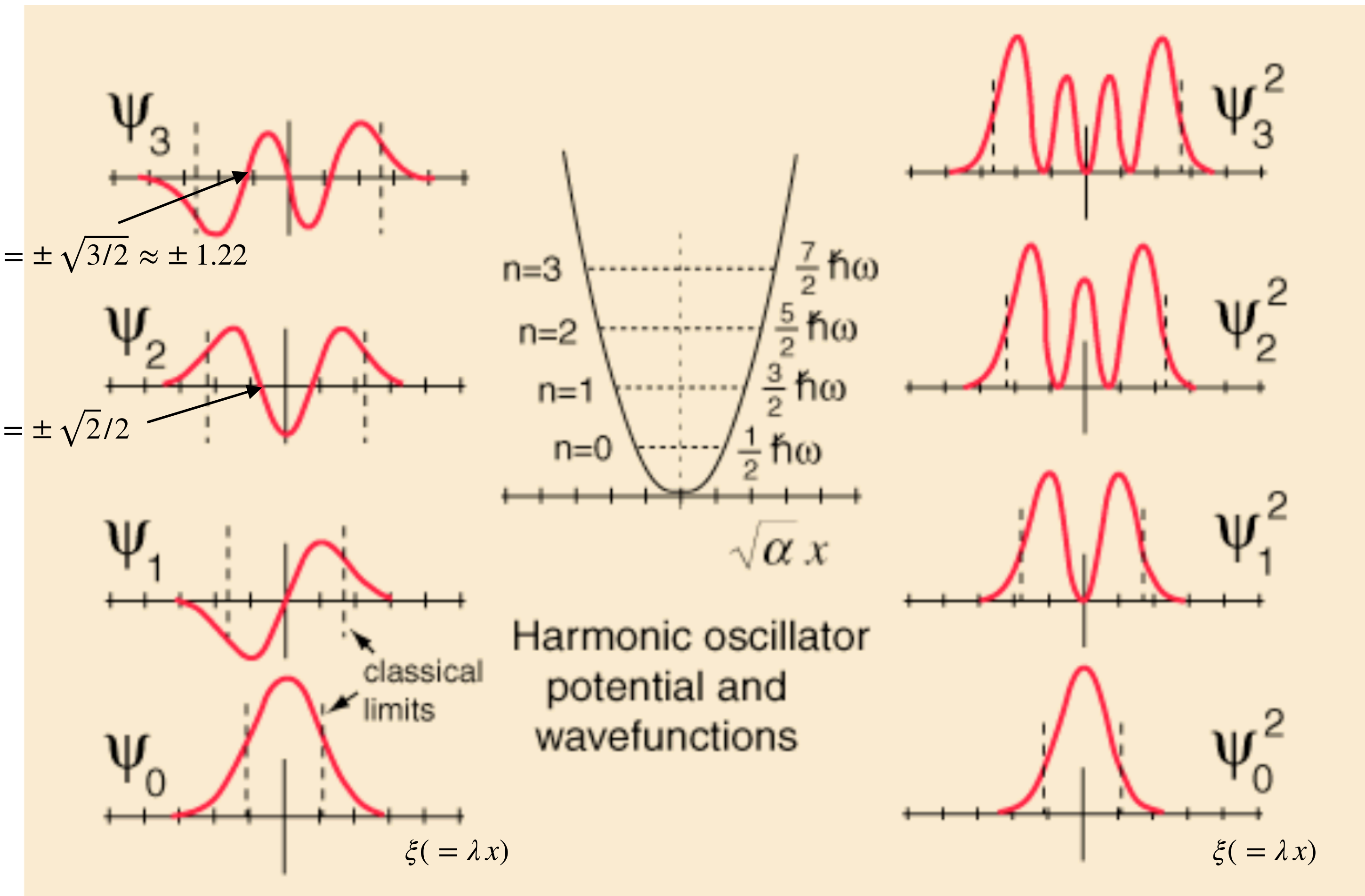
corresponding to discretized energies:

$$\varepsilon = n + \frac{1}{2} \quad \Rightarrow \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2, \ldots$$

n is a non-negative integer

harmonic oscillator:
1D Schroedinger eq.

Exact solution (plots):



$\mathscr{H}_3(\xi_0) = 0 \rightarrow \xi_0 = \pm\sqrt{3/2} \approx \pm 1.22$

$\mathscr{H}_2(\xi_0) = 0 \rightarrow \xi_0 = \pm\sqrt{2}/2$

The Numerov's method

To solve:

(g(x), s(x) given)

$$\frac{d^2y}{dx^2} = -g(x)y(x) + s(x)$$

idea: Taylor expansion of y(x), g(x), s(x), followed by a few manipulations

(details in the notes by prof. Giannozzi)

$$y_{n+1}\left[1 + g_{n+1}\frac{(\Delta x)^2}{12}\right] = 2y_n\left[1 - 5g_n\frac{(\Delta x)^2}{12}\right] - y_{n-1}\left[1 + g_{n-1}\frac{(\Delta x)^2}{12}\right] + (s_{n+1} + 10s_n + s_{n-1})\frac{(\Delta x)^2}{12} + O[(\Delta x)^6]$$

allows to obtain y_{n+1} starting from y_n and y_{n-1}, and recursively go on…

1D Schroedinger equation:
a form suitable for Numerov's method

The Scroedinger eq.:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x),$$

has the form:

$$\frac{d^2y}{dx^2} = -g(x)y(x) + s(x)$$

with:

$$g(x) = (2m/\hbar^2)[E - V(x)] \text{ and } s(x) = 0.$$

1D Schroedinger equation: harmonic oscillator - 1

In adimensional units:

$$\frac{d^2\psi}{d\xi^2} = -2\left(\varepsilon - \frac{\xi^2}{2}\right)\psi(\xi)$$

has the form:

$$\boxed{\frac{d^2y}{dx^2} = -g(x)y(x) + s(x)}$$

with:

$$g(x) = 2\left(\epsilon - \frac{x^2}{2}\right) \quad \text{and} \quad s(x) = 0$$

1D Schroedinger equation: harmonic oscillator - 2

Since $s(x) = 0$, the Numerov's formula reduces to :

$$y_{n+1}\left[1 + g_{n+1}\frac{(\Delta x)^2}{12}\right] = 2y_n\left[1 - 5g_n\frac{(\Delta x)^2}{12}\right] - y_{n-1}\left[1 + g_{n-1}\frac{(\Delta x)^2}{12}\right] + O[(\Delta x)^6]$$

Defining: $f_n \equiv 1 + g_n\dfrac{(\Delta x)^2}{12}$

we rewrite Numerov's formula as

$$y_{n+1} = \frac{(12 - 10f_n)y_n - f_{n-1}y_{n-1}}{f_{n+1}}$$

The value of the energy is now hidden into g_n and f_n.

1D Schroedinger equation: harmonic oscillator - 3

$$y_{n+1} = \frac{(12 - 10 f_n) y_n - f_{n-1} y_{n-1}}{f_{n+1}} \qquad (*)$$

The symmetry of the potential and the parity of the (still unknown) solutions allows to simplify the choice of the starting points

n even choose $y_0 = 0$ and whatever y_1 you want

n odd choose whatever y_0 (finite) you want;

y_1 is determined by Numerov's formula :

since $f_{-1} = f_1$ by symmetry, and $y_{-1} = y_1$; put into (*) and obtain :

$$y_1 = \frac{(12 - 10 f_0) y_0}{2 f_1}$$

harmonic0

The code prompts for some input data:

- the limit $x_{\max}$ for integration (typical values: $5 \div 10$);
- the number N of grid points (typical values range from hundreds to a few thousand); note that the grid point index actually runs from 0 to N, so that $\Delta x = x_{\max}/N$;
- the name of the file where ou output file written;
- the required number n of nodes (the code will stop if n is negative).

Finally the code prompts for a trial energy. You should answer 0 (*) in order to search for an eigenvalue with n nodes. The code will start iterating on the energy.

(*) It is however possible to specify an energy to force the code to perform an integration at fixed energy useful for testing purposes

new value of the number of nodes: answer -1 to stop

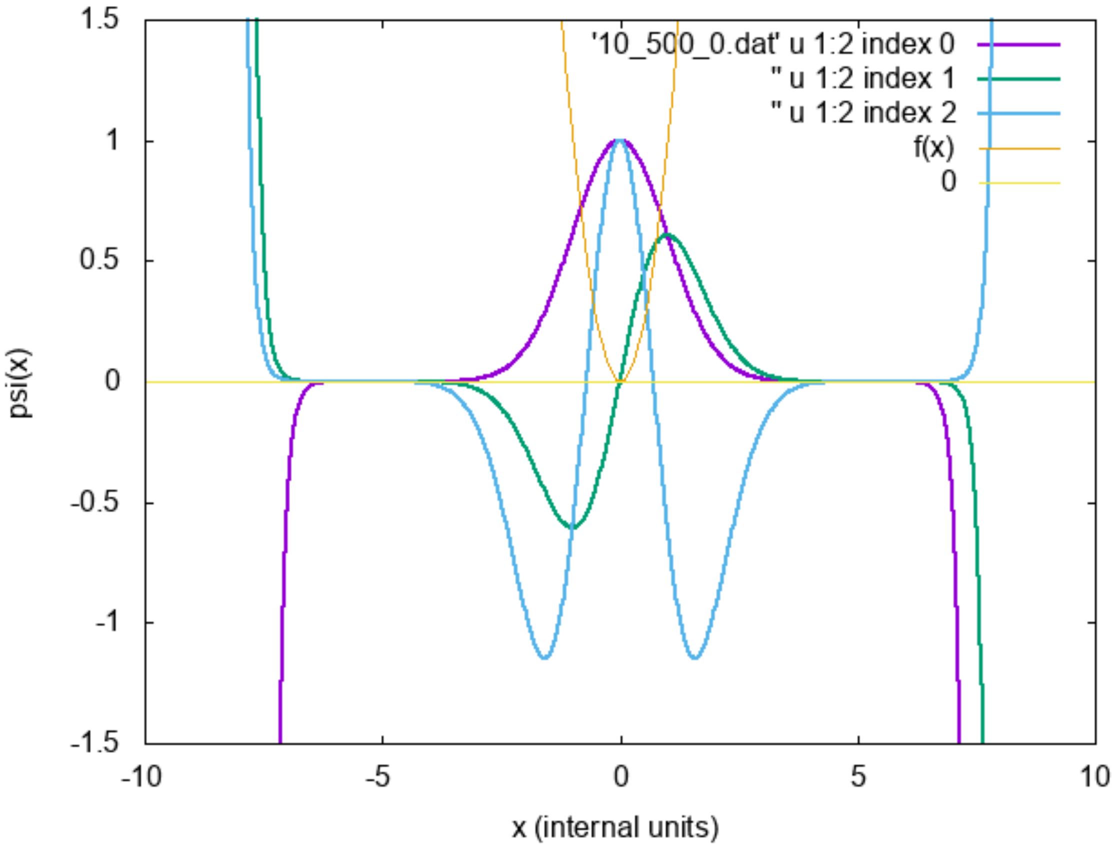
harmonic0

```
Max value for x (typical value: 10) > 10
Number of grid points (typically a few hundreds) > 500
output file name > 10_500.dat
nodes (type -1 to stop) > 0
Trial energy (0=search with bisection) > 0
           1    25.000000000000000              13           0
           2    12.500000000000000               7           0
           3    6.2500000000000000               3           0
           4    3.1250000000000000               2           0
```

Output file contains: $x,\ \psi(x),\ |\psi(x)|^2,\ \rho_{\mathrm{cl}}(x),\ V(x)$

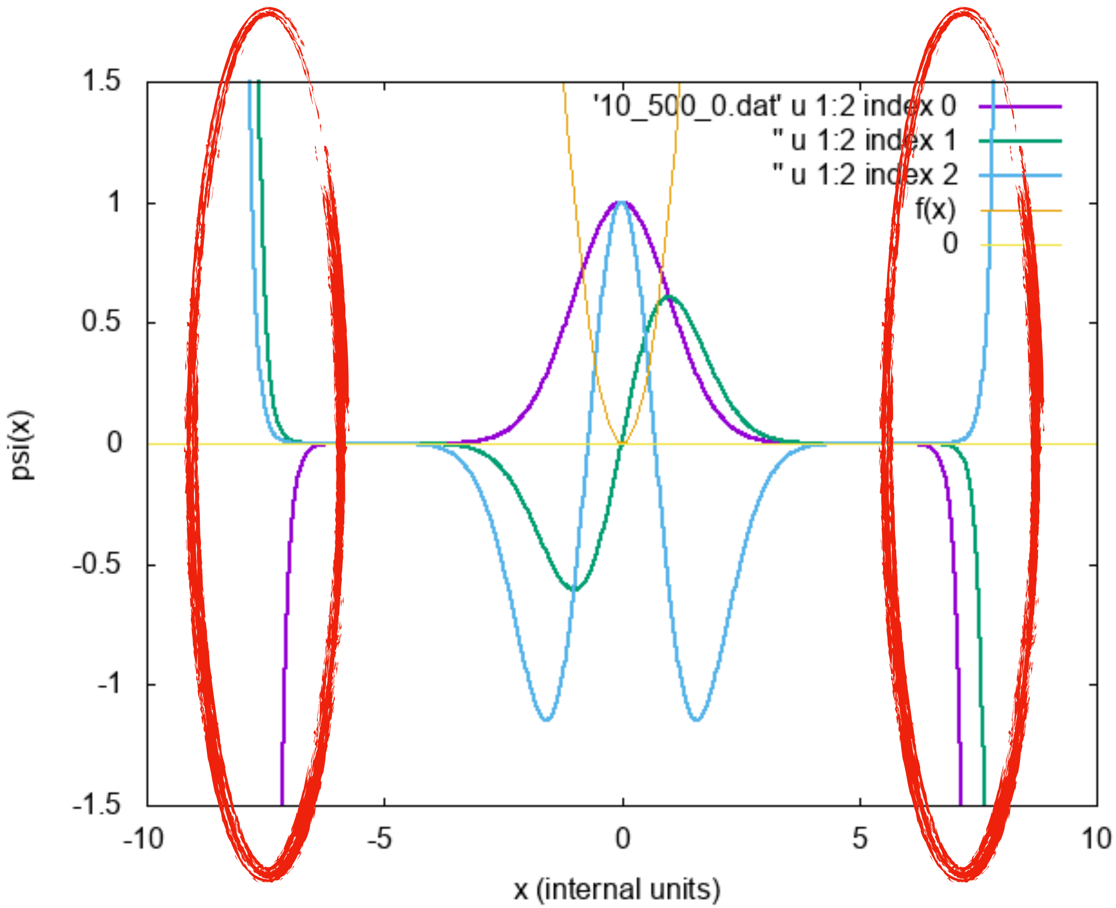
```
#    x          y(x)            y(x)^2          classical p(x)       V
-10.000 -0.41559380E+11  0.17271820E+22  0.00000000E+00   50.000000
 -9.980 -0.34101628E+11  0.11629210E+22  0.00000000E+00   49.800200
 -9.960 -0.27993466E+11  0.78363416E+21  0.00000000E+00   49.600800
 -9.940 -0.22988666E+11  0.52847878E+21  0.00000000E+00   49.401800
 -9.920 -0.18886279E+11  0.35669155E+21  0.00000000E+00   49.203200
```

Results



harmonic0

Results



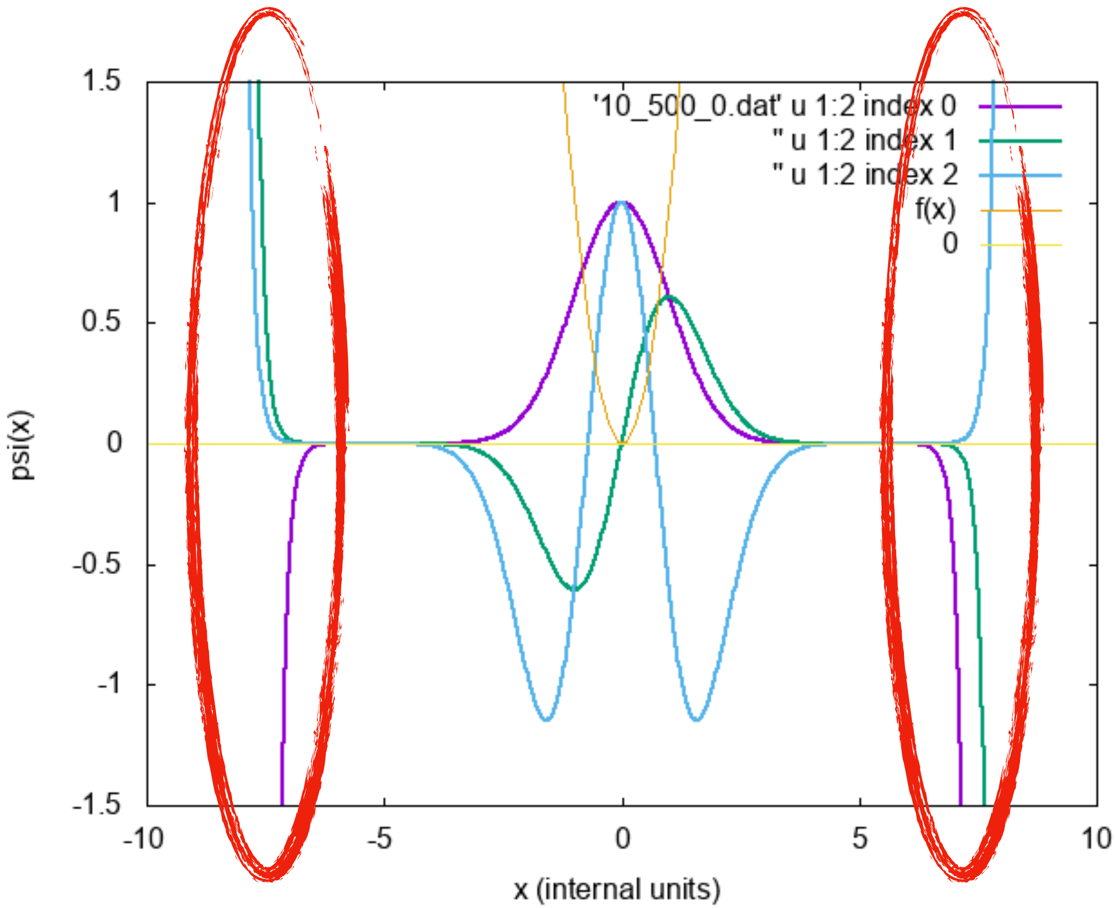
harmonic0

???

divergences!

… but can be hidden!

Results



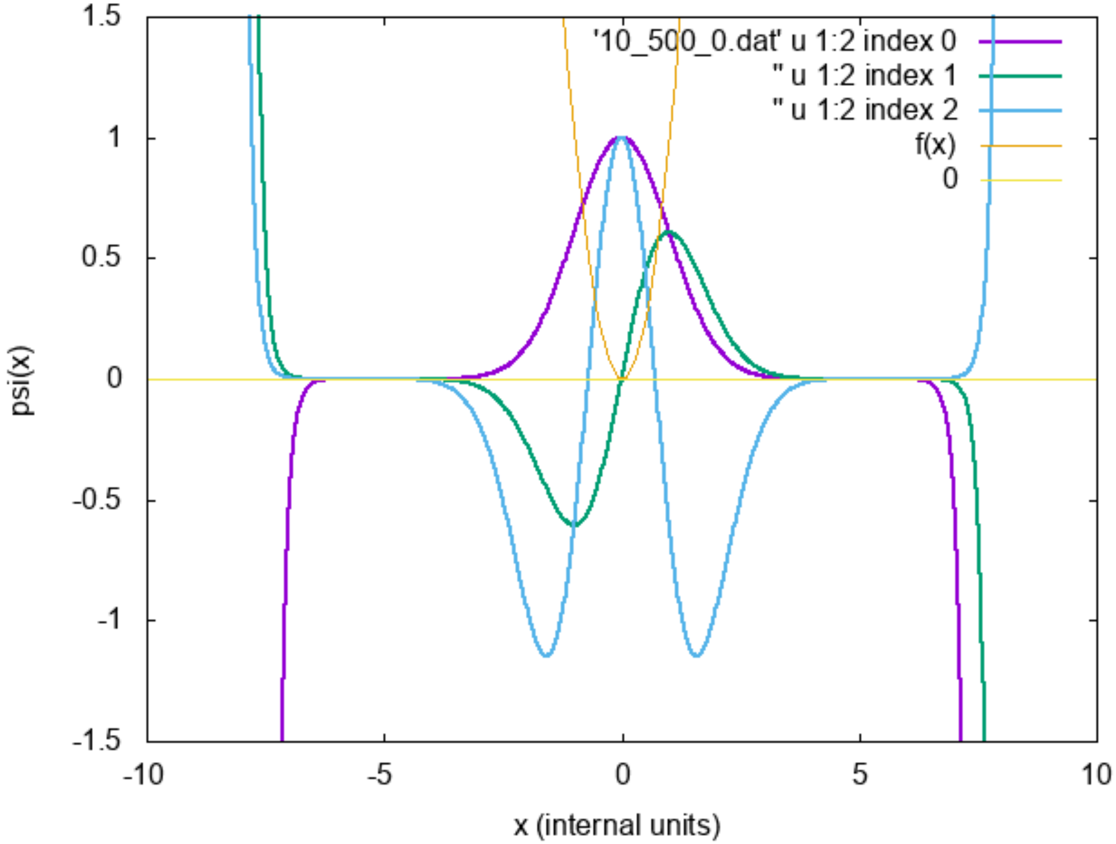
harmonic0

???

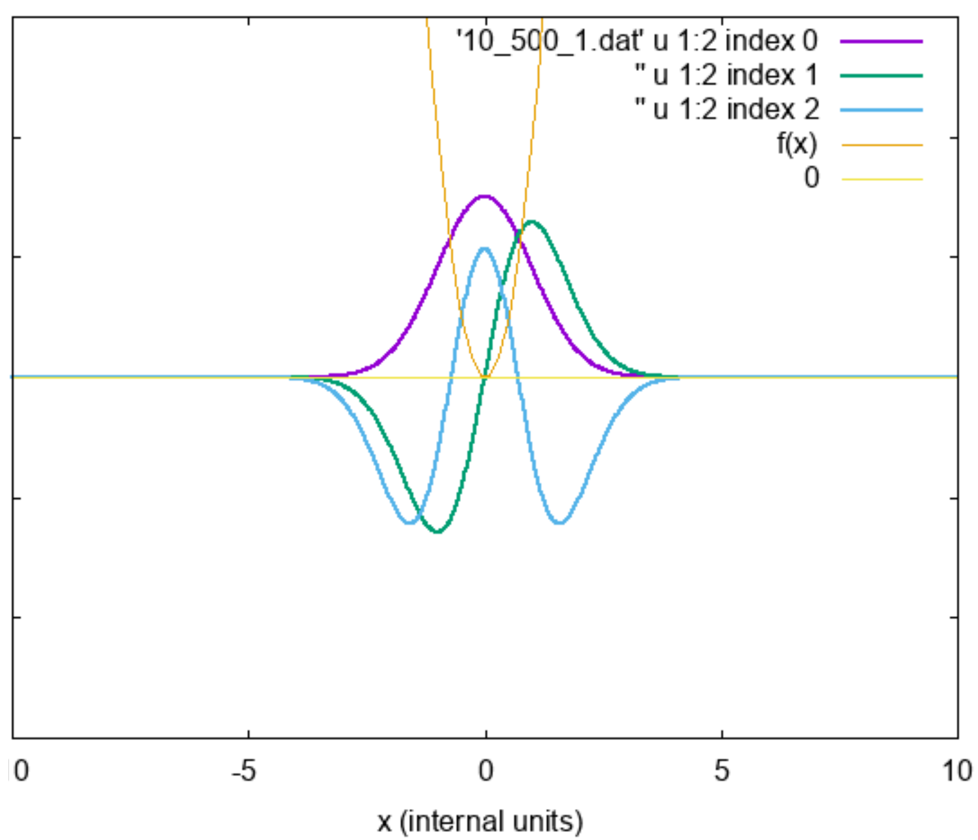
divergences!
… but can be hidden!

what's next?
integration
forward (from x=0 to x_max) and
backward (from x_max to 0)
=> harmonic1

Results



harmonic0



harmonic1

within the Numerov's method: the "shooting" step

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