A Few-Body Method for Bose-Einstein Condensates

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Study of A-boson Systems

What A?

$\Longrightarrow$ Typical number of atoms involved in the Bose-Einstein condensation (BEC):

$$A \sim 10^3 - 10^6$$

$\Longrightarrow$ Huge number of degrees of freedom

$\Longrightarrow$ Intractable numerical complexity

Thus, naturally one uses Monte Carlo type approaches:

- Variational Monte Carlo
- Diffusion Monte Carlo (DMC)
- Green Function Monte Carlo (GFMC).

Alternative methods: Based on Hyperspherical Harmonics:

- Hyperspherical Harmonics Expansion Method
- Integro–Differential Equation Approach (IDEA)

Faddeev-HH formalism

$$V(\mathbf{x}) = \sum_{ij} V_{ij}(r_{ij})$$

$$\Psi(\mathbf{x}) = \sum_{ij} \psi_{ij}(\mathbf{x})$$

$\Longrightarrow$ $\mathbf{x}$: Coordinates vector

$\Longrightarrow$ ψ_{ij}: Faddeev components

$$(T - E)\psi_{ij}(\mathbf{x}) = -V_{ij}(r_{ij}) \sum_{kl} \psi_{kl}(\mathbf{x})$$

Seek for states which are invariant by rotation in the $(D-3)$-dimensional space

Then

$$\psi_{ij}(\mathbf{x}) = F_{ij}(\mathbf{r}_{ij}, r)$$

Therefore,

$$(T - E)F_{ij}(\mathbf{r}_{ij}, r) = -V_{ij}(r_{ij}) \sum_{kl} F_{kl}(\mathbf{r}_{kl}, r)$$

Potential Harmonics $\mathcal{P}^{\ell,m}_{2K+\ell}(\Omega_{ij})$

$$\mathcal{P}^{\ell,m}_{2K+\ell}(\Omega_{ij}) = N_{K,\ell} Y_{\ell m}(\omega_{ij}) \left(\frac{r_{ij}}{r}\right)^{\ell} P_K^{\alpha,\beta+\ell}(2\frac{r_{ij}^2}{r^2} - 1)$$

$\alpha = (D-5)/2, \ \ \beta = 1/2, \quad D = 3(A-1)$

$Y_{\ell m}(\omega_{ij})$: Spherical Harmonics

$P_K^{\alpha,\beta+\ell}(z)$: Jacobi polynomial

$N_{K,\ell}$: Normalization constant,

$$\int_{(r=1)} \mathcal{P}^{\ell,m*}_{2K+\ell'}(\Omega_{ij}) \mathcal{P}^{\ell',m'}_{2K'+\ell'}(\Omega_{ij}) \, \mathrm{d}\Omega = \delta_{KK'} \delta_{\ell\ell'} \delta_{mm'} .$$

The $\mathcal{P}^{\ell,m}_{2K+\ell}(\Omega_{ij})$ are eigenfunctions of the operator $\hat{L}^2(\Omega)$

$$\left[\hat{L}^2(\Omega) + L(L+D-2)\right] \mathcal{P}^{\ell,m}_{2K+\ell}(\Omega_{ij}) = 0 \, , \quad L = 2K+\ell$$

with

$$\hat{L}^2(\Omega) = \frac{4}{W(z)} \frac{\partial}{\partial z} (1-z^2) W(z) \frac{\partial}{\partial z} + 2 \frac{\hat{\ell}^2(\omega_{ij})}{1+z} + 2 \frac{\hat{L}^2(\Omega_{N-1})}{1-z}$$

$W(z)$, known as weight function, is

$$W(z) = \frac{1}{2^{D/2}}(1-z)^{(D-5)/2}(1+z)^{1/2}$$

while z is an angular variable defined by

$$z = \cos 2\varphi = 2\frac{r_{ij}^2}{r^2} - 1\,, \qquad \cos\varphi = \frac{r_{ij}}{r}\,.$$

Expansion in PH $\mathcal{P}_{2K+\ell}^{\ell,m}(\Omega_{ij})$

$$F(\mathbf{r}_{ij}, r) = \sum_{K=0}^{\infty} \mathcal{P}_{2K+\ell}^{\ell,m}(\Omega_{ij}) U_K^{\ell}(r)$$

Two options:

- Obtain, as usual, a system of differential equations for the radial functions $U_K^{\ell}(r)$
- Use the definition in terms $F(\mathbf{r}_{ij}, r)$

$$U_K^{\ell}(r) = \int \mathcal{P}_{2K+\ell}^{\ell,m}(\Omega_{ij}) F^{\ell}(\mathbf{r}_{ij}, r) \, \mathrm{d}\Omega \, .$$

Then:

Expansion of the Faddeev components $F^{\ell}(\mathbf{r}_{ij}, r)$ leads instead to an Integrodifferential Equation (IDEA).

IDEA equation for A–particle systems

Let $P(z,r) = F(r_{ij},r)\, r^{\mathcal{L}_m+1}$,

$$-\frac{\hbar^2}{m}\left[H_r + \frac{4}{r^2}T(z)\right]P(z,r) = -\left[V(r_{ij}) - V_0^{[L_m]}(r)\right]\left[P(z,r)\right.$$

$$\left. + \int_{-1}^{+1} \mathcal{F}_{[L_m]}(z,z')\; P(z',r)\; dz'\right]$$

with

$$H_r = \frac{\partial^2}{\partial r^2} - \frac{\mathcal{L}_m(\mathcal{L}_m+1)}{r^2} + \frac{A(A-1)}{2}V_0^{[L_m]}(r)$$

$T(z)$ is the kinetic energy term

$$\hat{T}(z) = \frac{1}{W_{[L_m]}(z)}\,\frac{\partial}{\partial z}\,(1-z^2)W_{[L_m]}(z)\,\frac{\partial}{\partial z}$$

and $W_{[L_m]}(z)$ is the weight function which, for bosonic systems, is given by

$$W_{[L_m]}(z) = (1-z)^{\alpha}(1+z)^{\beta}$$

with

$$\begin{aligned}\alpha &= \frac{(D-5)}{2} + L_m - 2\ell_m \\ &= \frac{3}{2}A - 4 + L_m - 2\ell_m \\ \beta &= \frac{1}{2} + \ell_m\end{aligned}$$

The kernel $\mathcal{F}_{[L_m]}(z, z')$ is the projection function which is expressed in terms of the Jacobi polynomials $P_K^{\alpha,\beta}(z)$,

$$\mathcal{F}_{[L_m]}(z, z') = W_{[L_m]}(z') \sum_K \frac{(f_K^2 - 1)}{h_K} P_K^{\alpha,\beta}(z) P_K^{\alpha,\beta}(z')$$

The normalization h_K is given by

$$h_K = \int_{-1}^{+1} \left(P_K^{\alpha,\beta}(z) \right)^2 W_{[L_m]}(z) dz$$

and the function f_K by

$$f_K^2 - 1 = \frac{2(A-2) P_K^{\alpha,\beta}(-1/2) + \frac{(A-2)(A-3)}{2} P_K^{\alpha,\beta}(-1)}{P_K^{\alpha,\beta}(+1)}$$

Characteristics of the IDEA

- Describes A-Body systems
- Includes two-body correlations exactly
- Three-body correlations can be easily included, if wanted
- Typical accuracy: $\sim 0.2\%$
- For Low A (such as $A = 4$) the equation can be easily solved.

What about large A?

Example: For $A = 100000$

- $(1 - z)^{\alpha} \sim (1 - z)^{1.5A}$

  $\Longrightarrow$ δ-function behavior around $z = -1$

$$(1 - z)^{\alpha} \underset{\alpha \to \infty}{\longrightarrow} 2^{150000}$$

- $P_K^{\alpha,1/2}(z) \sim P_K^{150000,1/2}(z)$

  $\Longrightarrow$ Uncontrollable oscillations

  $\Longrightarrow$ Calculations impossible

Same problems for HHEM

Transformation for Large A

$$r_{\rm ij} = r\zeta/\sqrt{\alpha}$$

with

$z = 2\zeta^2/\alpha - 1$

$\alpha = (D-5)/2 = (3(A-1)-5)/2 \sim 3A/2$ (large A, $\ell = 0$)

Why?

- Transforms $P_K^{\alpha,1/2}$

$$P_K^{\alpha,\beta}(2r_{ij}^2/r^2 - 1) \underset{\alpha\to\infty}{\longrightarrow} (-1)^K L_K^{1/2}(\alpha r_{ij}^2/r^2)$$

$$\equiv (-1)^K L_K^{1/2}(\zeta^2)$$

$L_K^{1/2}$ Laguerre Polynomials which are independent of α

- Transform $(1-z)^\alpha$

$$W(z) = C_W \frac{2^{\alpha+1/2}}{\sqrt{\alpha}} \zeta \mathrm{e}^{-\zeta^2}$$

- Transform h_K

$$\begin{aligned} h_K &= \int_{-1}^{+1} \left(P_K^{\alpha,\beta}(z) \right)^2 W_{[L_m]}(z)\, \mathrm{d}z \\ &\xrightarrow[\alpha\to\infty]{} \int_0^{\sqrt{\alpha}} \left[L_K^{1/2}(\zeta^2) \right]^2 \mathrm{e}^{-\zeta^2} \zeta^2\, \mathrm{d}\zeta \\ &= \frac{1}{2} \frac{\Gamma(K+3/2)}{K!}. \end{aligned}$$

IDEA-E

$$P(\zeta, r) = \frac{e^{\zeta^2/2}}{\zeta} Q(\zeta, r) \,.$$

$\Longrightarrow$ For bosons in the ground state:

$$\frac{\hbar^2}{m}\left[H_r + \frac{\alpha}{r^2} H_\zeta - E\right] Q(\zeta, r)$$
$$= -\left[V(r_{ij}) - V_0(r)\right]$$
$$\left[Q(\zeta, r) + \int_0^{\sqrt{\alpha}} \mathcal{F}_E(\zeta, \zeta') \; Q(\zeta', r) \; d\zeta'\right]$$

where

$$H_r = -\frac{\partial^2}{\partial r^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + \frac{A(A-1)}{2} V_0(r)$$

$$H_\zeta = \frac{\alpha}{4}\left[-\frac{\partial^2}{\partial \zeta^2} + \zeta^2 - 3\right].$$

$$\mathcal{F}_E(\zeta,\zeta') =$$
$$\zeta e^{-\zeta^2/2} \sum_K C_K L_K^{1/2}(\zeta^2) L_K^{1/2}(\zeta'^2) \zeta' e^{-\zeta'^2/2},$$

$$C_K = \frac{2\,K!}{\Gamma(K+3/2)}(f_K^2 - 1)$$

IDEA-I

More simplifications!

The summation $\sum_K$ can be carried out analytically!

$$\frac{\hbar^2}{m}\left[H_r + \frac{\alpha}{r^2}H_\zeta - E\right]Q(\zeta,r)$$
$$= -\left[V(r_{ij}) - V_0(r)\right]$$
$$\left[Q(\zeta,r) + \int_0^{\sqrt{\alpha}} \mathcal{F}_I(\zeta,\zeta')\ Q(\zeta',r)\ \mathrm{d}\zeta'\right]$$

with

$$\mathcal{F}_I(\zeta,\zeta') =$$
$$\frac{2(A-2)}{\sqrt{3}}\left\{\left[A-3-\frac{2}{3}(\zeta^2-\frac{3}{2})(\zeta'^2-\frac{3}{2})\right]\zeta\zeta'\mathrm{e}^{-(\zeta^2+\zeta'^2)/2}\right.$$
$$\left.+\frac{4}{\sqrt{3}}\left[\mathrm{e}^{-(5(\zeta-\zeta')+2\zeta\zeta')} - \mathrm{e}^{-(5(\zeta+\zeta')-2\zeta\zeta')}\right]\right\}$$

In the presence of a trapping potential $V_{\rm trap}(r)$:

$$H_r = -\frac{\partial^2}{\partial r^2} + \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + V_{\rm trap}(r)$$

Adiabatic Approximation

Let

$$Q(\zeta, r) = Q_\lambda(\zeta, r) u_\lambda(r)$$

Then

$$\begin{aligned} \frac{\hbar^2}{m}\left[\frac{4}{r^2}H_\zeta \right. &+& \left. U_\lambda(r)\right] Q_\lambda(\zeta, r) = -\left[V(\frac{r}{\sqrt{\alpha}}\zeta) - V_0(r)\right] \\ &\times& \left[Q_\lambda(\zeta, r) + \int_0^{\sqrt{\alpha}} \mathcal{F}_I(\zeta, \zeta')Q_\lambda(\zeta', r)\,\mathrm{d}\zeta'\right] \end{aligned}$$

and k_λ^2: Eigen-energy

$$u_\lambda^{''}(r) + \left[k_\lambda^2 + V_{\rm eff}(r)\right] u_\lambda(r) = 0$$

$V_{\rm eff}$: Effective potential

$$V_{\rm eff}(r) = \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + \frac{A(A-1)}{2} V_0(r) - U_\lambda(r) + V_{\rm trap}(r)$$

Results

- Expansion of $f_K^2 - 1$ as $\alpha \to \infty$.

$$T_1 = (A-2)2P_K^{\alpha,1/2}(-1/2)/P_K^{\alpha,1/2}(1)$$

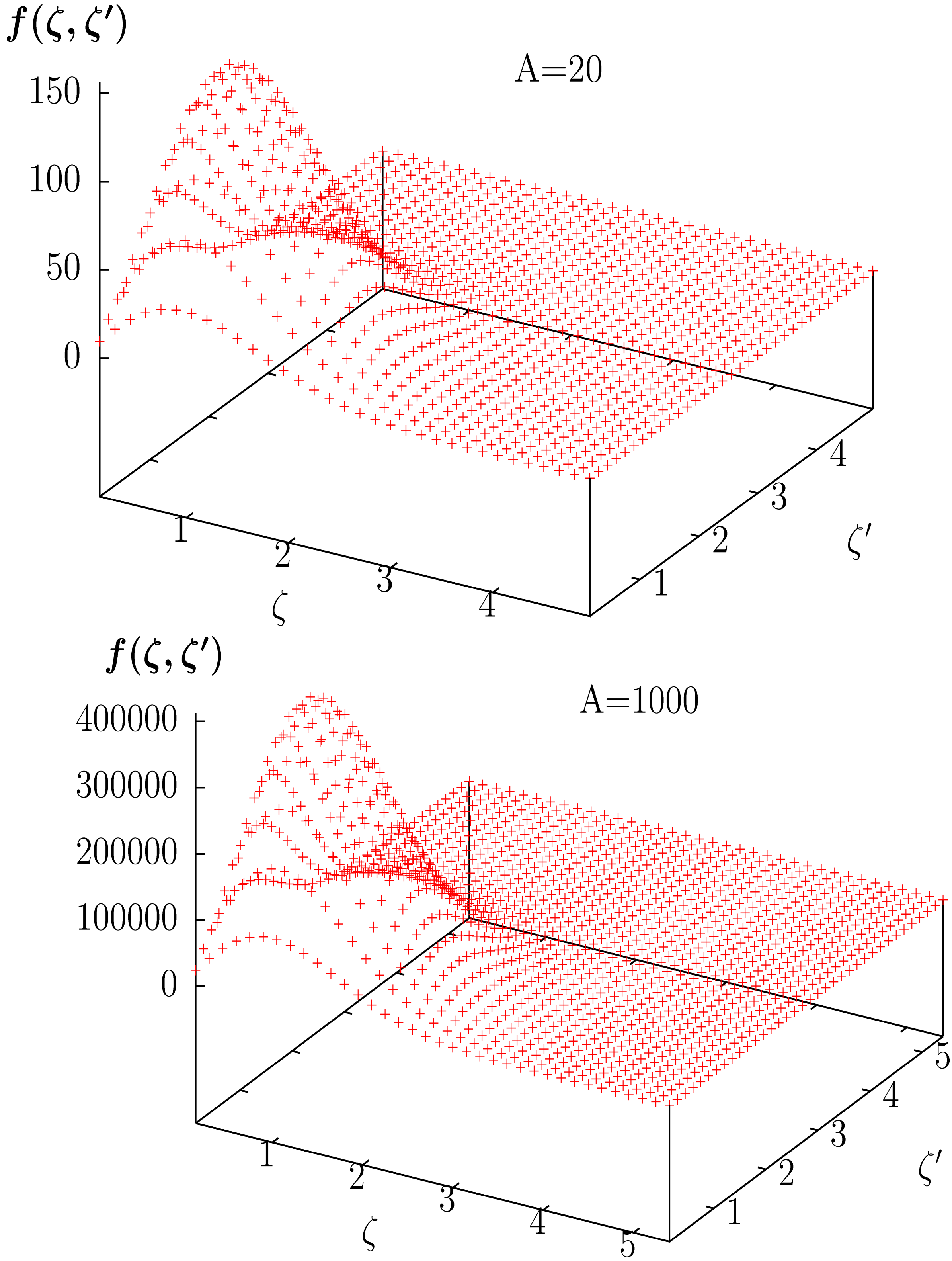
$$T_2 = (A-2)(A-3)/2\ P_K^{\alpha,1/2}(-1)/P_K^{\alpha,1/2}(1)$$

$$f_K^2 - 1 = T_1 + T_2$$

	$A = 20$		
K	T_1	T_2	$f_K^2 - 1$
0	36.	153	189
1	7.5	-8.5	-1
2	1.1004464	0.7589286	1.8593750
3	0.0729391	-0.0915948	-0.0186557
4	-0.0086754	0.0137392	0.0050638
5	-0.0016333	-0.0024376	-0.0040709
6	0.0002636	0.0004951	0.0007588
7	0.0000479	-0.0001125	-0.0000646
10	0.0000012	0.0000022	0.0000035

	$A = 1000$		
K	T_1	T_2	$f_K^2 - 1$
0	1996.0000000	497503.	499499.
1	497.5000000	-498.5000000	-1.0000000
2	123.5018775	0.8319426	124.3338201
3	30.5345323	-0.0019425	30.5325898
4	7.5185722	0.0000058	7.5185780
5	1.8437195	-0.0000000	1.8437195
6	0.4502550	0.0000000	0.4502550
7	0.1095002	-0.0000000	0.1095002
10	0.0015358	0.0000000	0.0015358

Strength, shape, and spread of $\mathcal{F}(\zeta, \zeta')$



The ^{16}O system

Wigner Force only

- Volkov potential Soft core

$$V(r_{ij}) = v_1 \exp[-(r_{ij}/b_1)^2] + v_2 \exp[-(r_{ij}/b_2)^2]$$

($v_1 = -83.34002\,\mathrm{MeV}$, $v_2 = 144.84341\,\mathrm{MeV}$
$b_1 = 1.6\,\mathrm{fm}$, $b_2 = 0.82\,\mathrm{fm}$)

- Afnan and Tang S3 potential

$$V(r_{ij}) = \sum_{i=1}^{5} v_i \exp[-b_i r_{ij}^2]$$

(v_i being 1000.0, -163.345, -9.8025, -82.0, and
-11.5 MeV,
b_i are 3., 1.05, 0.6, 0.8, and 0.4 fm^{-2})

- Yukawa type MT-V potential

$$V(r_{ij}) = \frac{v_1}{r_{ij}} \exp[-b_1 r_{ij}] + \frac{v_2}{r_{ij}} \exp[-b_2 r_{ij}]$$

($v_1 = -578.09\,\mathrm{MeV\,fm}$, $v_2 = 1458.05\,\mathrm{MeV\,fm}$)
$b_1 = 1.55\,\mathrm{fm}^{-1}$, $b_2 = 3.11\,\mathrm{fm}^{-1}$)

Table 1: Binding energies (in MeV) obtained for $A = 16$ with nuclear forces)

Potential	IDEA-I	IDEA(exact)	HHEM
Volkov	1643	1640	–
S3	1247	1246	1235
MT-V	1377	1376	1363

Bosons confined in magnetic trap

Trap: Spherically symmetric harmonic oscillator potential

$$V_{\mathrm{trap}}(r) = \sum_{i=1}^{A} \frac{1}{2} m\omega^2 x_i^2 = \frac{1}{4} m\omega r^2$$

Potential: Gaussian

$$V(r_{ij}) = V_0 \exp[-r_{ij}^2/r_0^2]$$

$V_0 = 3.1985 \times 10^6$ o.u and $r_0 = 0.005$ o.u **Note:**

Oscillator units (o.u)

Energy: $\hbar\omega$

Length: $\sqrt{\hbar/m\omega}$

ω is the harmonic oscillator circular frequency

$\hbar^2/m = 1$.

Table 2: Results (in o.u) obtained with IDEA-E and IDEA-I using the Gaussian potential

A	IDEA-E	IDEA-I	PHEM
3	6.009	6.009	4.500
5	7.758	7.758	7.505
10	15.003	15.003	15.034
15	22.501	22.501	22.567
20	30.000	30.001	30.107
25	37.501	37.501	37.654
30	45.009	45.001	45.207
35	52.509	52.501	52.768

- For $A = 3$: 25%,
- For $A = 5$: 3.26%.
- For $A = 10$: 0.2%
- Beyond $A > 10$ differences within numerics

Second example

$$V(r_{ij}) = V_0 \,\mathrm{sech}^2(r_{ij}/r_0)$$

$V_0 = 1.81847 \times 10^9\,\mathrm{o.u}$, $r_0 = 0.001\,\mathrm{o.u.}$.

A	IDEA-I	PHEM	DMC
10	15.143	15.1490	15.1539
20	30.625	30.6209	30.639
50	78.701	78.8704	
100	165.038	164.907	

For very large A plethora of eigenpotentials close to each other

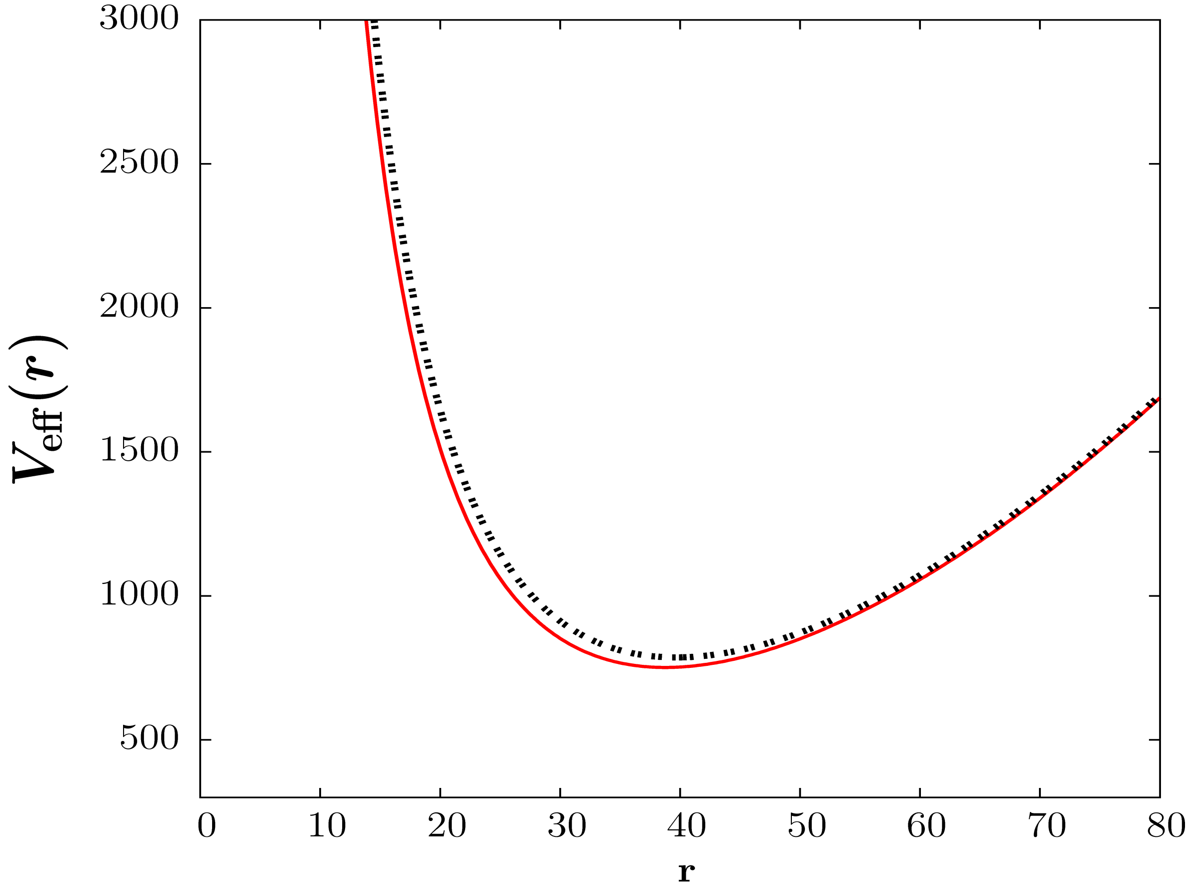


Figure 1: Two eigenpotentials $U_{\rm eff}(r)$ corresponding to $\lambda = 1$ and $\lambda = 20$ for $A = 500$.

Conclusions

- Equation can be used in studies of bound A-boson systems
- Approximations should become better with increasing A $i.e$ for $\alpha \to \infty$
- Numerics must be improved