Iterative methods for Solving the Schroedinger Eq.

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Two separate examples

1. Effect of long range potentials, Born-like series

2. Non-linear Gross-Pitaevskii Eq. for Bose-Einstein Condensates

Basic strategy: work with the L-S intergral eq.

Integral Eq.

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} \right] \psi(r) = V(r)\psi(r)$$

$$\downarrow$$

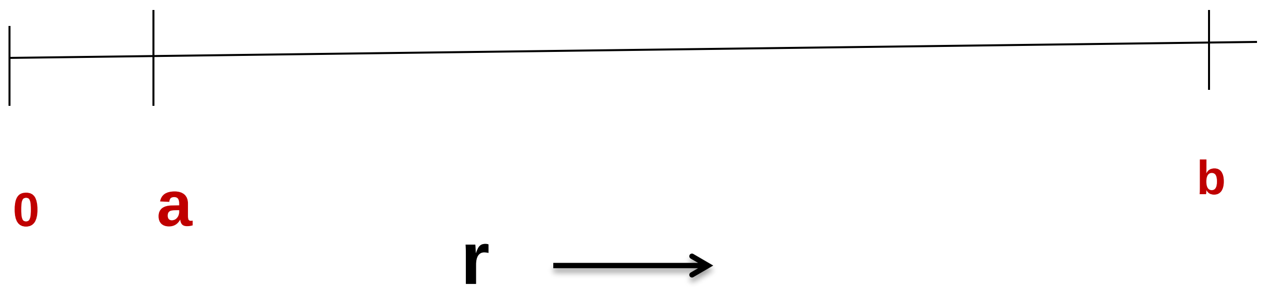
$$\psi_L(r) = f_L(r) + \int_0^\infty \mathcal{G}_L(k;r,r')V(r')\psi_L(r')\, dr'$$

$$\int_0^\infty \mathcal{G}_L(k;r,r')V(r')\psi_L(r')\, dr' =$$
$$-(1/k)h_L(r)\int_0^r f_L(r')\, V(r')\psi_L(r')dr' +$$
$$-(1/k)f_L(r)\int_r^\infty h_L(r')\, V(r')\psi_L(r')dr'$$

f_L and h_L are spherical Bessel functions

Part 1 : Long range potentials

Propagate psi from r = a to r = b



$$\psi_L(r) = \alpha_L Y_L(r) + \beta_L Z_L(r) \qquad a < r < b$$

Two independent sol. of the Schr. Eq

determine α_L and β_L by

Matching psi to Y and Z at r = a,

Two independent solutions Y(r) and Z(r)
In the radial interval [a,b]

$$Y_L(r) = f_L(r) + \int_a^b \mathcal{G}_L(k;r,r')V(r')Y_L(r')\,dr'$$

$$Z_L(r) = h_L(r) + \int_a^b \mathcal{G}_L(k;r,r')V(r')Z_L(r')\,dr'$$

$$\mathcal{G}_L(k;r,r') = -\frac{1}{k} f_L(kr_<)h_l(kr_>)$$

The iteration procedure for Y

$$Y_L(r) = f_L(r) + \chi_L^{(Y)}(1,r) + \chi_L^{(Y)}(2,r) + \ \dots, \ a \leq r \ \leq b$$

$$\chi_L^{(Y)}(n+1,r) = \int_a^b \mathcal{G}_L(r,r')V(r')\chi_L^{(Y)}(n,r')dr'$$

$$n = 0,1,2\dots \chi_L^{(Y)}(0,r) = f_L(r)$$

Iteration (n+1) in terms of (n)
No equations, only integrals

Asymptotic Limit, r = b

$$\chi_L^{(Y)}(n,b) = A_L(n)h_L(b)$$

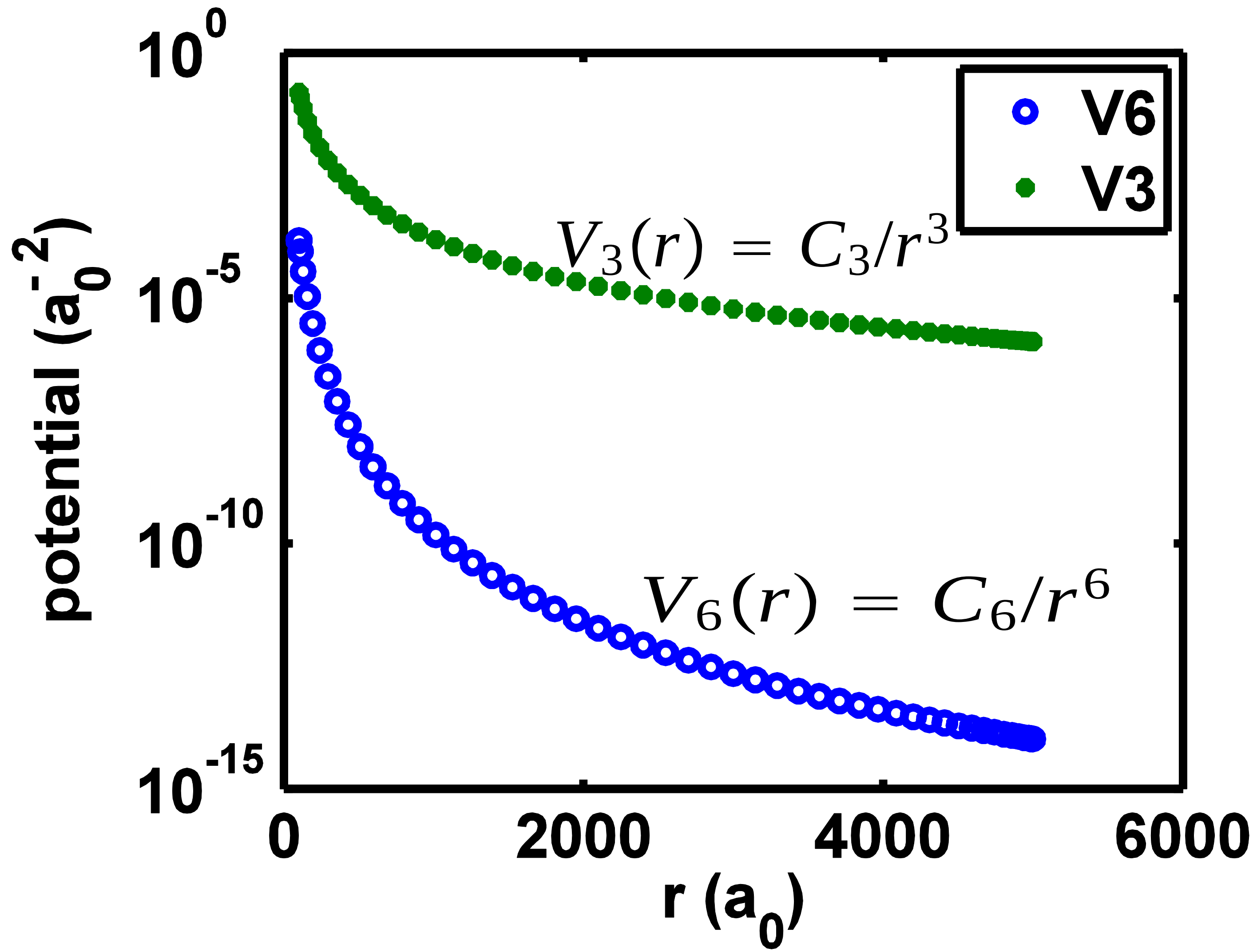
$$\chi_L^{(Z)}(n,b) = B_L(n)h_L(b)$$

$$A_L(n) = -(1/k)\int_a^b f_L(r')\ V(r')\chi_L^{(Y)}(n,r')dr'$$

$$B_L(n) = -(1/k)\int_a^b f_L(r')\ V(r')\chi_L^{(Z)}(n,r')dr'$$

C3 = 89*1822.9*1

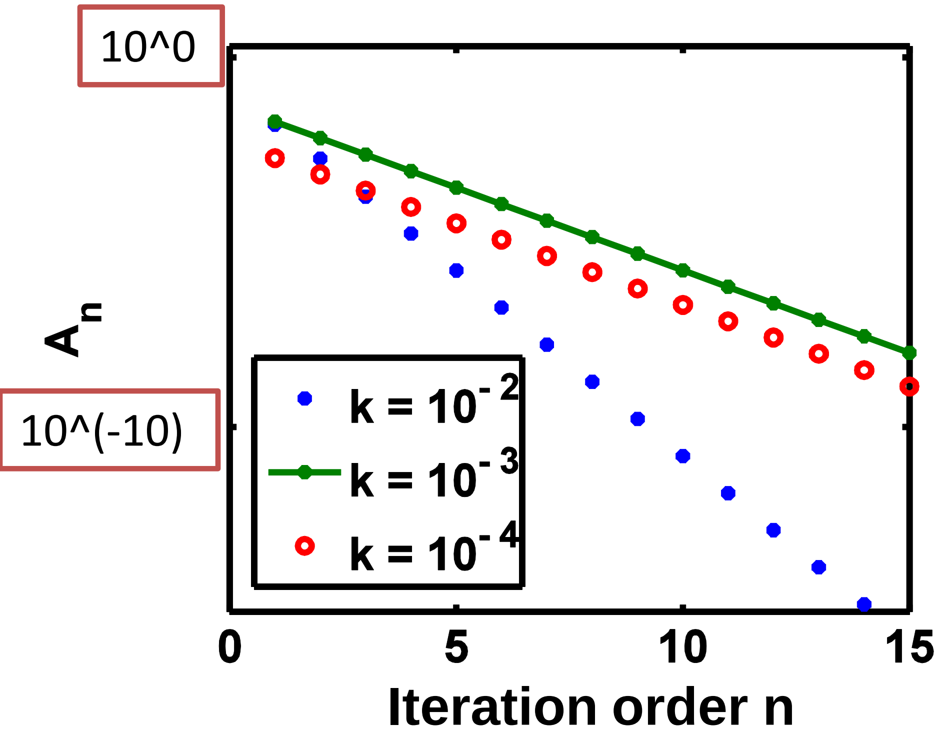
C6 = 89*1822.9*10^3

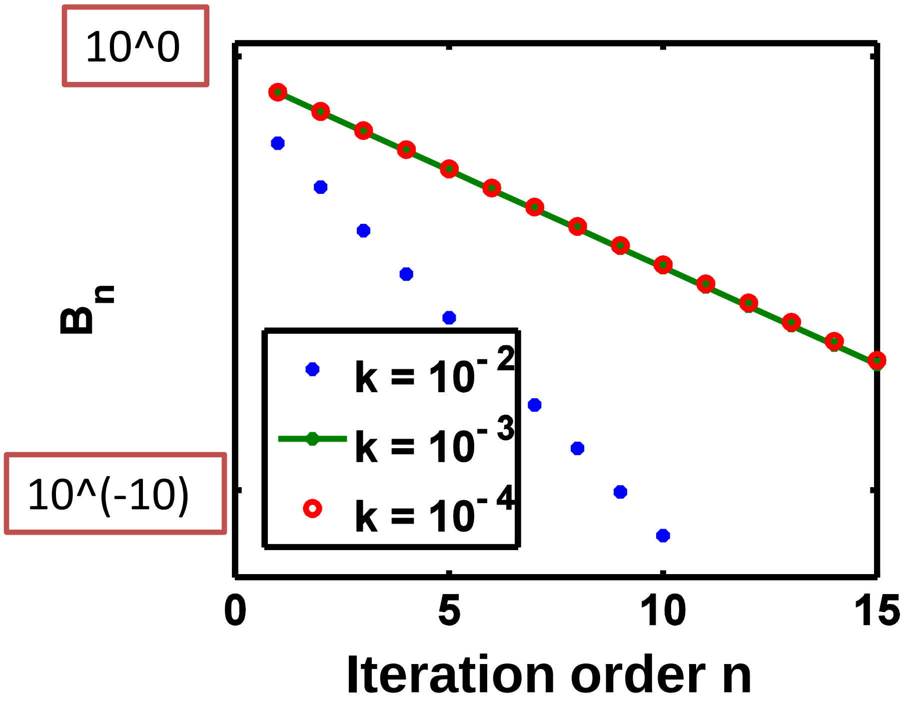


V6, L= 0

Rate of convergence

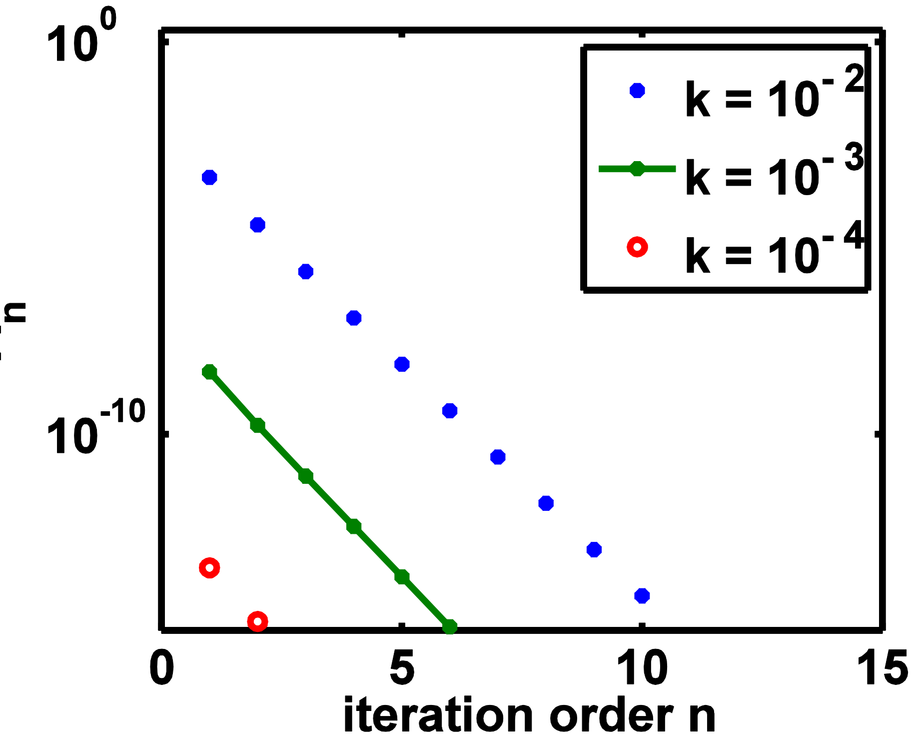
a=100 < r < b=1000

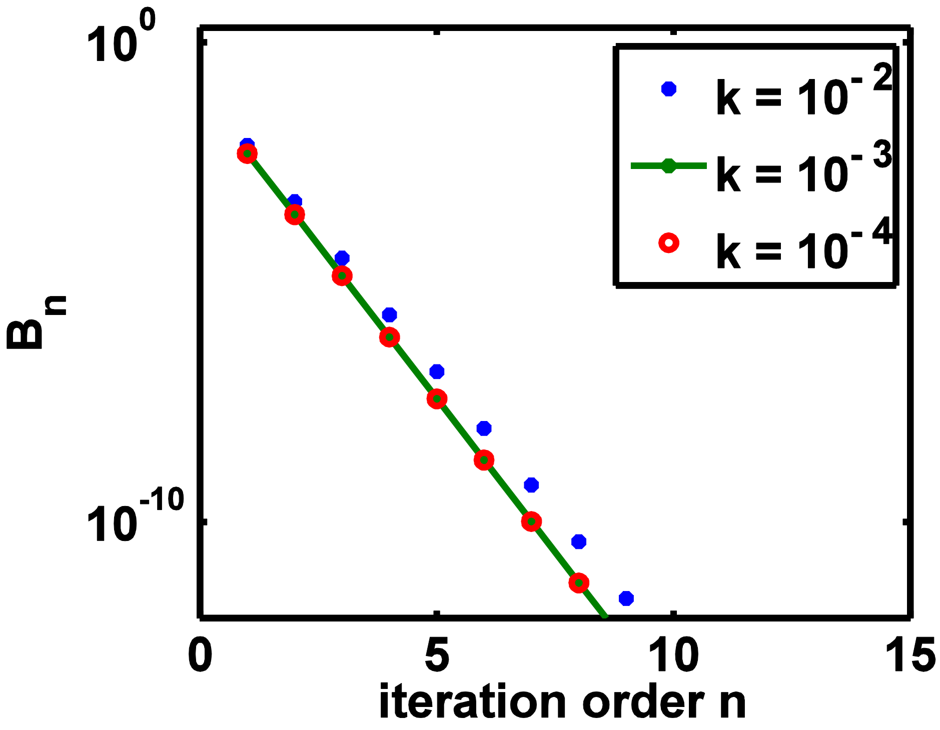




V6, L = 2

100 < r < 1000





Conclusions for part 1

1. Integral equations permit iterations (Born-like series)

2. It is now possible to include the long range part of the potentials accurately by avoiding the conventional solution of the Schr. Eq.

3. Only integrals are involved in $a < r < b$

Part 2

Non-linear Gross-Pitaevskii Eq.

For a Bose-Einstein Condensate of

cold trapped atoms

3 - dimension

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g|\Psi|^2\right]\Psi(\vec{r},t),$$

$$g = N\frac{\hbar^2}{2m}8\pi a,$$

N = # of atoms, a = scattering length

$$\mu\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g|\psi(\vec{r})|^2\right]\psi(\vec{r})$$

eigenvalue

Partial wave, L = 0

$$\psi(\vec{r}) \rightarrow \psi(r) = \phi(r)/(r\sqrt{4\pi})$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{ext}(r) + \frac{g}{4\pi}|\phi(r)/r|^2\right]\phi(r) = \mu\phi(r)$$

$$\int_0^\infty |\phi(r)|^2 dr = 1.$$

$V_H(r)$ Hartree Potential

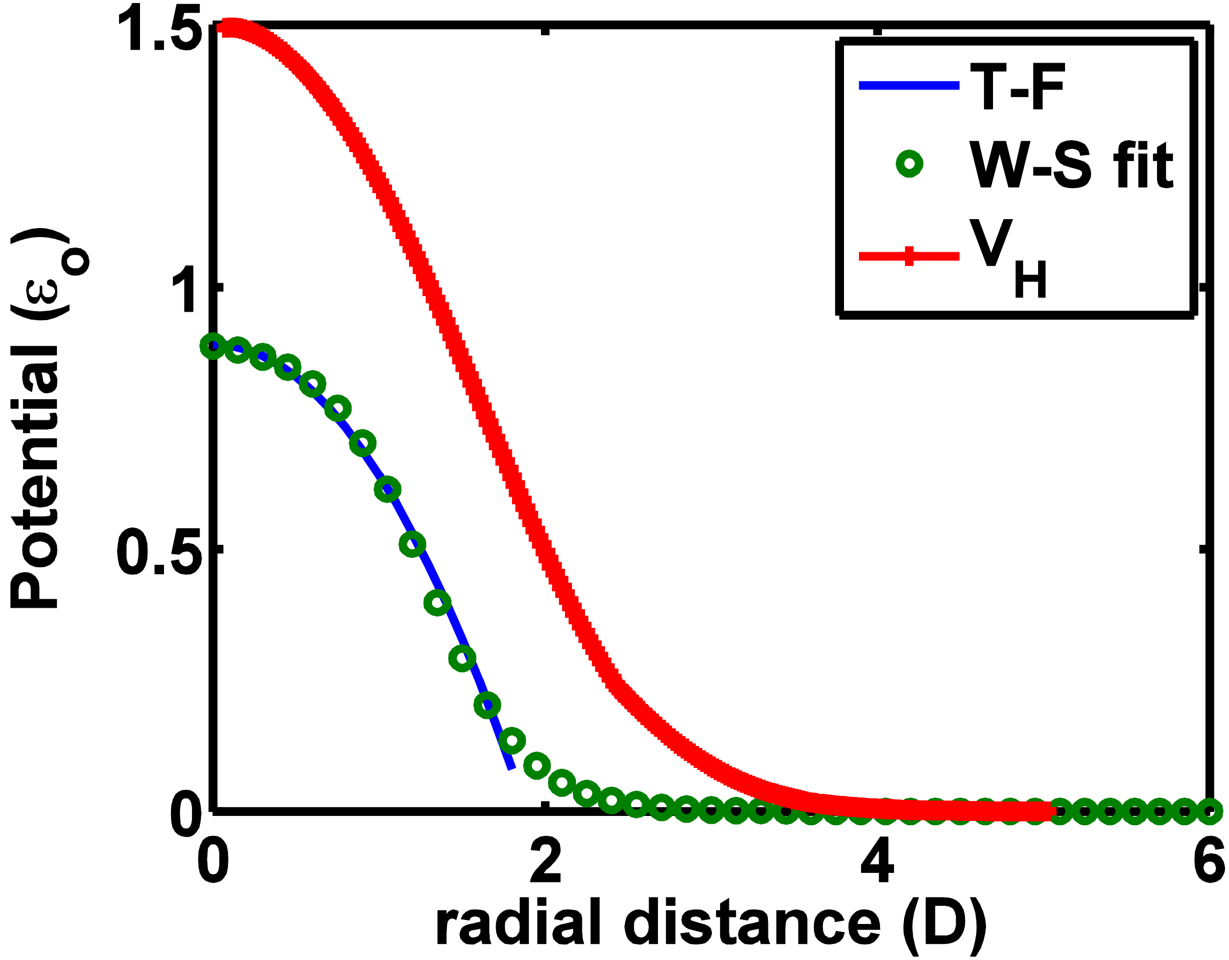
Iterate

$$V_H^{(n)}(r) = N\frac{g}{4\pi}|\phi^{(n)}(r)/r|^2, \quad n = 0, 1, 2, \ldots,$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{ext}(r) + V_H^{(n)}(r)\right]\phi^{(n+1)}(r) = \mu^{(n+1)}\phi^{(n+1)}(r)$$

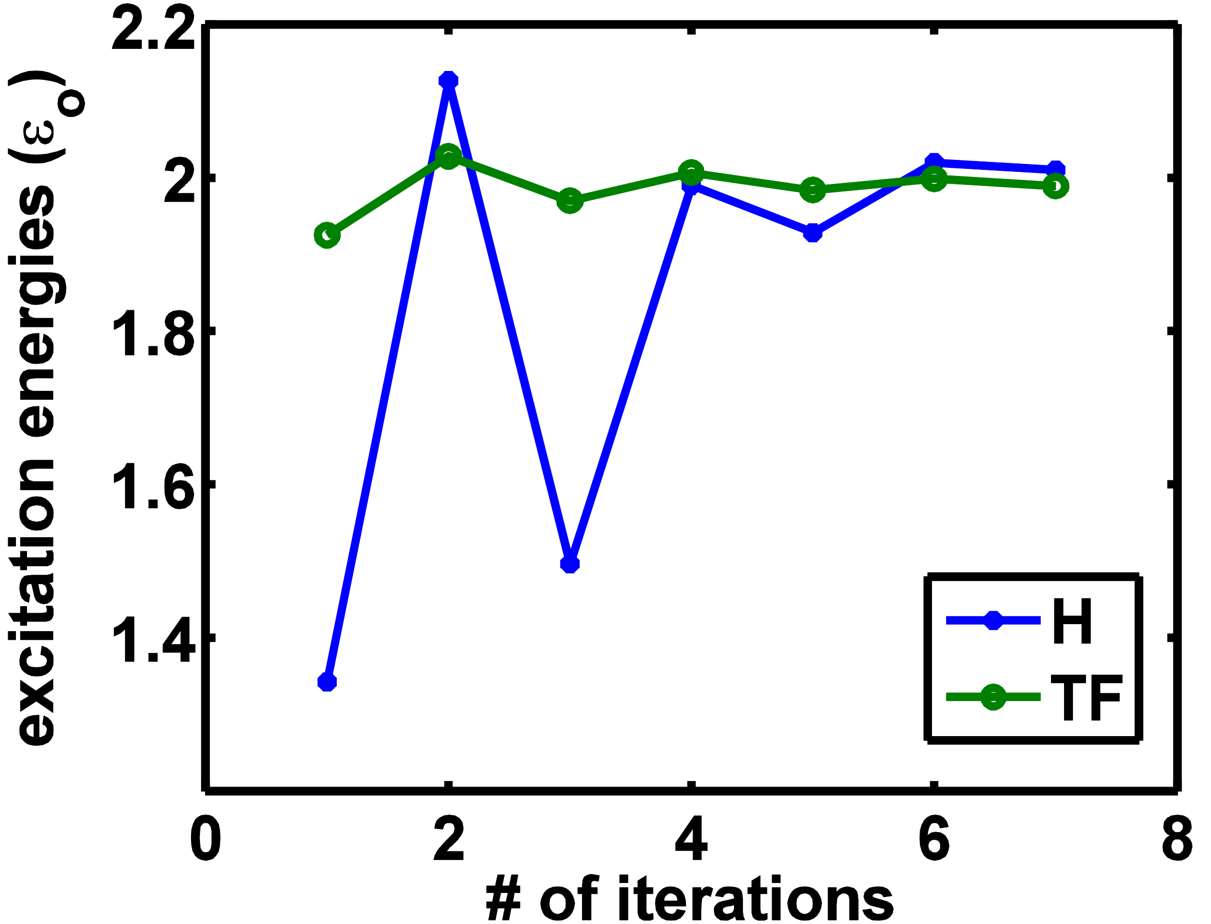
Look for both $\phi^{(n+1)}(r)$ *and* $\mu^{(n+1)}$

Results

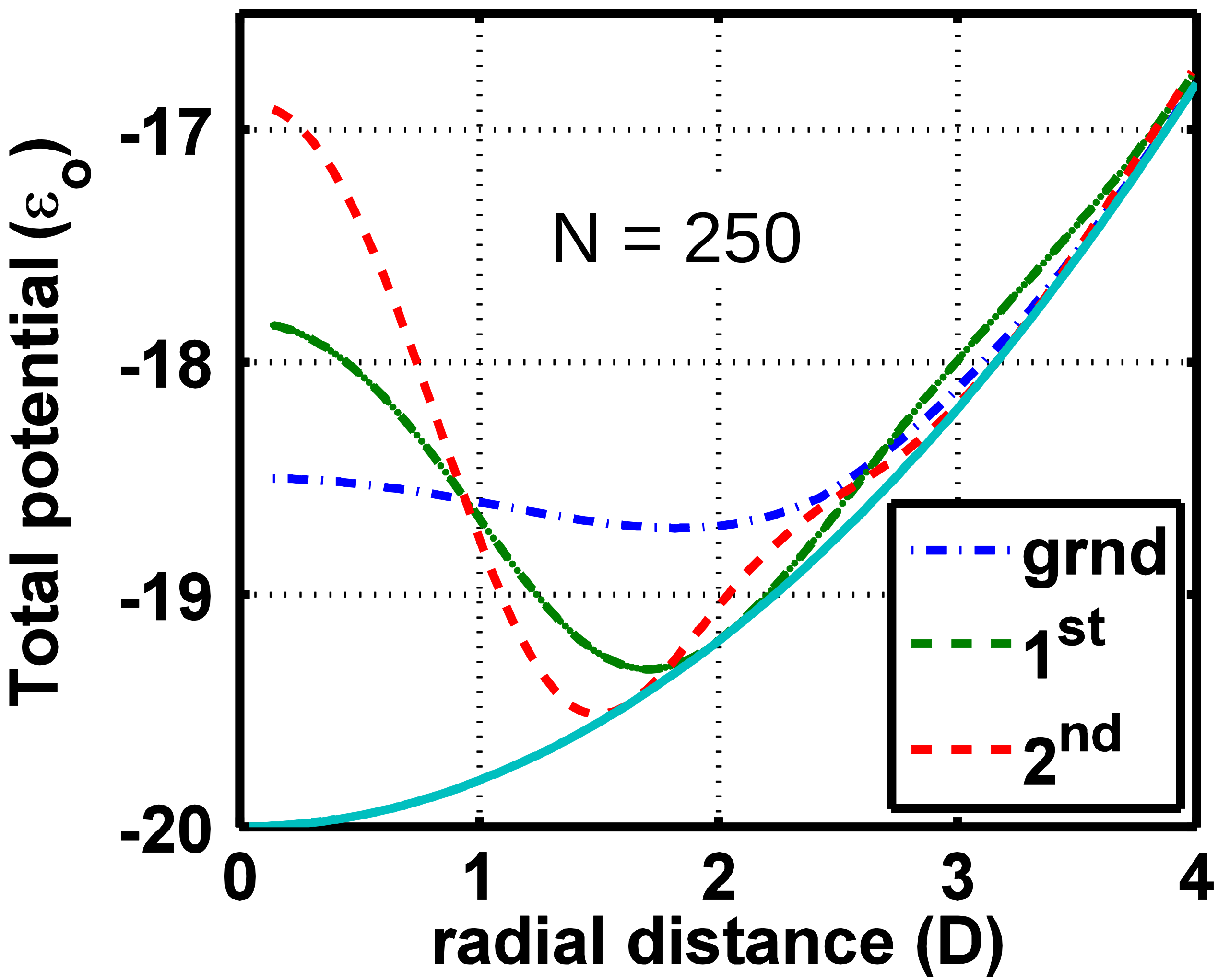


1.5
1
0.5
0
0
2
4
6
Potential (ε_o)
radial distance (D)
T-F
W-S fit
V_H

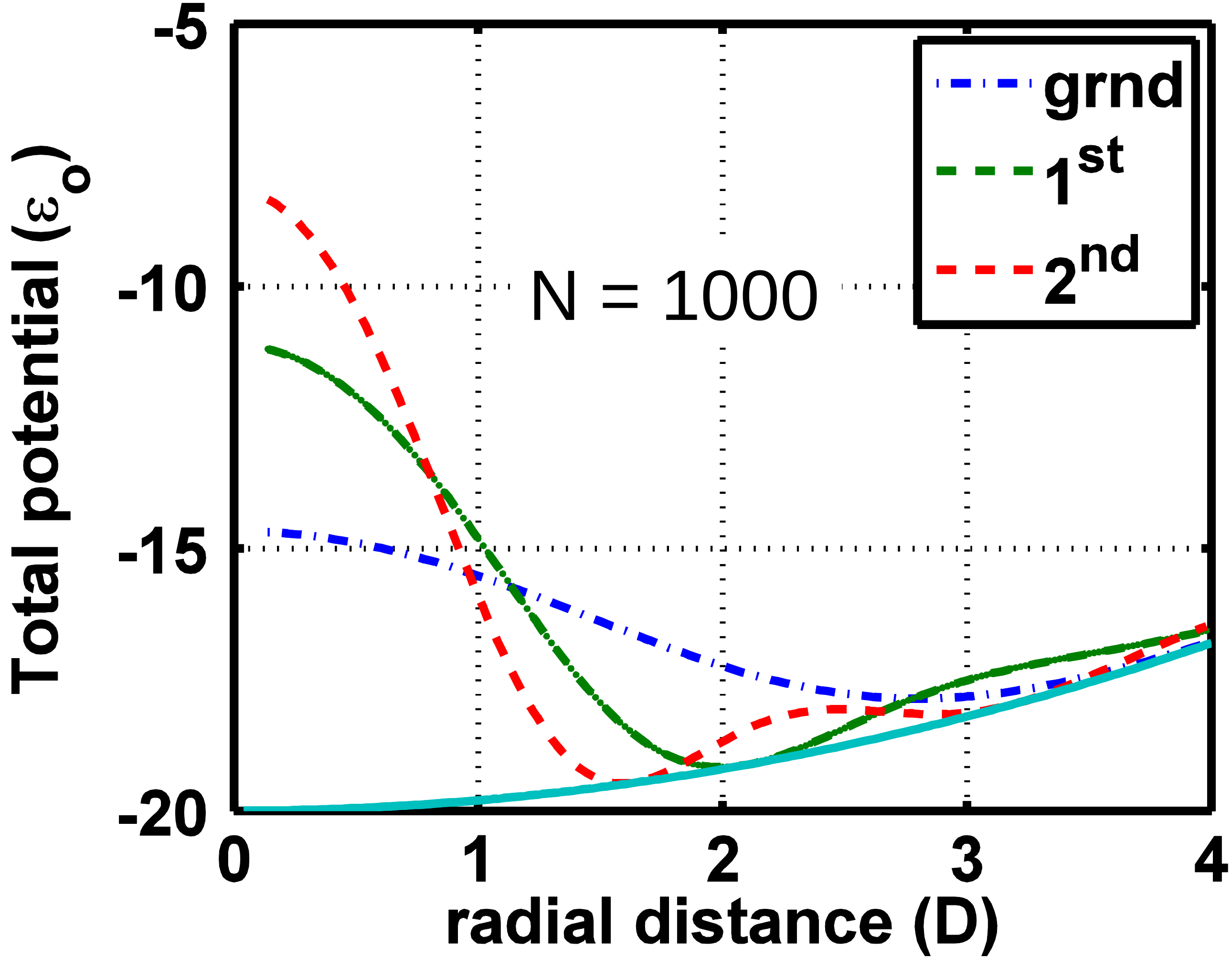
Convergence of Bound State Energies



Harm.Osc. Pot'l + Hartree Pot'l



Harm.Osc. Pot'l + Hartree Pot'l



Summary

1. Iterations of the non-linear Gross-Pitaevskii Eq, based on the Hartree potentials are physically intuitive and converge. Applied Mathematics, Nov 2013

2. Long-Ranged potentials can be included iteratively based on a Born Approximation scheme using the integral equation for the Schr. Eq. PRA, **87**, 032708 (2013)

Examples: V6 = C6 / (r ^ 6); V3 = C3/ (r ^ 3)

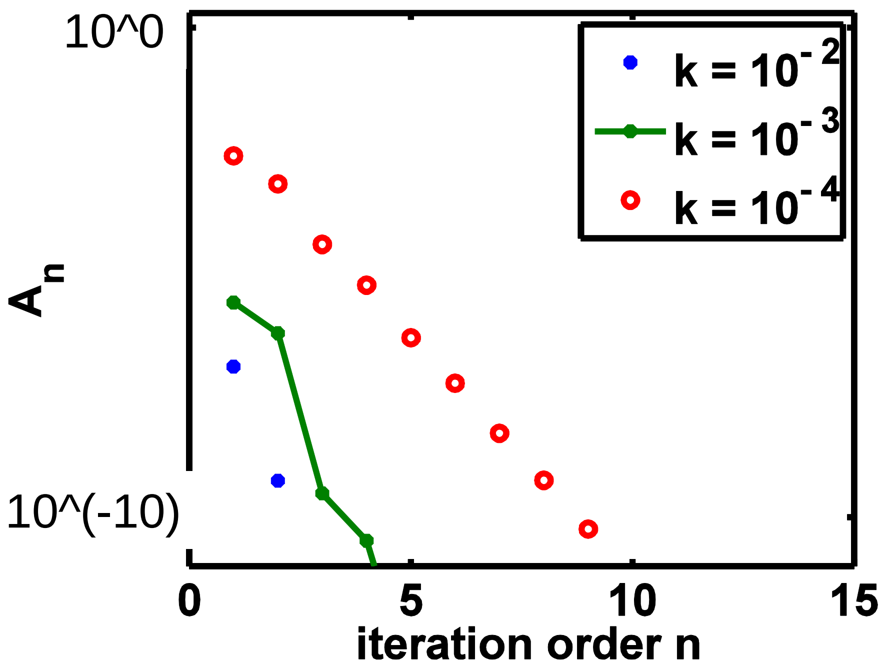
Reduced Mass of colliding atoms 89 u / 2 Rubidium

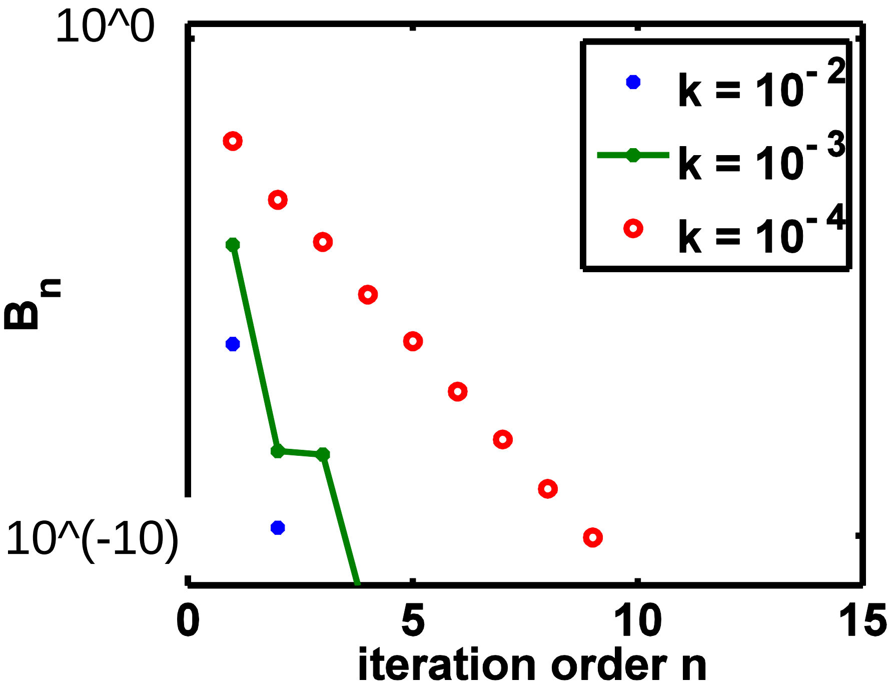
C6 = - 10^3 C3 = -1 in amu units

$k\ (a_0)$	10^{-5}	10^{-4}	10^{-3}	10^{-2}
$T\ (K)$	10^{-10}	10^{-8}	10^{-6}	10^{-4}

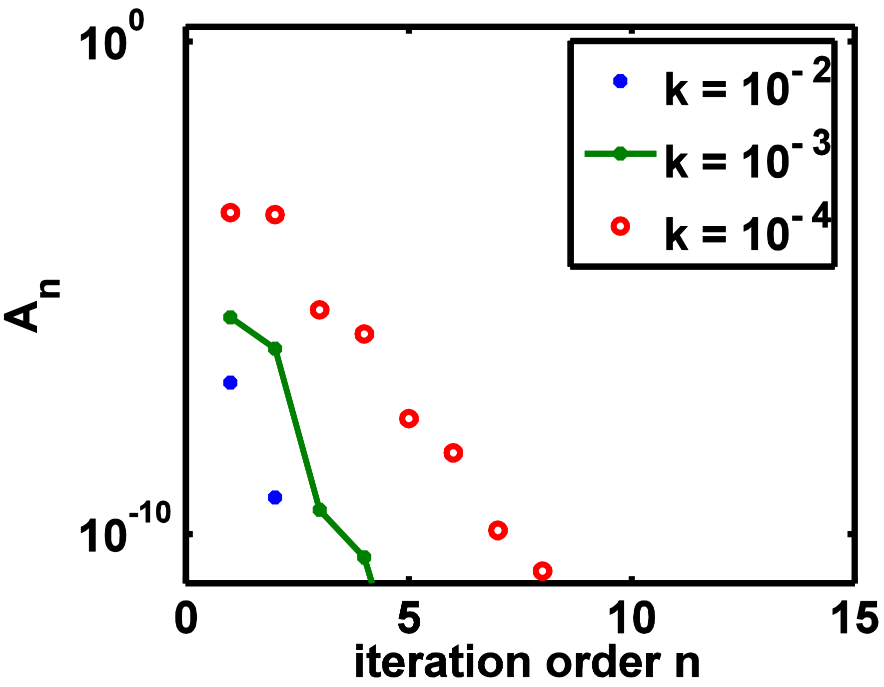
V3 10,000 < r < 100,000 L = 0

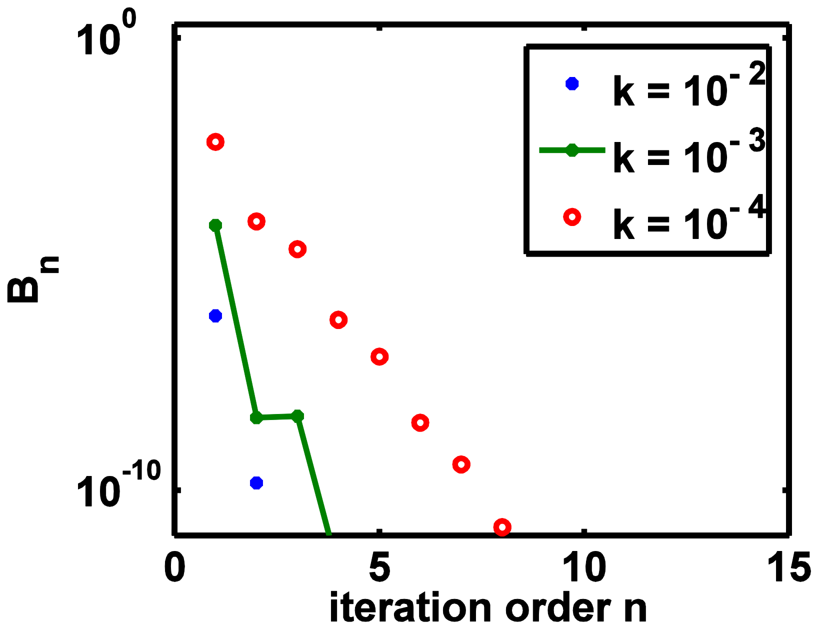
Rate of convergence



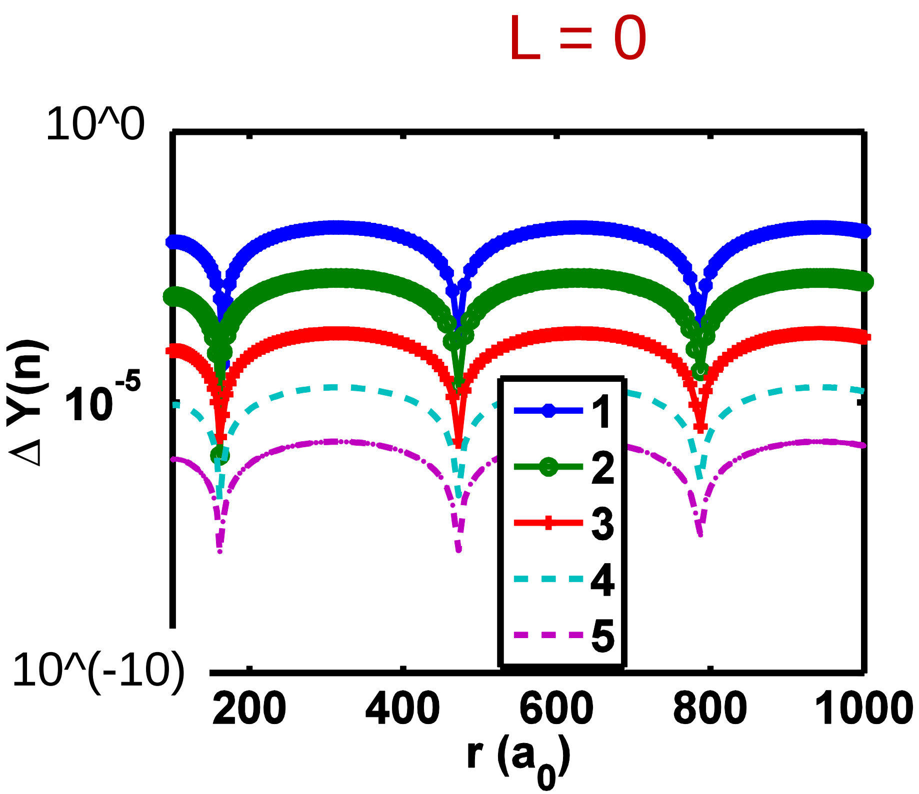


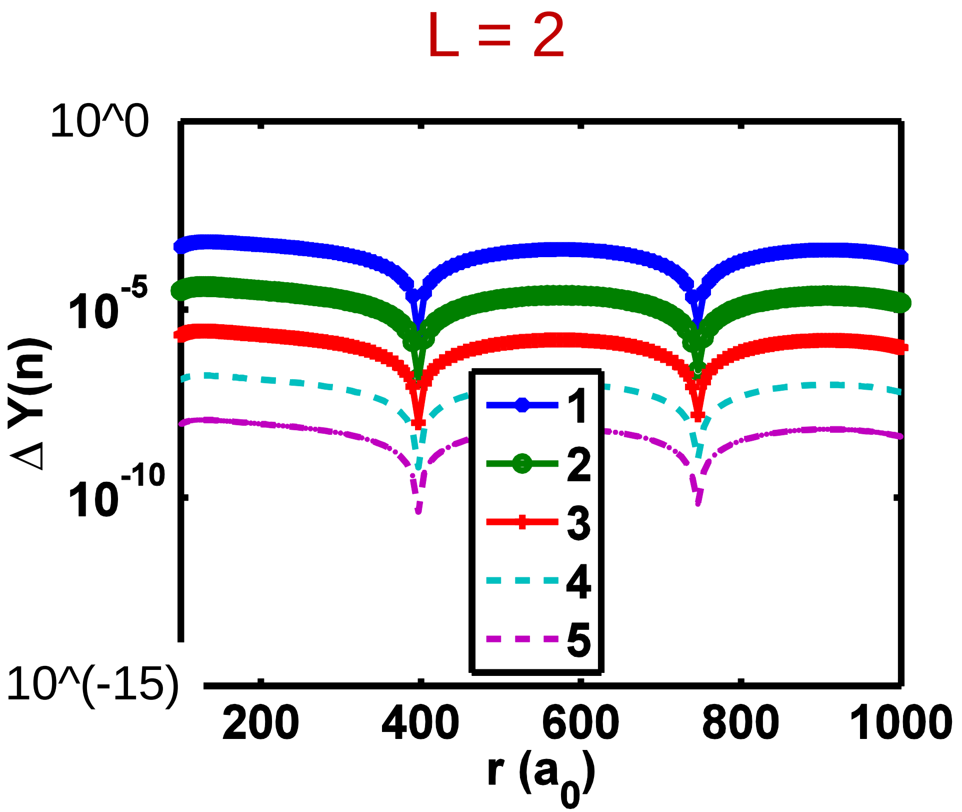
V3 10,000<r<100,000 L = 2





V6, k=0.01, error in Y after n iterations

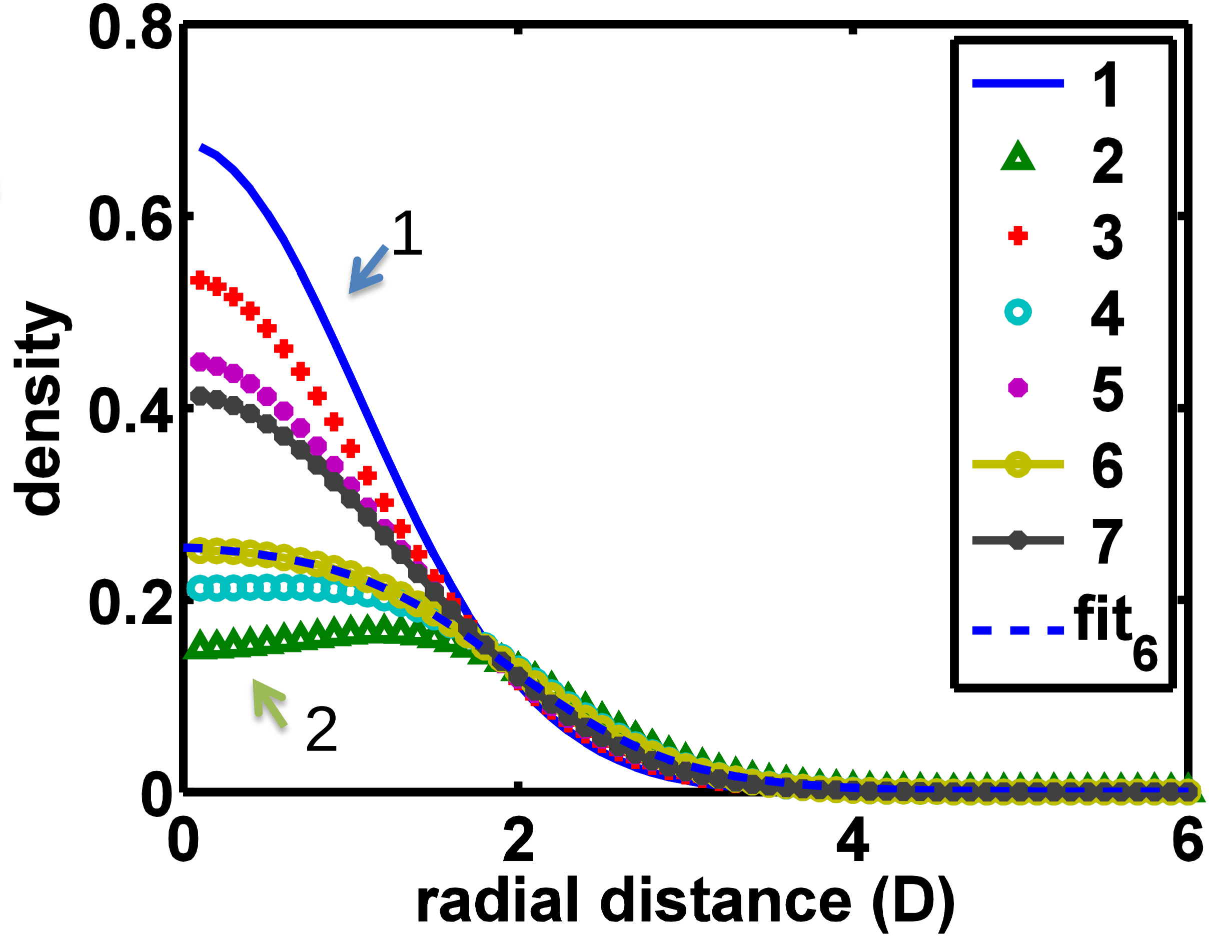




Radial distance r

Convergence of wave functions

$$density = |\phi^{(n)}(r)/r|^2$$

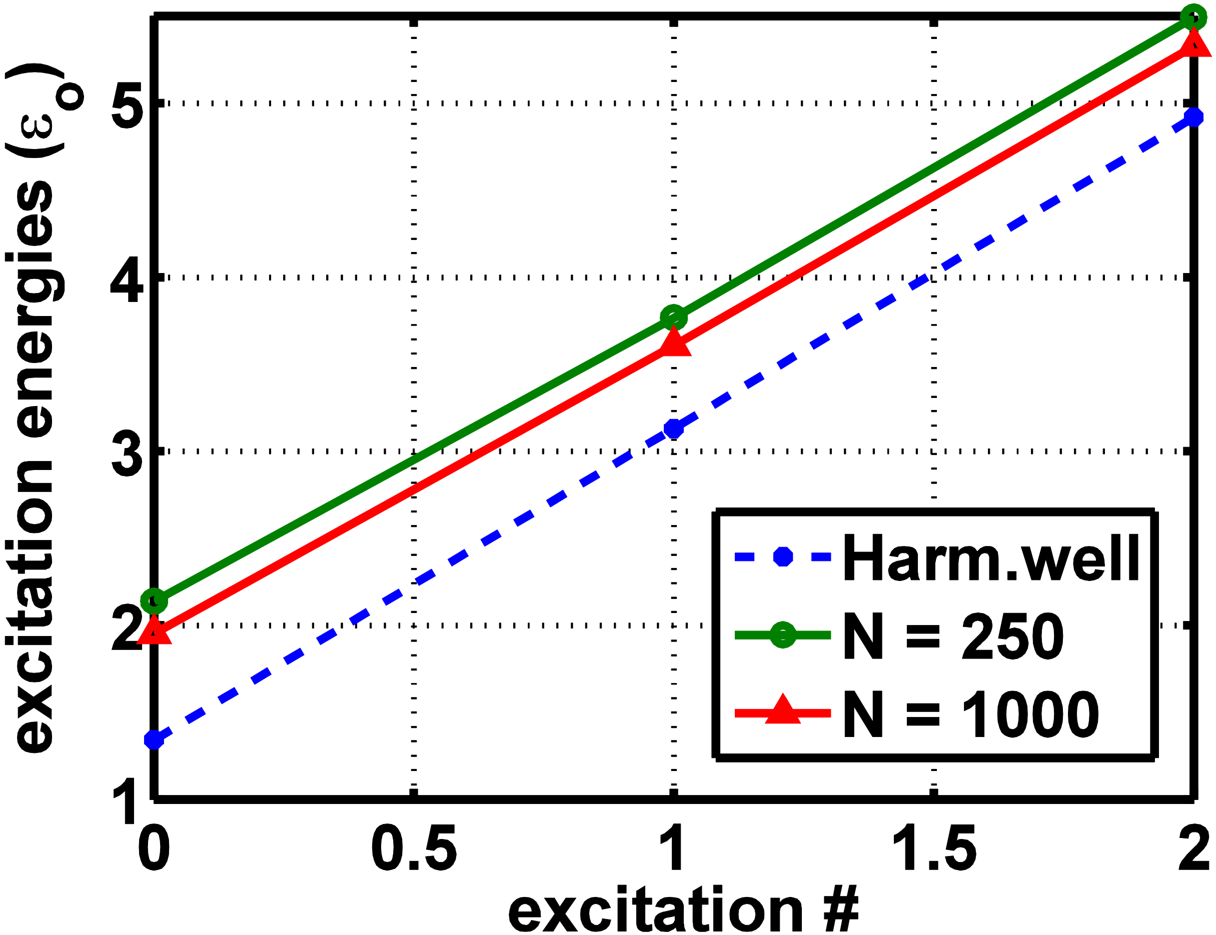


For r = b (asymptotic limit)

$$Y_L = f_L(b) + A_L h_L(b), \quad Z_L = (1 + B_L) h_L(b)$$

$$A_L = -(1/k) \int_a^b f_L(r') \, V(r') Y_L(r') dr'$$

$$B_L - (1/k) \int_a^b f_L(r') \, V(r') Z_L(r') dr'$$



excitation energies (ε_o)
1
2
3
4
5
0
0.5
1
1.5
2
excitation #
Harm.well
N = 250
N = 1000