The DVR Basis:

An Efficient Alternative to the HO Basis for Nuclear Physics

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Discrete Variable Representation (DVR)

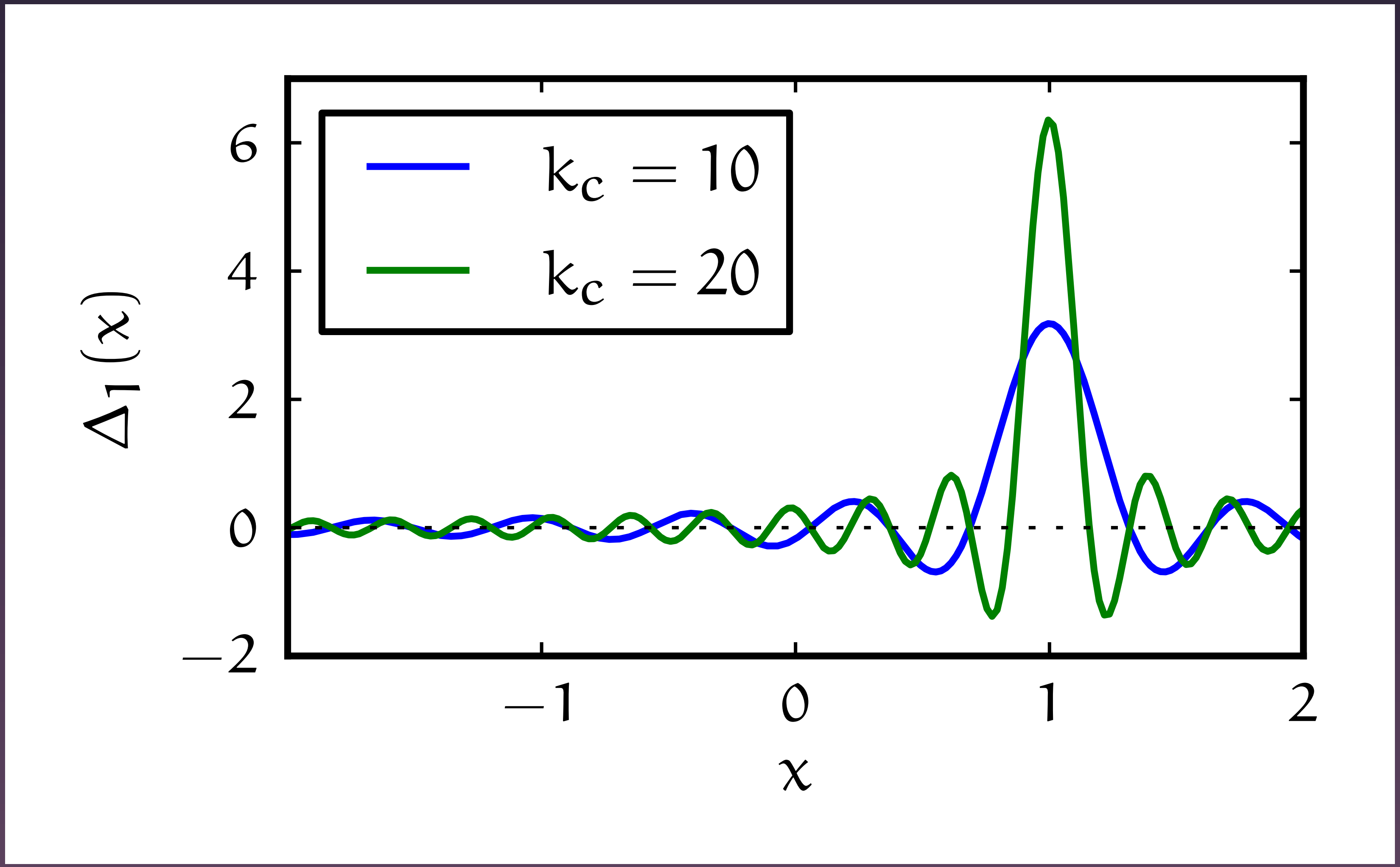
- Quasi-local (projected delta functions)
  - $F_n(x_m) \propto \delta_{mn}, \quad \langle F_m|V|F_n\rangle \approx \delta_{mn}V(x_n)$
- Analytic form for Kinetic Energy
- Exponential convergence
  - for appropriate potentials, boundary conditions etc.

Standard DVR Basis

$$\Delta_n(x) \propto F_n(x) \propto L_n(x)$$

- Projected delta-functions: $\Delta_n(x)$
  - Let $\langle x|x_n\rangle = \delta(x-x_n)$, then $|\Delta_n\rangle = P|x_n\rangle$
- Interpolating functions: $L_n(x)$
  - $|f\rangle = \sum_n f(x_n)\ |L_n\rangle$
- Orthonormal basis functions: $F_n(x)$
  - $\langle F_m|F_n\rangle = \delta_{mn}$

Projected Delta Functions



$$P = \sum_{k<k_c} |k\rangle \langle k|$$

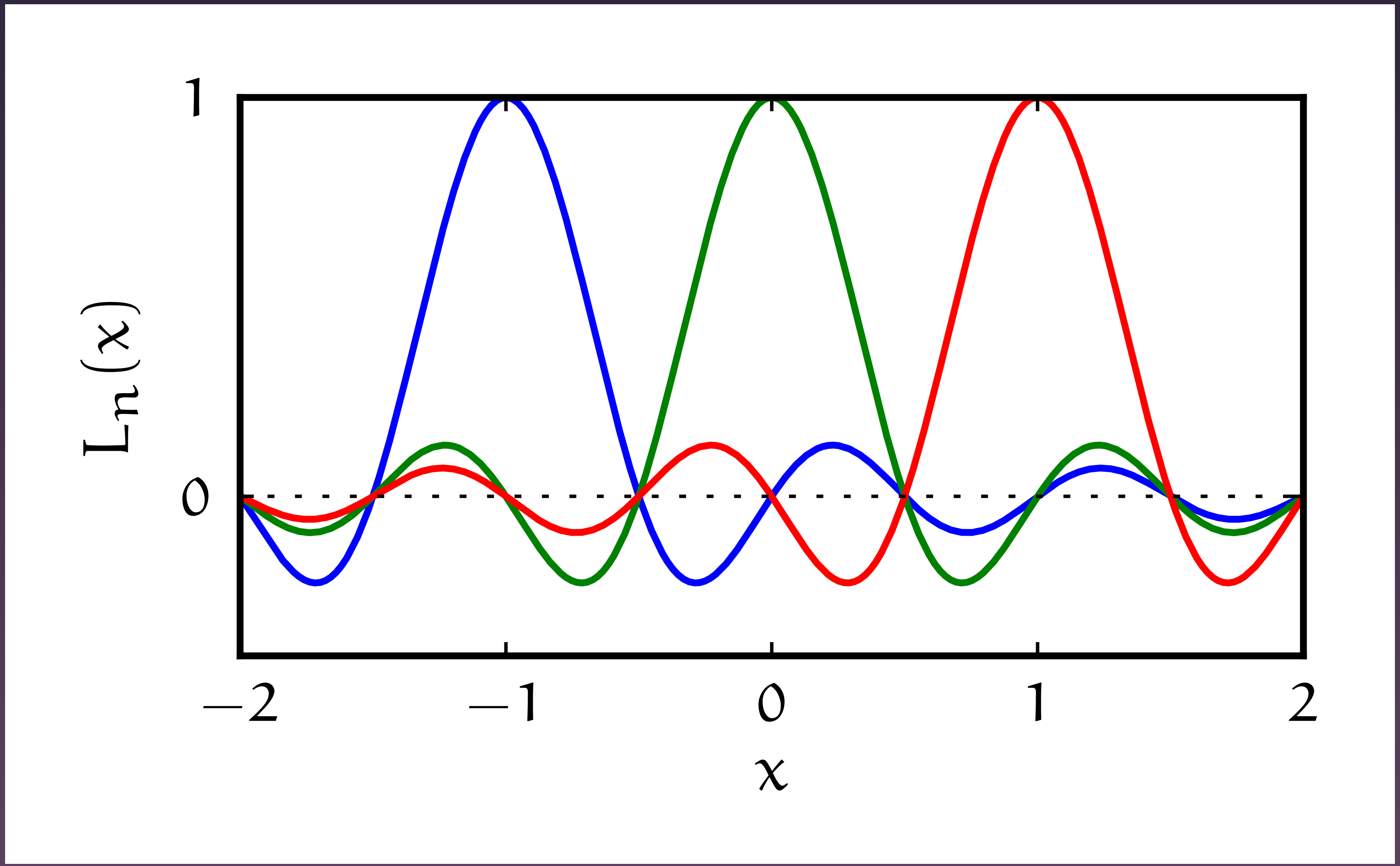
$$\langle x|x_n\rangle = \delta(x - x_n)$$

$$|\Delta_n\rangle = P\,|x_n\rangle$$

$$|F_n\rangle = |\hat{\Delta}_n\rangle = \frac{|\Delta_n\rangle}{\sqrt{\langle \Delta_n|\Delta_n\rangle}}$$

Monday, April 8, 13

Non-trivial Consistency of Abscissa

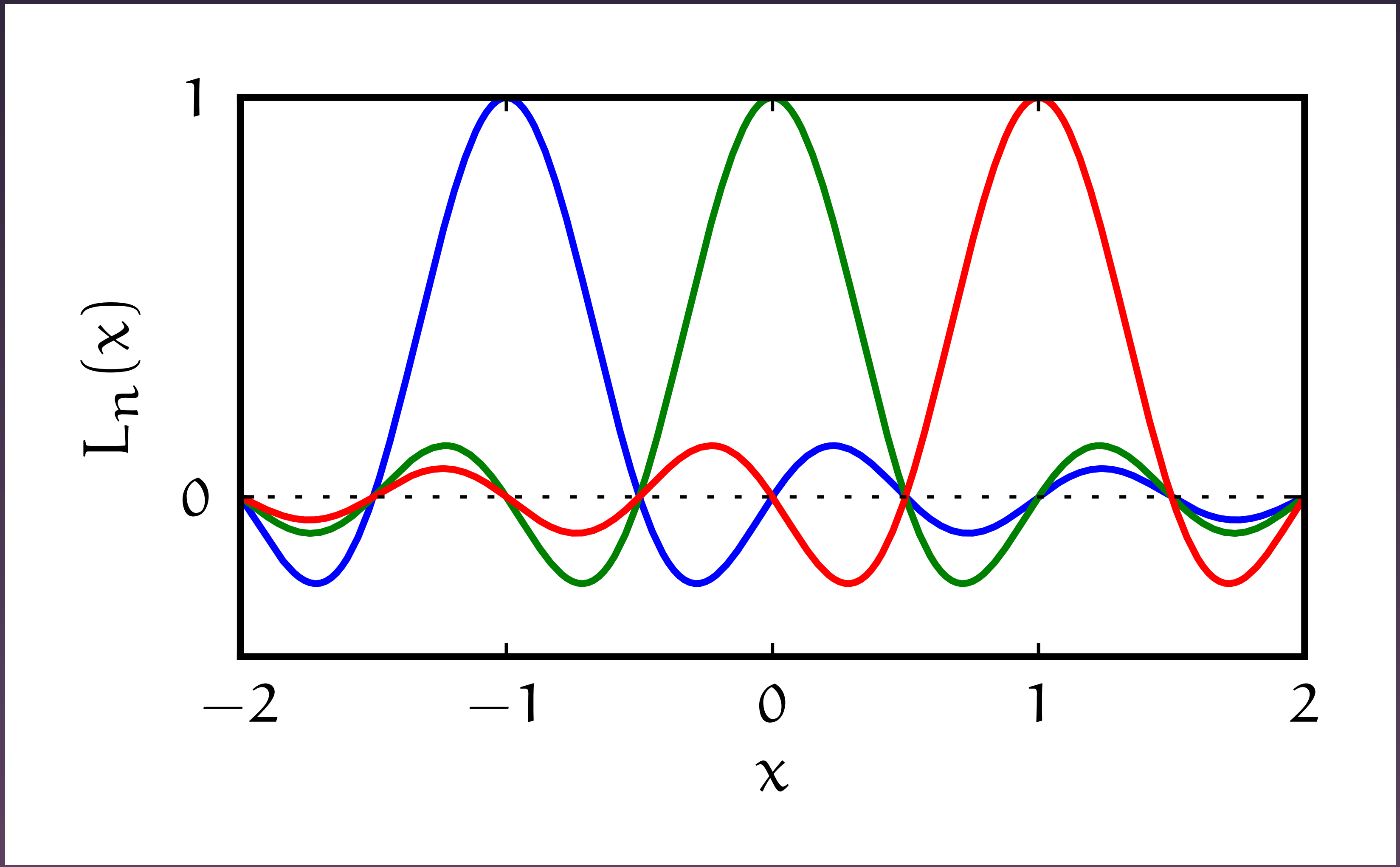


Abscissa must be nodes of $\Delta_m(x)$

$$\Delta_m(x_n) = \delta_{mn}/w_n$$

Associated with orthogonal polynomials

Interpolating Functions



Just evaluate $f(x_n)$ at the abscissa:

$$|f\rangle = \sum_n f_n \, |F_n\rangle$$
$$= \sum_n f(x_n) \, |L_n\rangle$$

Integration Weights

- $w_n = 1/\langle \Delta_n | \Delta_n \rangle = 1/\Delta_n(x_n)$
- $L_n(x) = w_n{}^{1/2} F_n(x) = w_n \Delta_n(x)$
- Gaussian quadrature wights for functions in basis:
  - $\langle f|g \rangle = \sum_n w_n f^*(x_n) g(x_n)$
- But... make sure to integrate functions in basis (or add more abscissa)

Diagonal Potential Energy

$$\langle F_m | V | F_n \rangle \approx \delta_{mn} V(x_m)$$

- Not exact, but eigenvalues and eigenvectors still have exponential convergence
- No overlap integrals needed
- Trivial 3 and 4-body operators

Analytic Kinetic Energy

$$K_{mn} = \langle F_m | \frac{\hbar^2 \nabla^2}{2m} | F_n \rangle \,, \quad K_{mn} = \langle F_m | \frac{\hbar^2}{2m} \frac{d^2}{dr^2} - \frac{\nu^2 - \frac{1}{4}}{r^2} | F_n \rangle$$

- Include singularities here
  - They can spoil convergence

DVR Examples

- Fourier basis (rearrangement): use FFTW

$$L_n(x) = \frac{\sin k_c(x - x_n)}{N \sin \frac{k_c(x-x_n)}{N}} = \frac{1}{N} \sum_{m=-(N-1)/2}^{(N-1)/2} e^{ik_m(x-x_n)}$$

$$K_{m\neq n} = \frac{2\pi^2(-1)^{m-n}}{L^2} \frac{\cos \frac{k_c(x_m-x_n)}{N}}{\sin^2 \frac{k_c(x_m-x_n)}{N}},$$

$$K_{nn} = \frac{\pi^2}{3a^2}\left(1 - \frac{1}{N^2}\right).$$

DVR Examples

- Sinc function basis
- K_{mn} dense (but only in each dimension)

$$L_n(x) = \text{sinc}\Big(k_c(x - x_n)\Big)$$

$$K_{m \neq n} = \frac{2(-1)^{m-n}}{(x_m - x_n)^2}, \qquad K_{nn} = \frac{\pi^2}{3a^2}.$$

DVR Examples

- Bessel Function Basis: Spherical/Cylindrical symmetry

$$J_\nu(z_{\nu n}) = 0, \quad w_n = \frac{2}{k_c z_{\nu n} J'_\nu(z_{\nu n})^2},$$

$$F_n(r) = (-1)^{n+1} \frac{k_c z_{\nu n}\sqrt{2r}}{k_c^2 r^2 - z_{\nu n}^2} J_\nu(k_c r),$$

$$K_{m\neq n} = \frac{8k_c^2(-1)^{m-n} z_{\nu n} z_{\nu m}}{(z_{\nu n}^2 - z_{\nu m}^2)^2},$$

$$K_{nn} = \frac{k_c^2}{3}\left[1 + \frac{2(\nu^2-1)}{z_{\nu n}^2}\right]$$

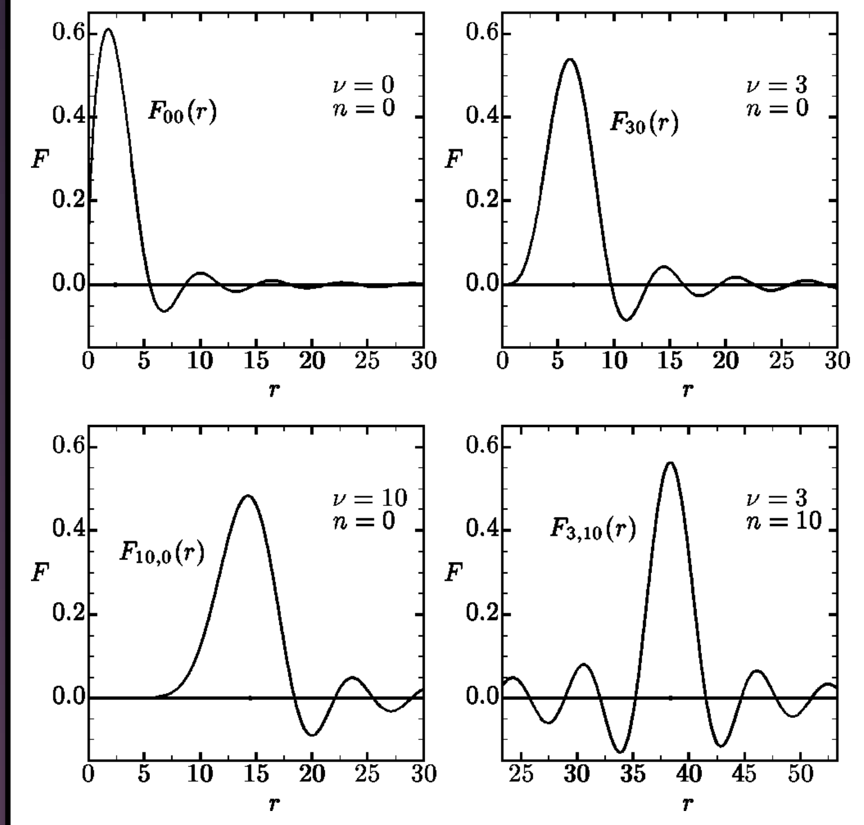


FIG. 2. Plots of the Bessel DVR functions $F_{\nu n}(r)$ for $K=1$ and for selected values of ν and n.

DVR Examples

- Bessel Function Basis: Spherical/Cylindrical symmetry
- In principle: one basis for each l
- In practice (3D):
  - use l=0, for even l
  - use l=1, for odd l
- (may need extra point to represent densities etc.)

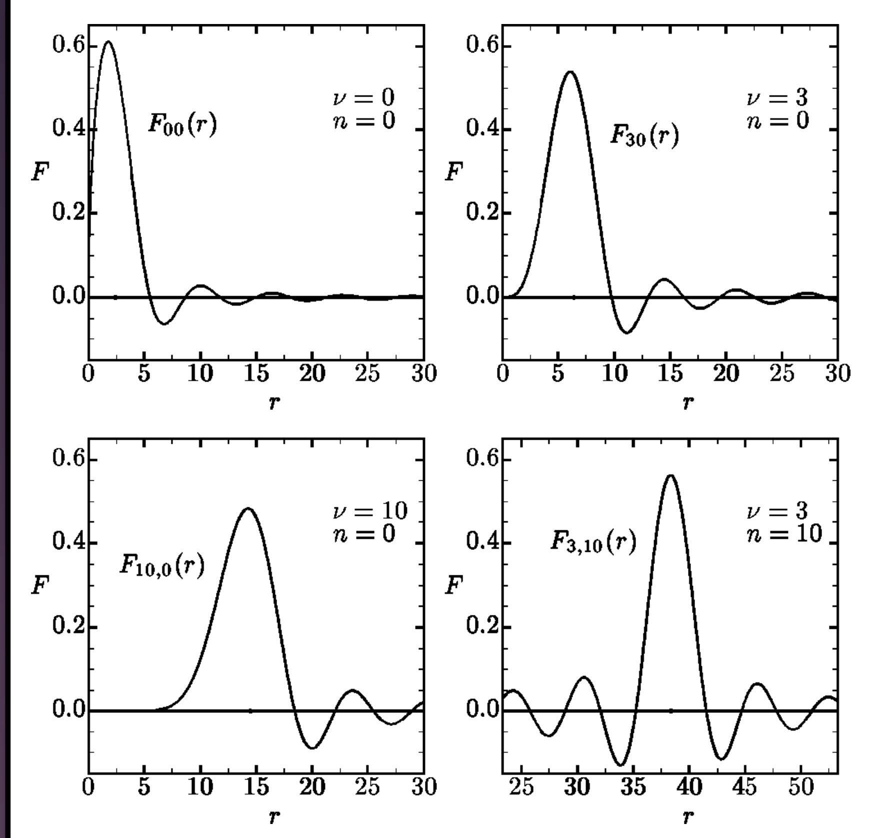


FIG. 2. Plots of the Bessel DVR functions $F_{\nu n}(r)$ for $K=1$ and for selected values of ν and n.

Simple Implementation

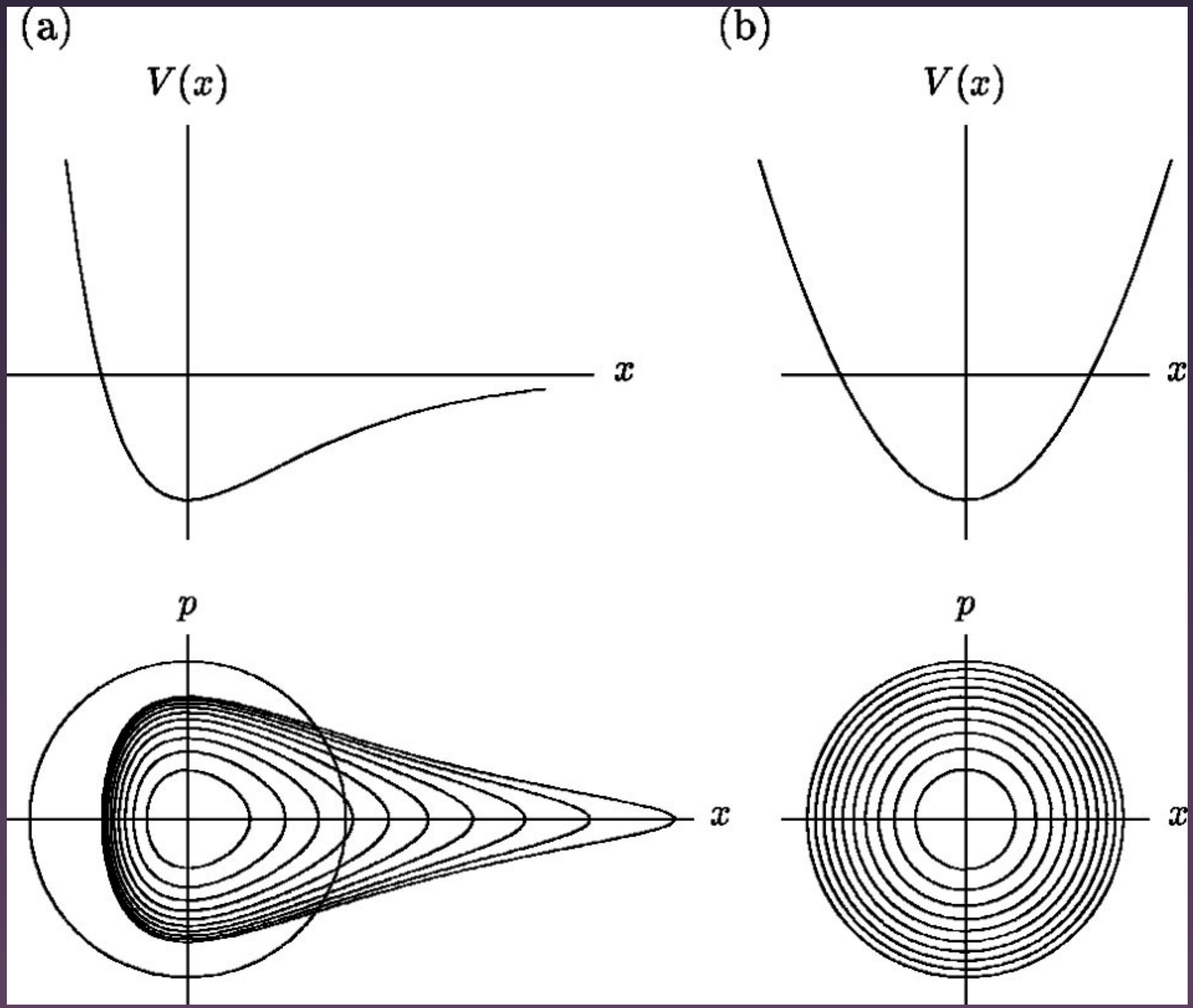
- MATLAB

```
N     = 32;
n     = (1:N);
[k,l] = meshgrid(n,n);
a     = 1;    %  lattice constant
x     = a*(-N/2:1:N/2-1)';
V     = x.^2/2;   %potential
p     = 2*pi/L*(-N/2:1:N/2-1);

Tk  = 2*(-1).^(k-l)./((sin(pi*(k-l)/N)).^2 + eps)/N^2;
Tk  = Tk - diag(diag(Tk));
Tk  = (Tk + eye(N)*(1+2/N^2)/3)*pi^2/a^2/2;
H   = Tk +diag(V);
energy  = eig(H);
```

- Python

```
class DVR1D(object):
    r"""Sinc function basis for non-periodic functions over
     an interval`xo +- L/2` with `N` points."""
    def __init__(self, N, L, xo=0.0):
        L = float(L)
        self.N = N
        self.L = L
        self.xo = xo
        self.a = L/N
        self.n = np.arange(N)
        self.x = self.xo + self.n*self.a - self.L/2.0 + self.a/2.0
        self.k_max = np.pi/self.a

    def H(self, V):
        """Return the Hamiltonian with the give potential."""
        _m = self.n[:, None]
        _n = self.n[None, :]
        K = 2.0*(-1)**(_m-_n)/(_m-_n)**2/self.a**2
        K[self.n, self.n] = np.pi**2/3/self.a**2
        K *= 0.5    # p^2/2/m
        V = np.diag(V(self.x))
        return K + V
```

Phase-Space Coverage



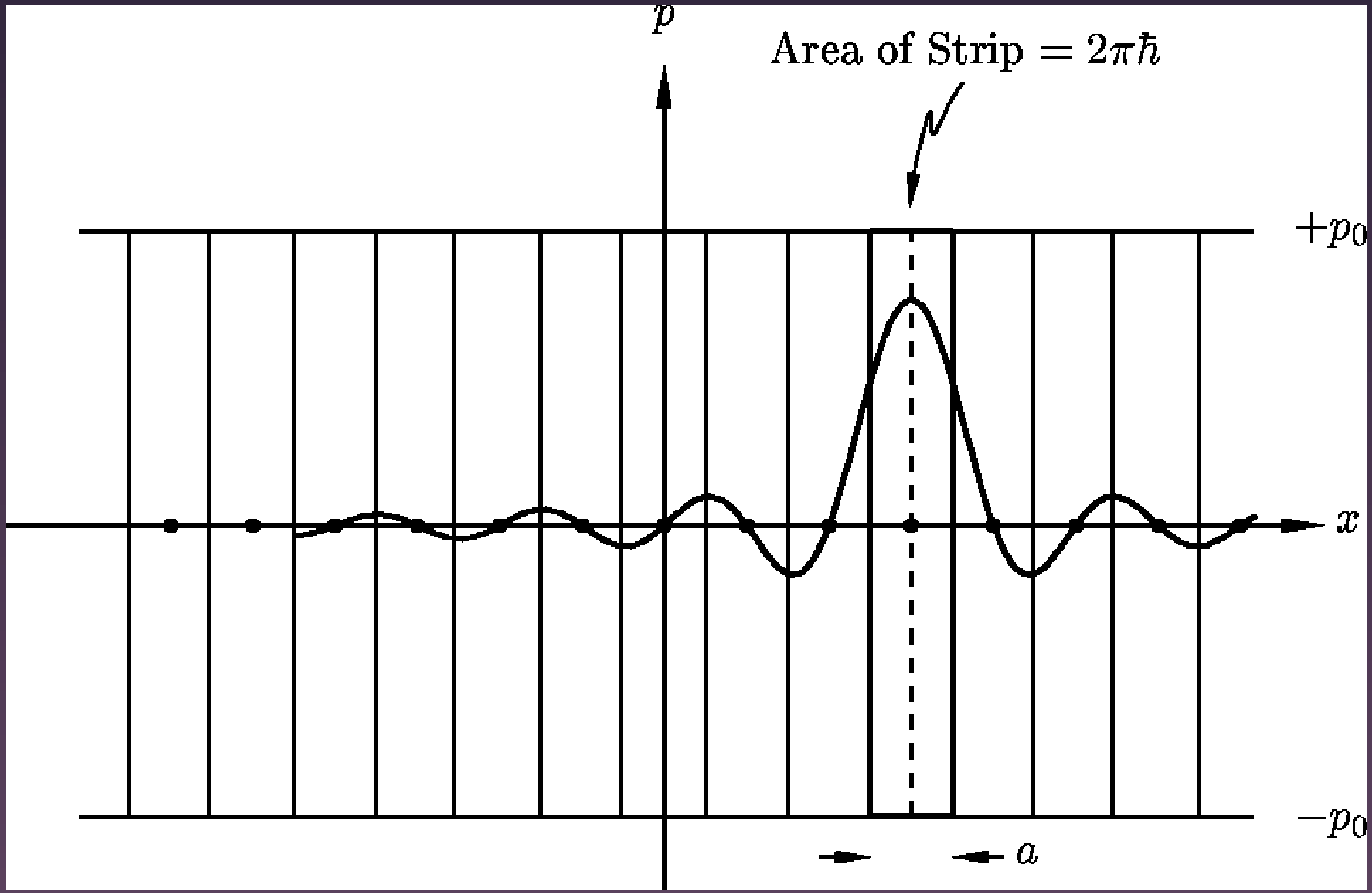
Littlejohn et al. J. Chem. Phys. 116 (2002) 8691

For convergence:

- Must cover same semi-classical phase space

- Consider modeling the Morse (left) potential with HO basis (right)

Phase-Space Coverage

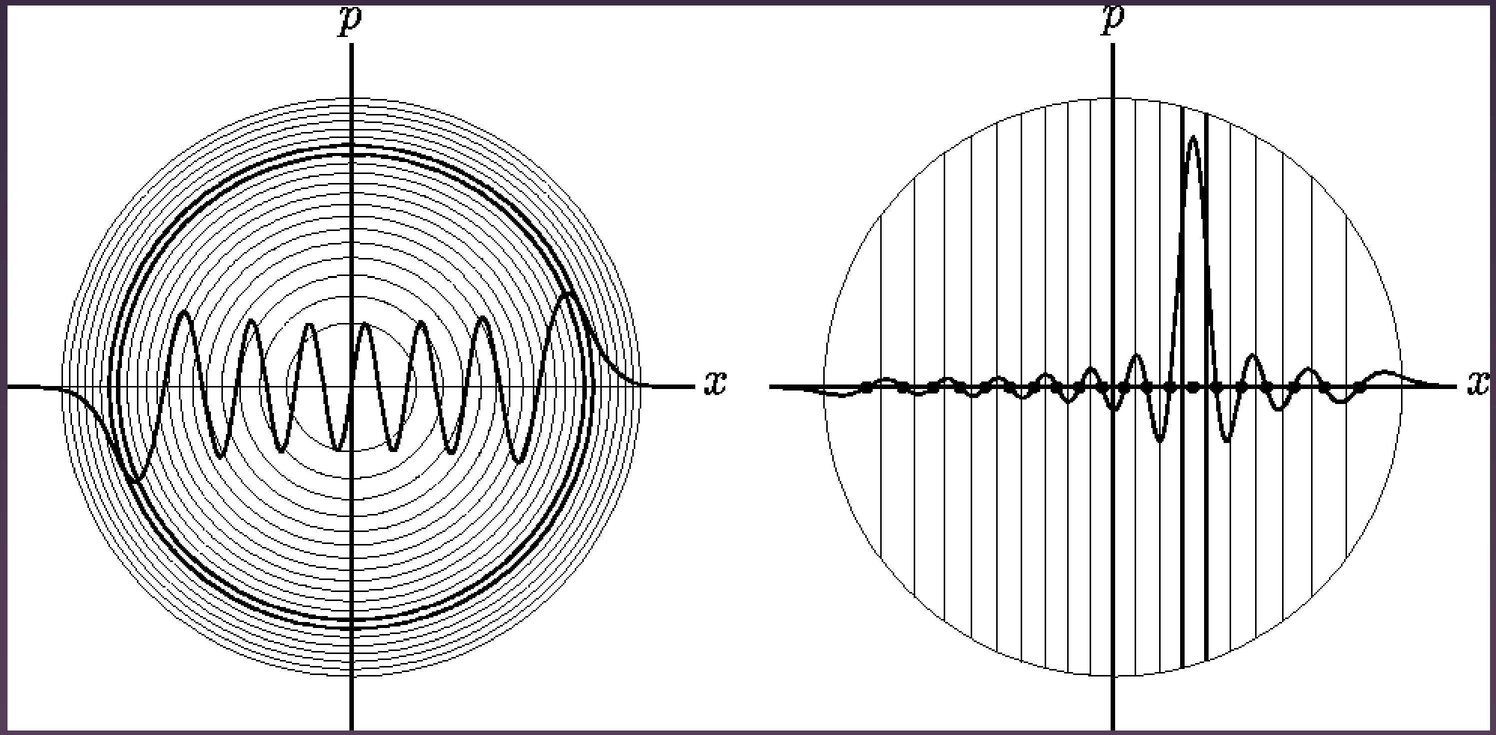


DVR basis slices phase space into strips

Efficient coverage of typical rectangular "model spaces" with simple IR and UV cutoffs

Littlejohn et al. J. Chem. Phys. 116 (2002) 8691

Phase-Space Coverage

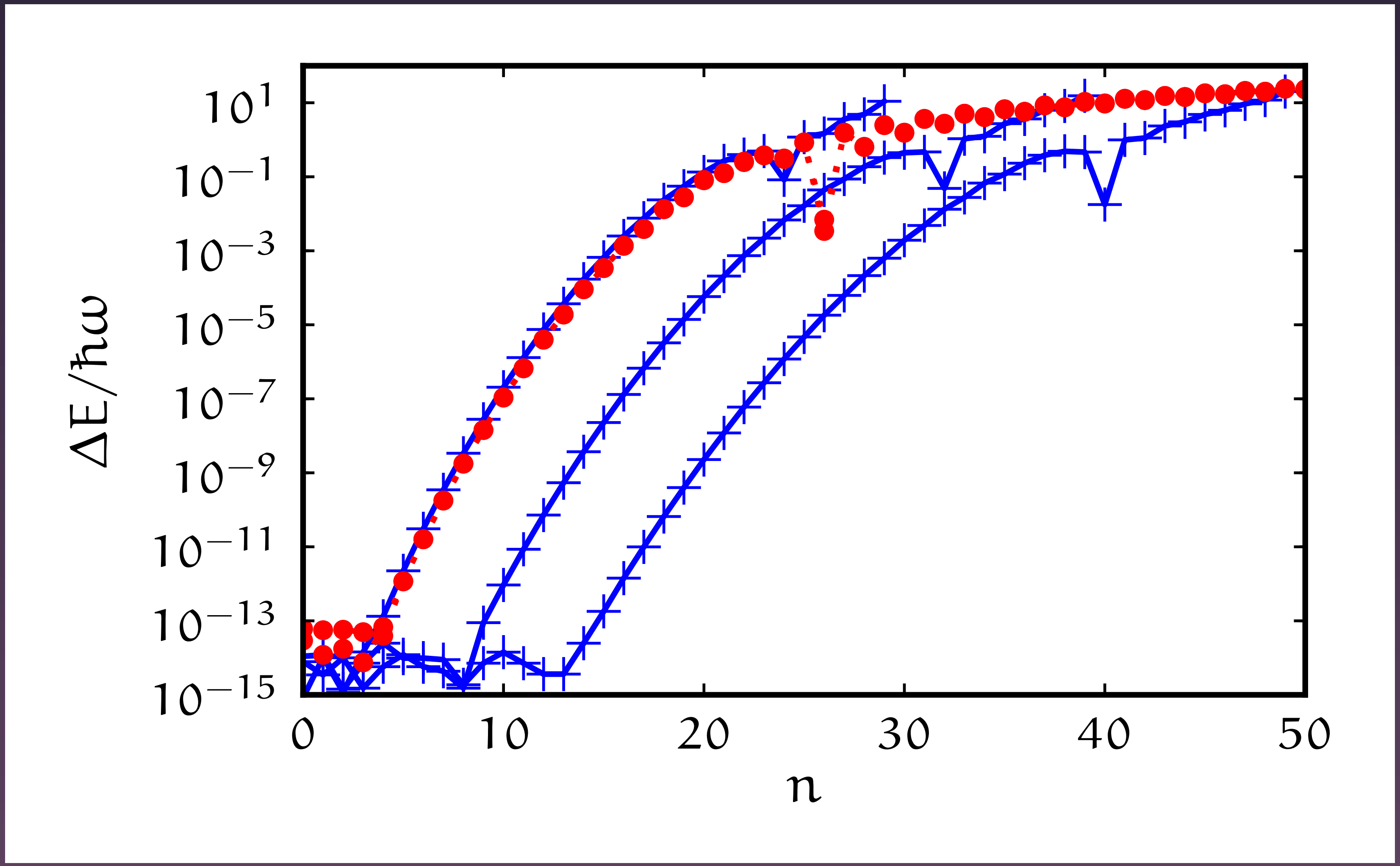


Optimal coverage of a HO with a DVR basis

Note: adding more states efficiently expands the space

Littlejohn et al. J. Chem. Phys. 116 (2002) 8691

HO Eigentstates with DVR basis



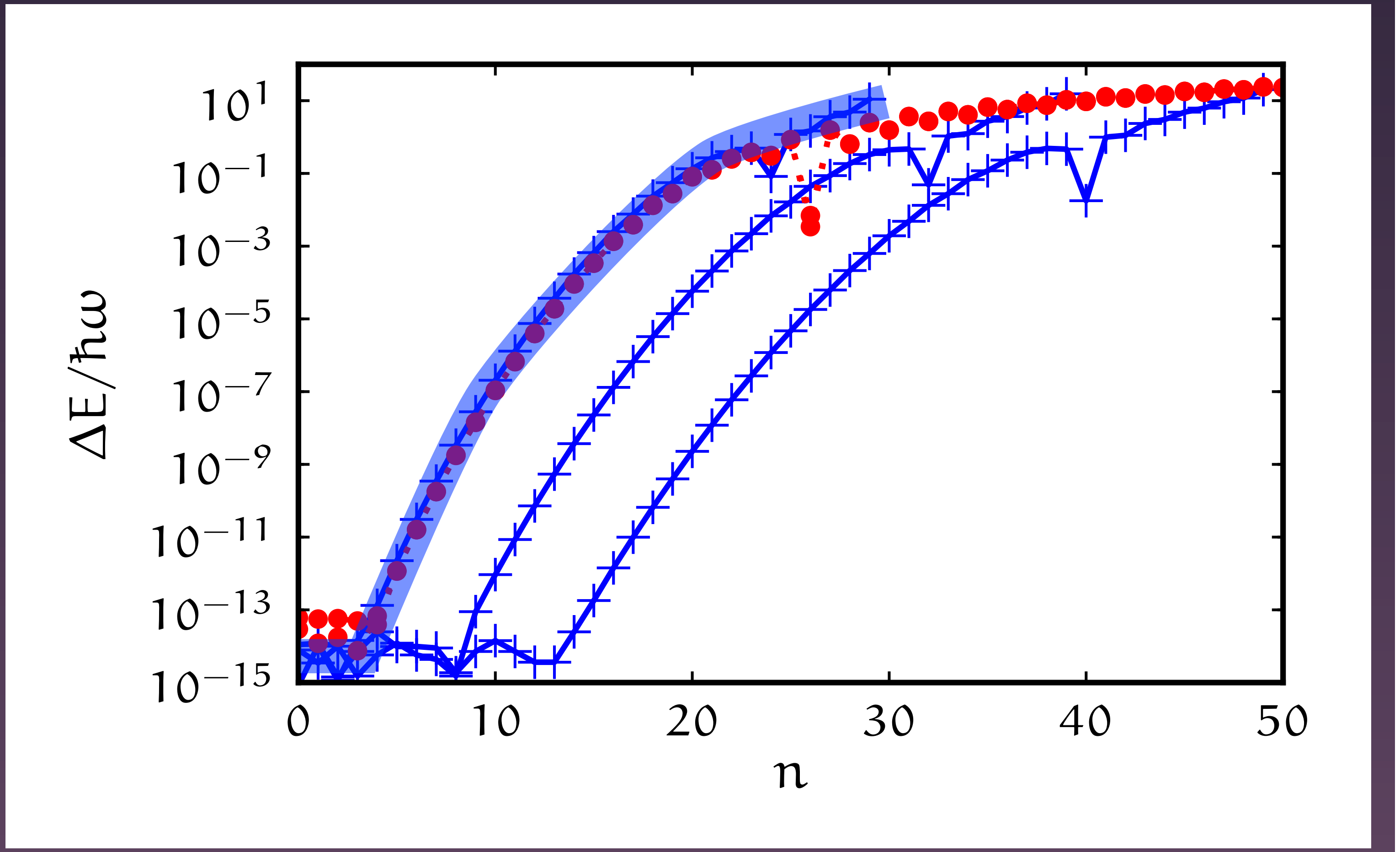
Ho potential with optimally tuned DVR basis

Bulgac & Forbes arXiv:1301.7354

N=L=30

Optimal phase space coverage

- 5 energies to machine precision
- 24 reasonable energies (10%)



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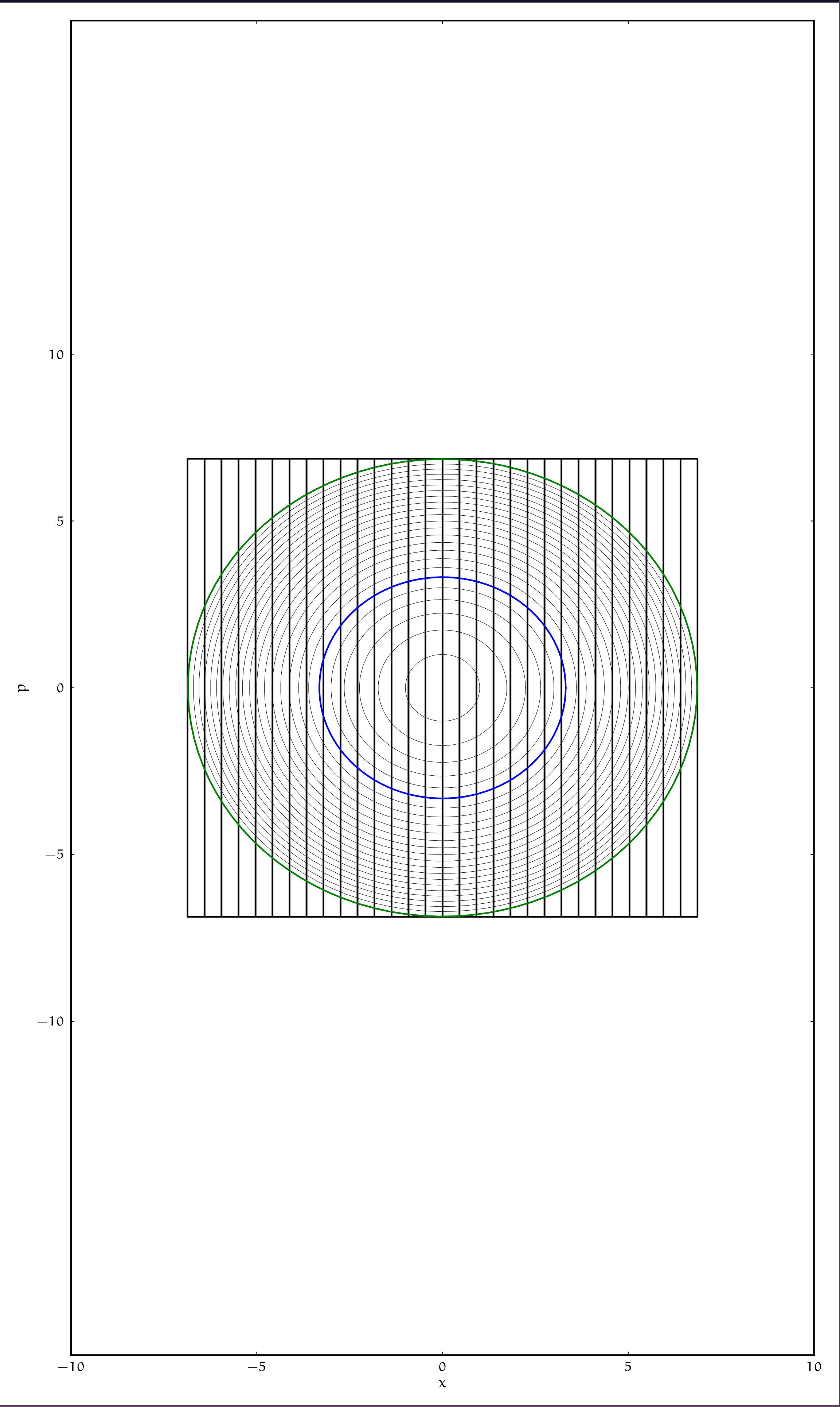
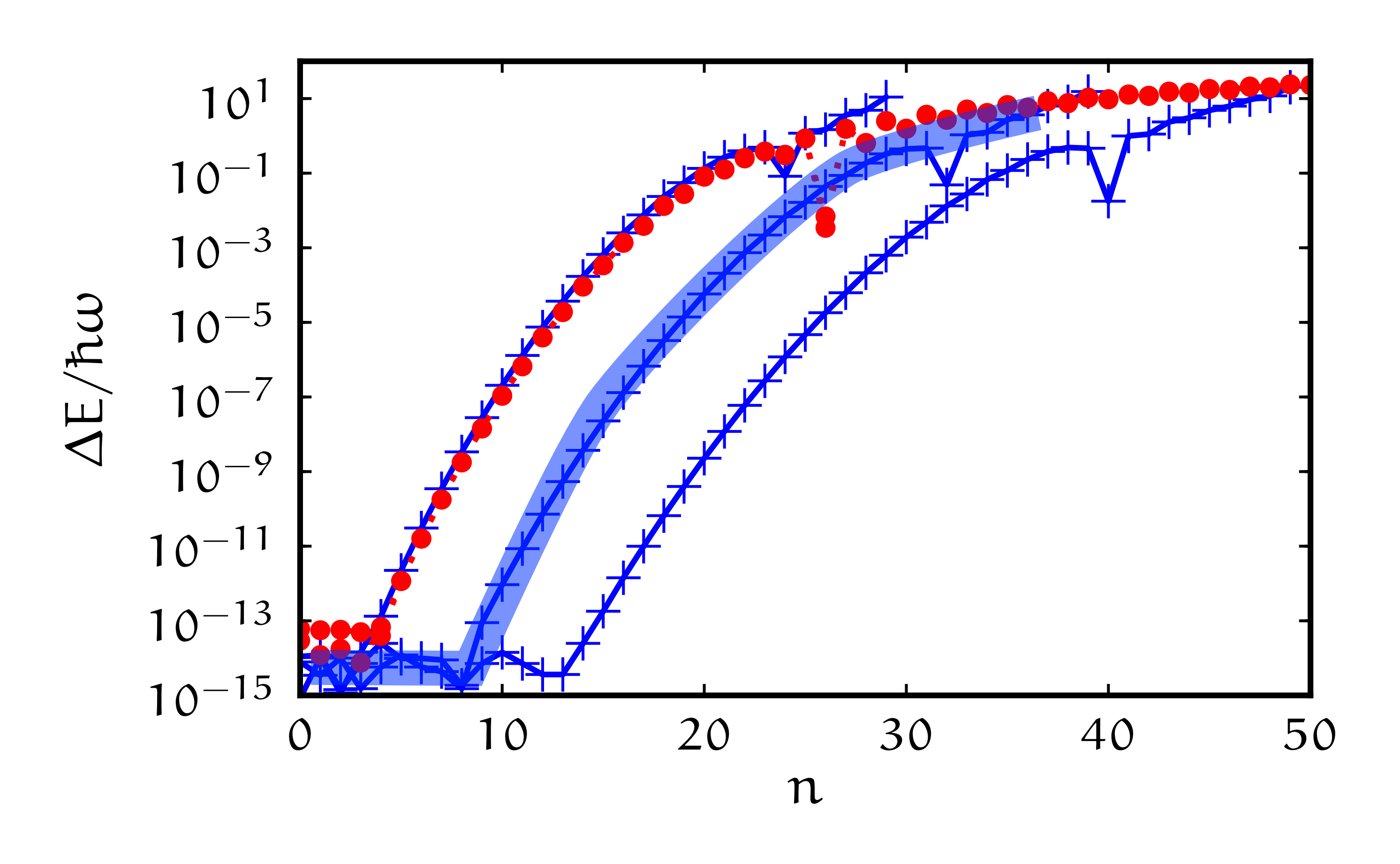
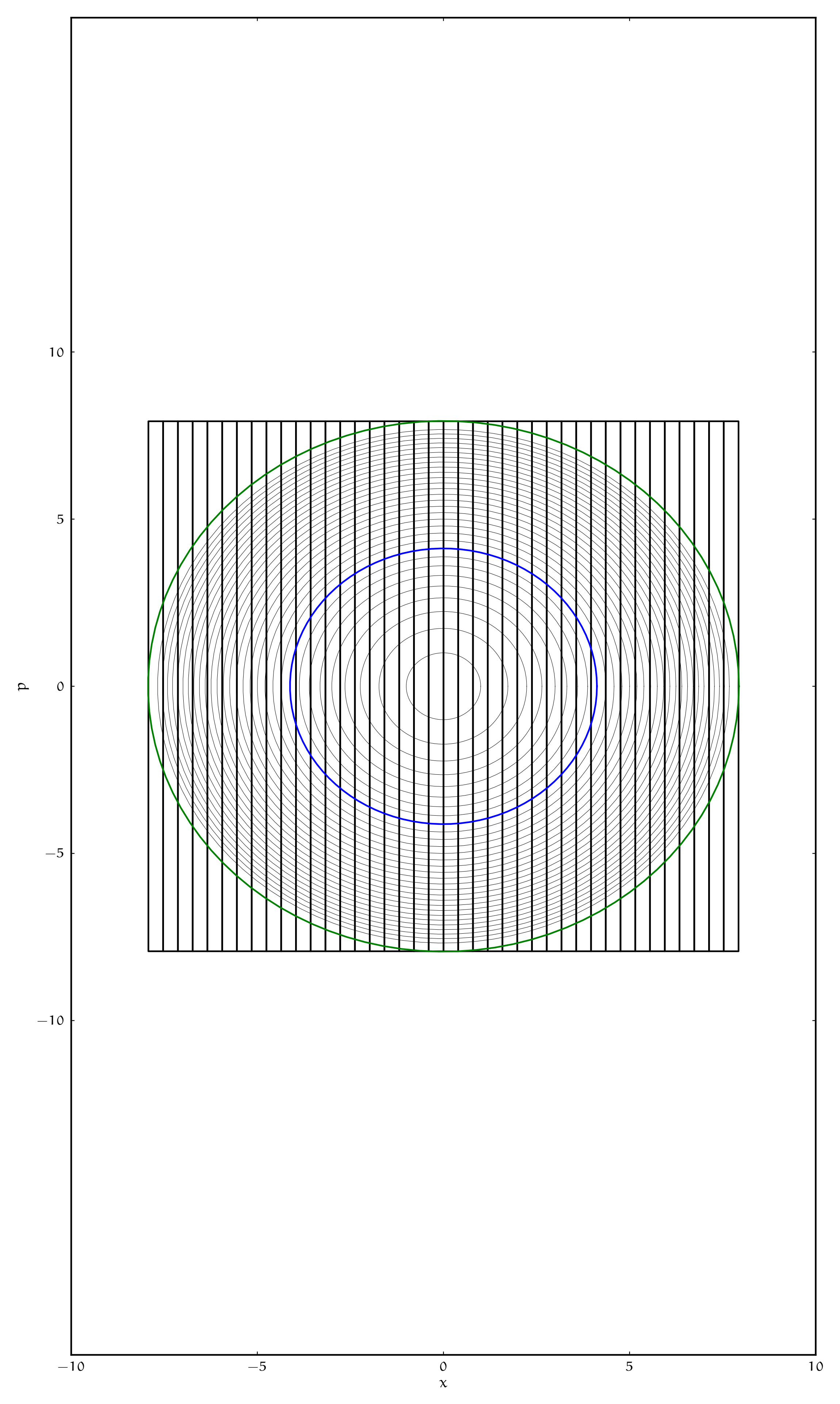


N=L=40

Optimal phase space coverage

- 8 energies to machine precision
- 32 reasonable energies (10%)



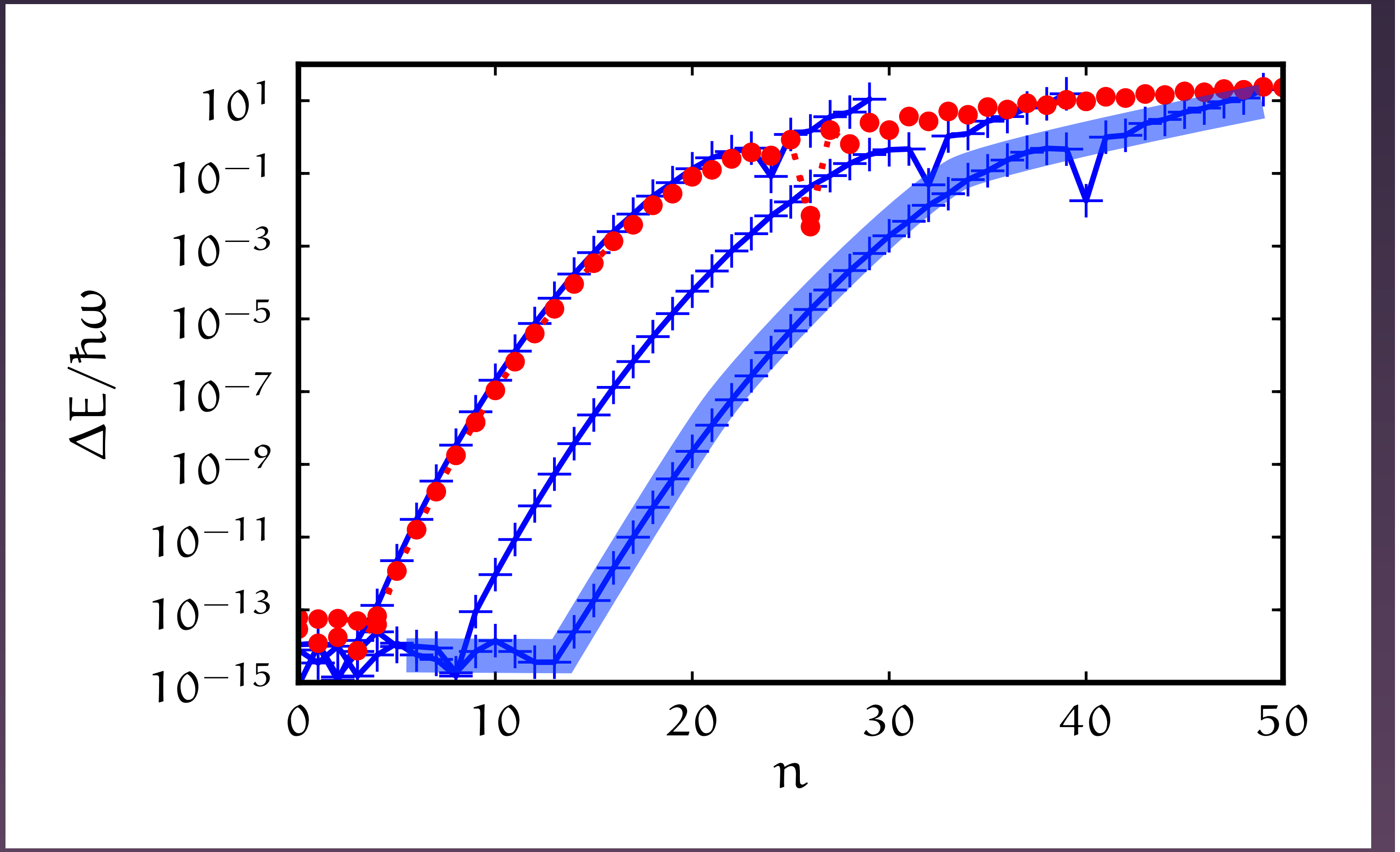


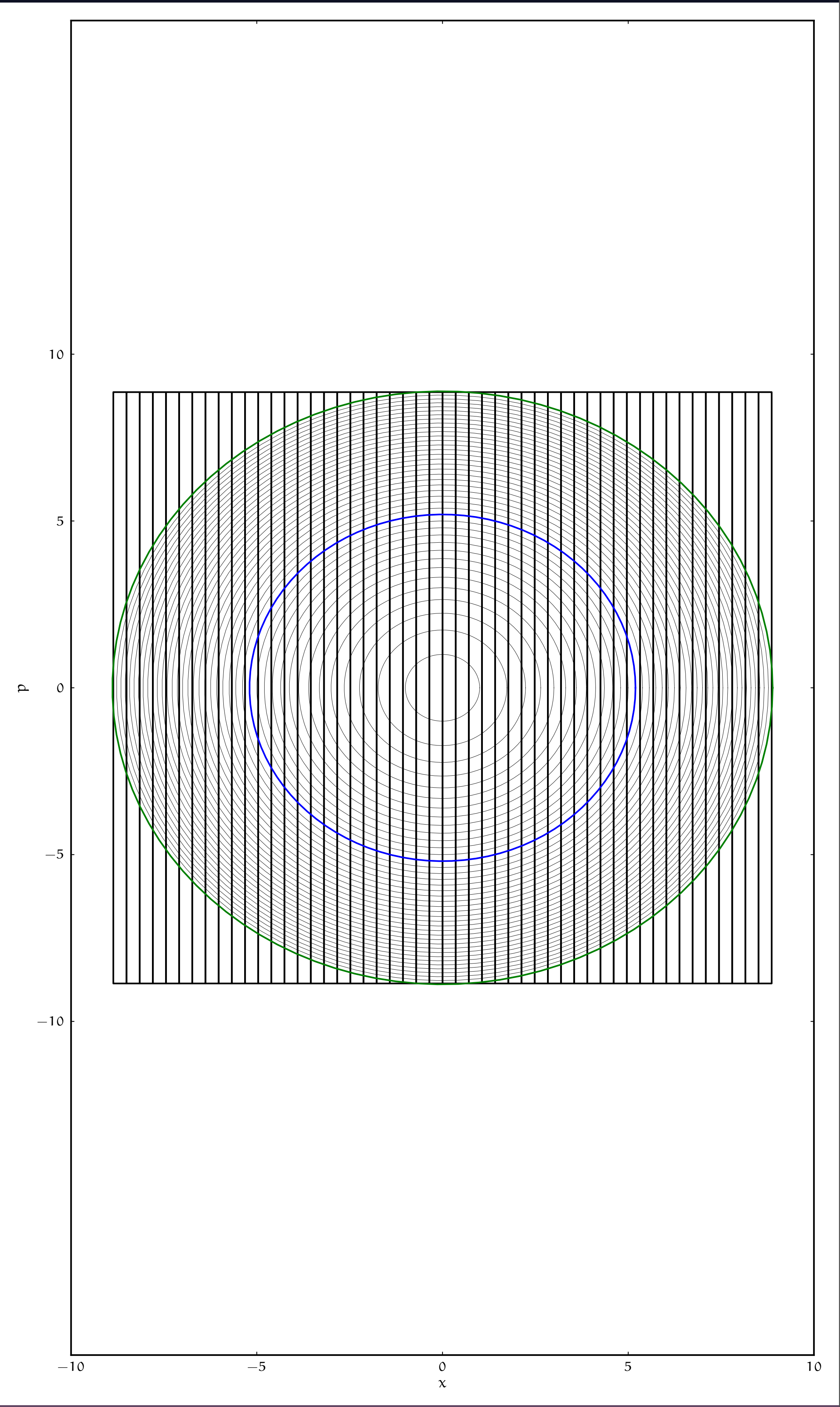
Bulgac & Forbes arXiv:1301.7354

N=L=50

Optimal phase space coverage

- 14 energies to machine precision
- 40 reasonable energies (10%)



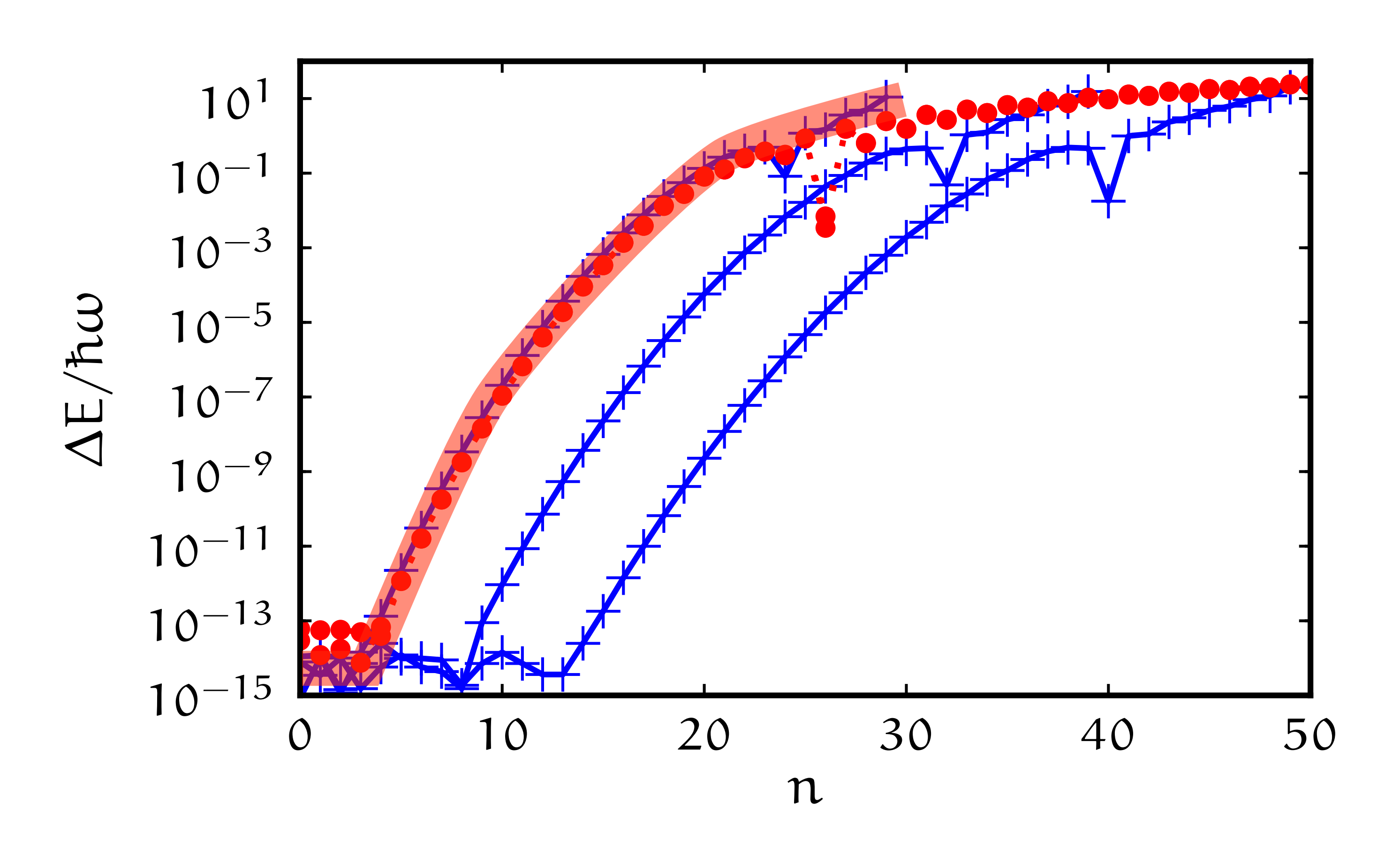


Bulgac & Forbes arXiv:1301.7354

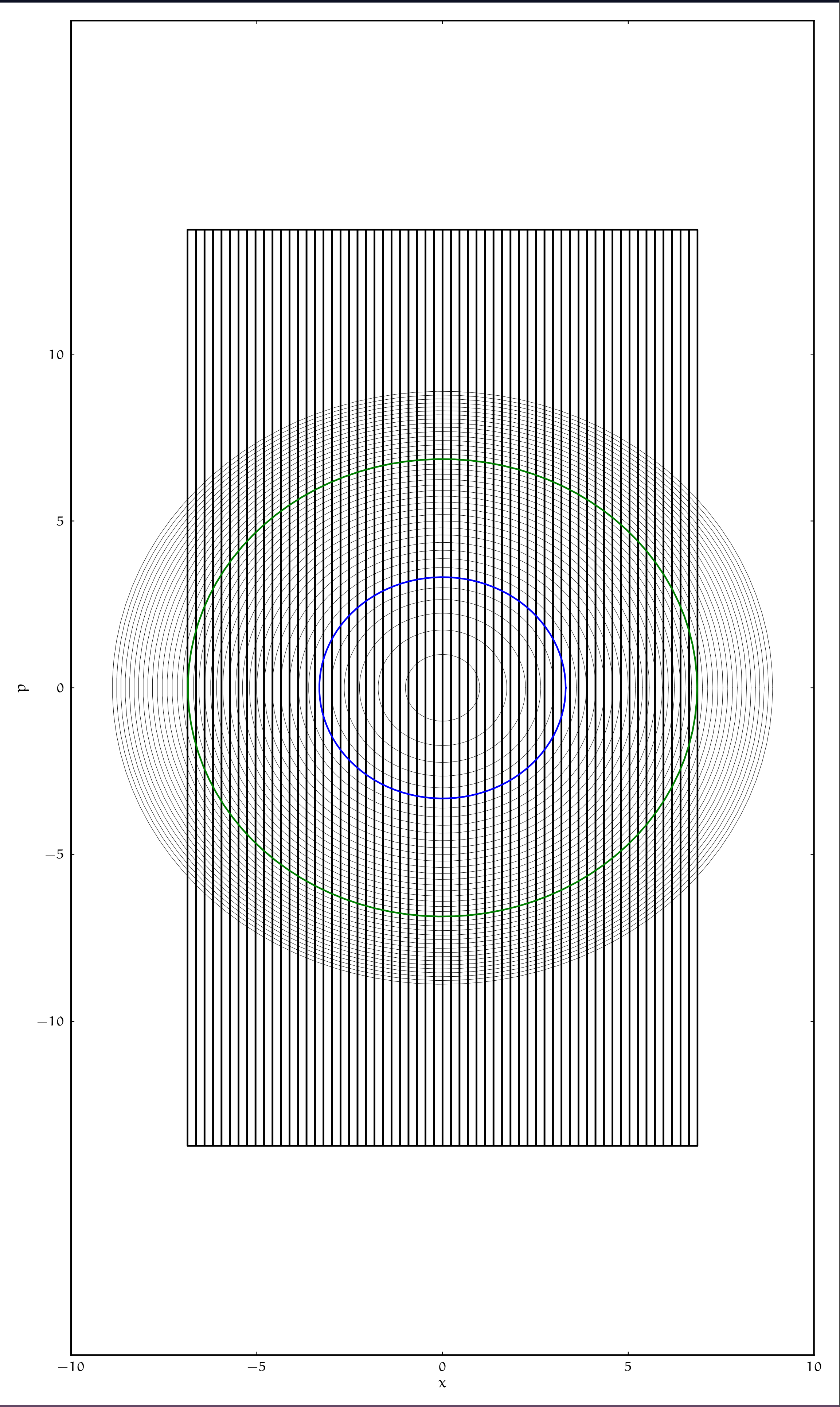
N=60, L=30

Higher UV cutoff does not help

- 5 energies to machine precision
- 24 reasonable energies (10%)



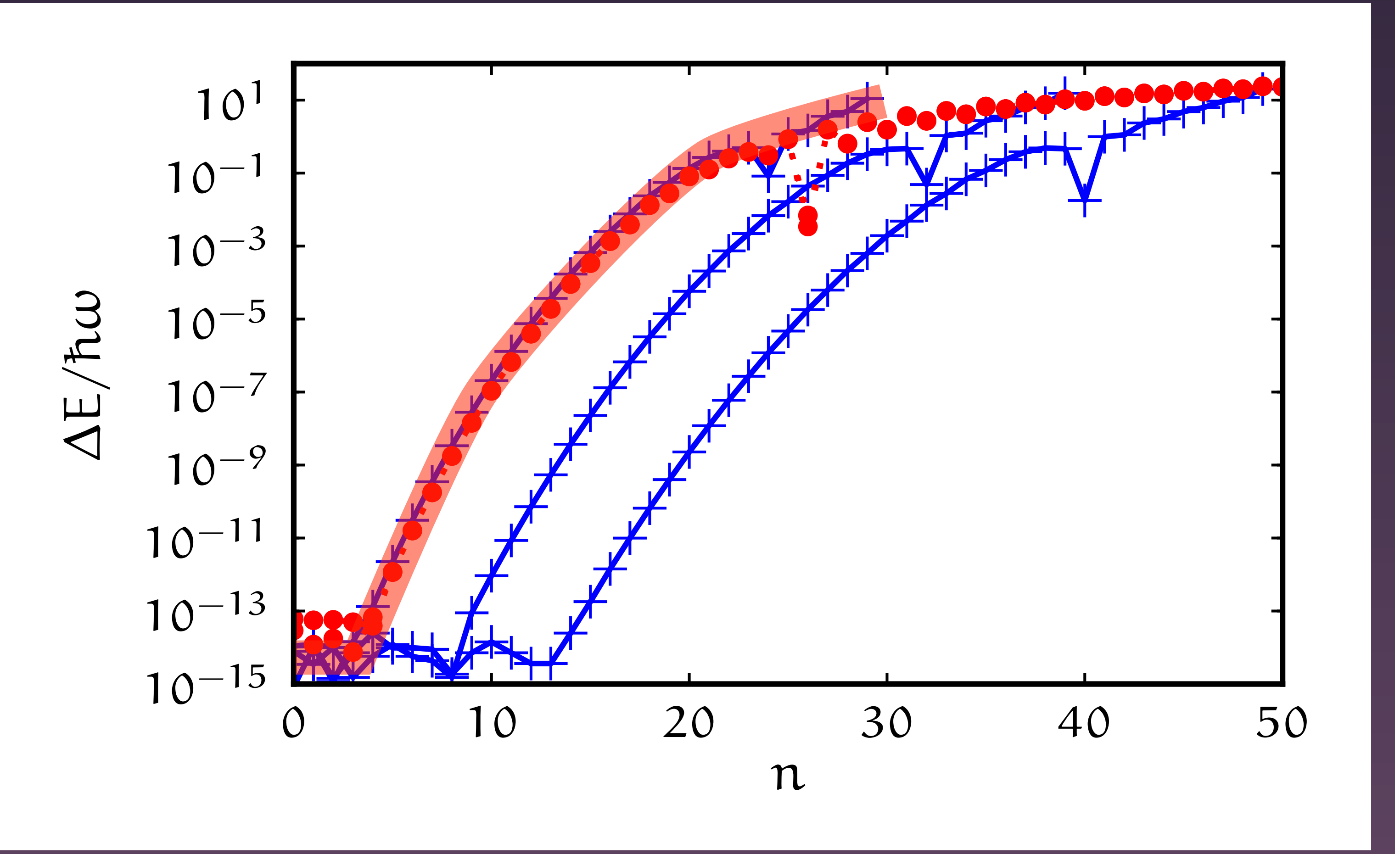
Bulgac & Forbes arXiv:1301.7354

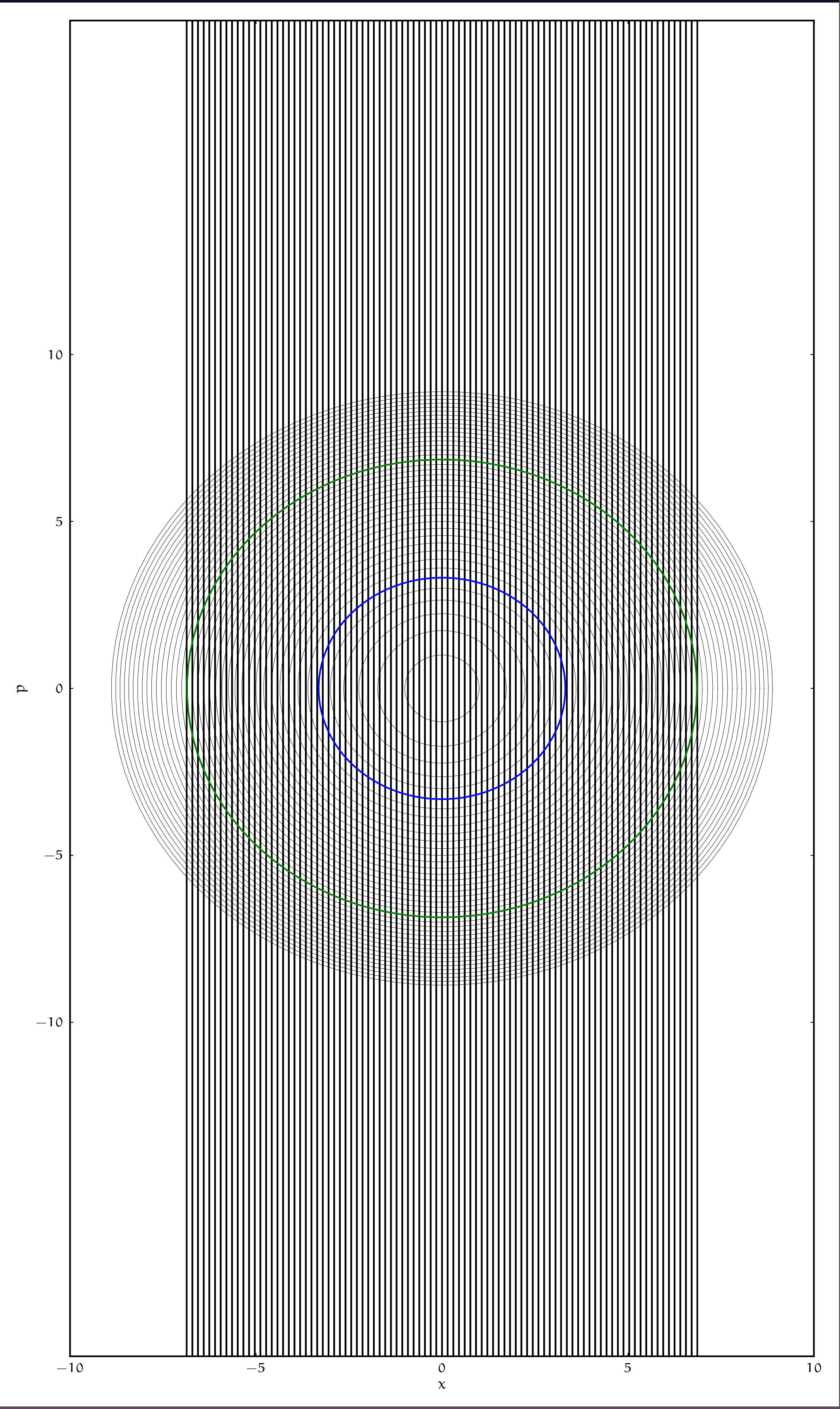


N=90, L=30

Higher UV cutoff does not help

- 5 energies to machine precision
- 24 reasonable energies (10%)





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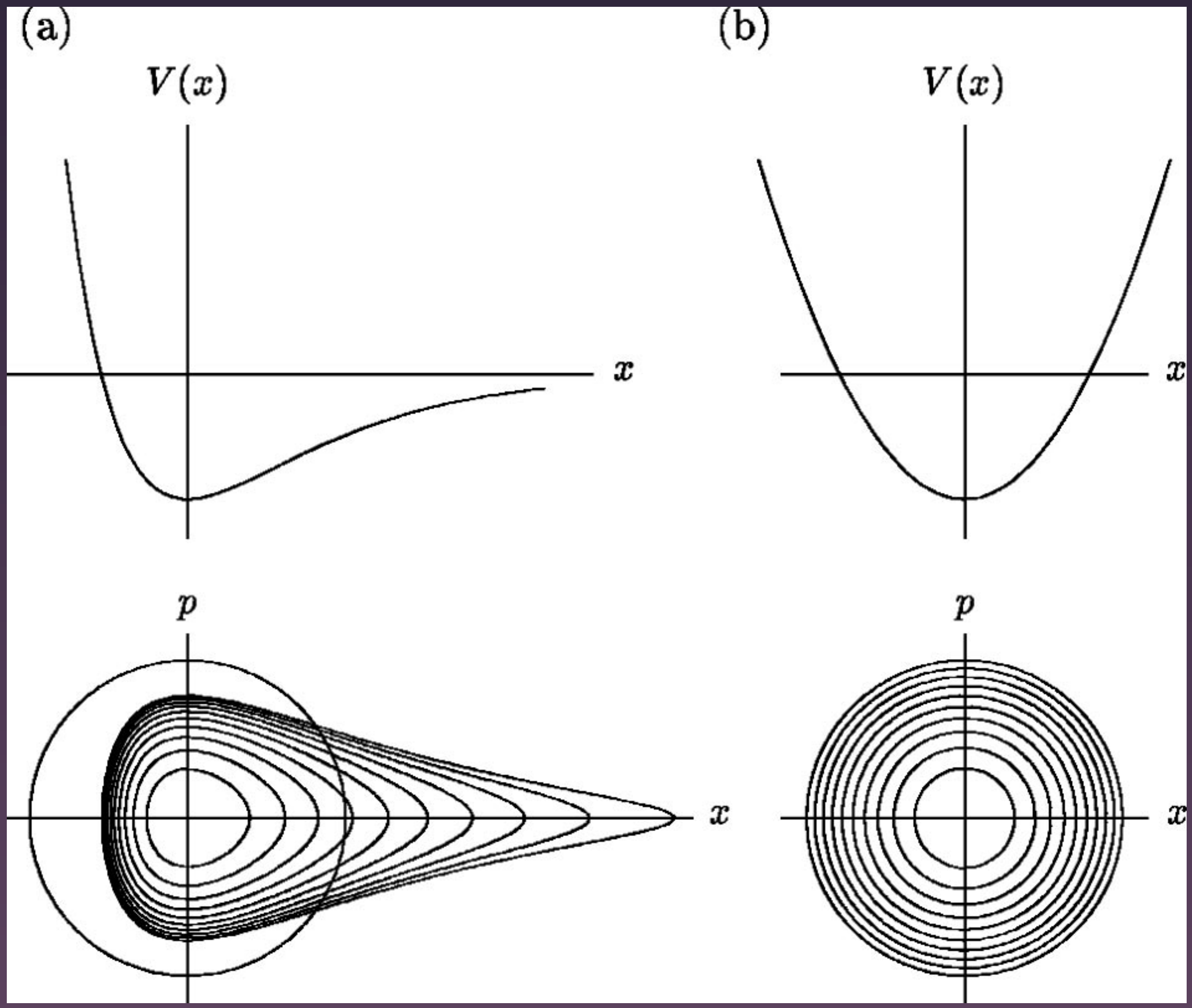
Difficulties with HO Basis



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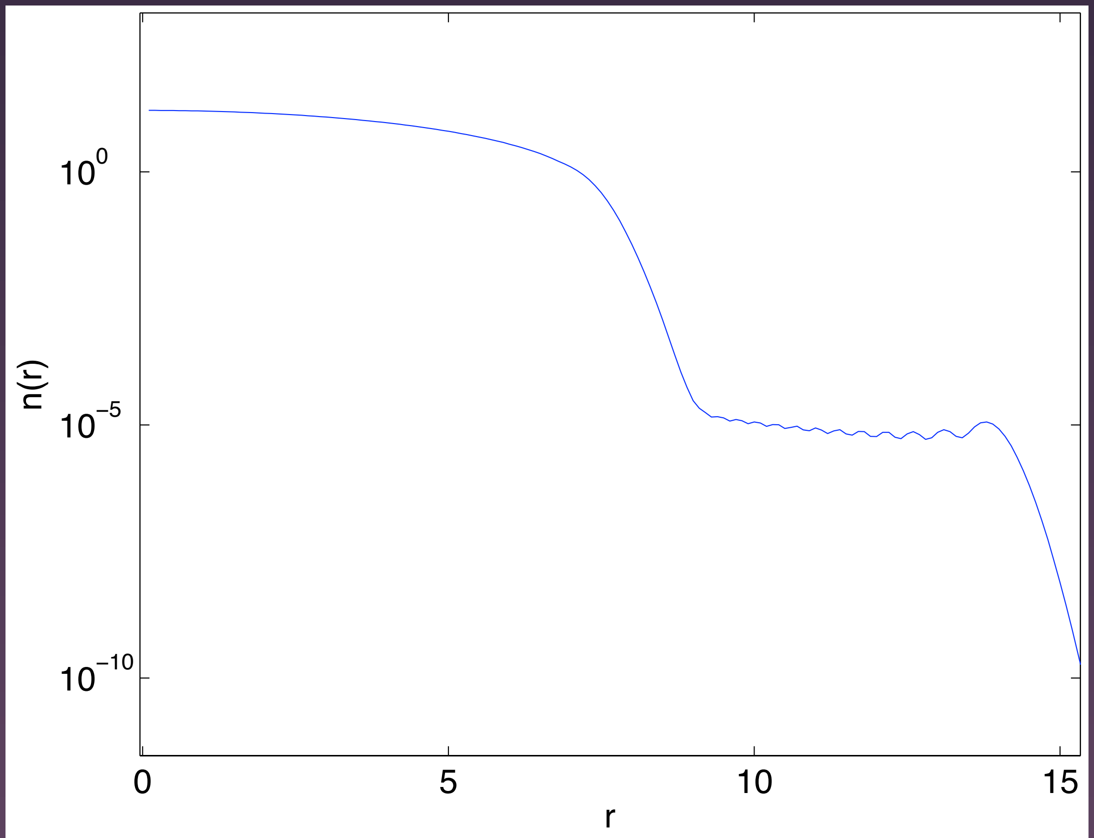
For convergence:

- Must cover same semi-classical phase space
- Consider modeling the Morse (left) potential with HO basis (right)

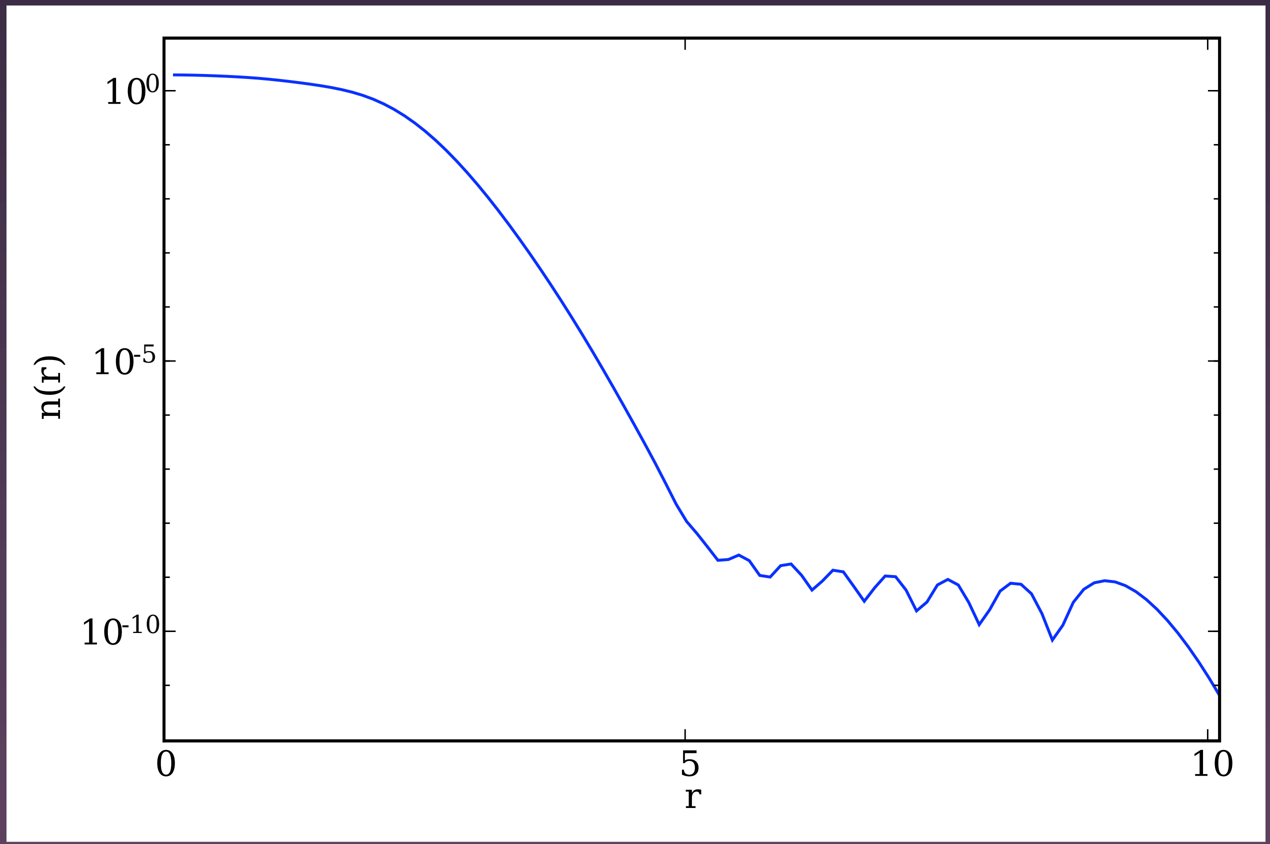
Difficulties with HO Basis

- Large Radius of HO wavefunctions introduce artifacts
- Need large number of states to correct
- (Requires HO wavefunction to high precision!)

Grasso and Urban, BCS Code



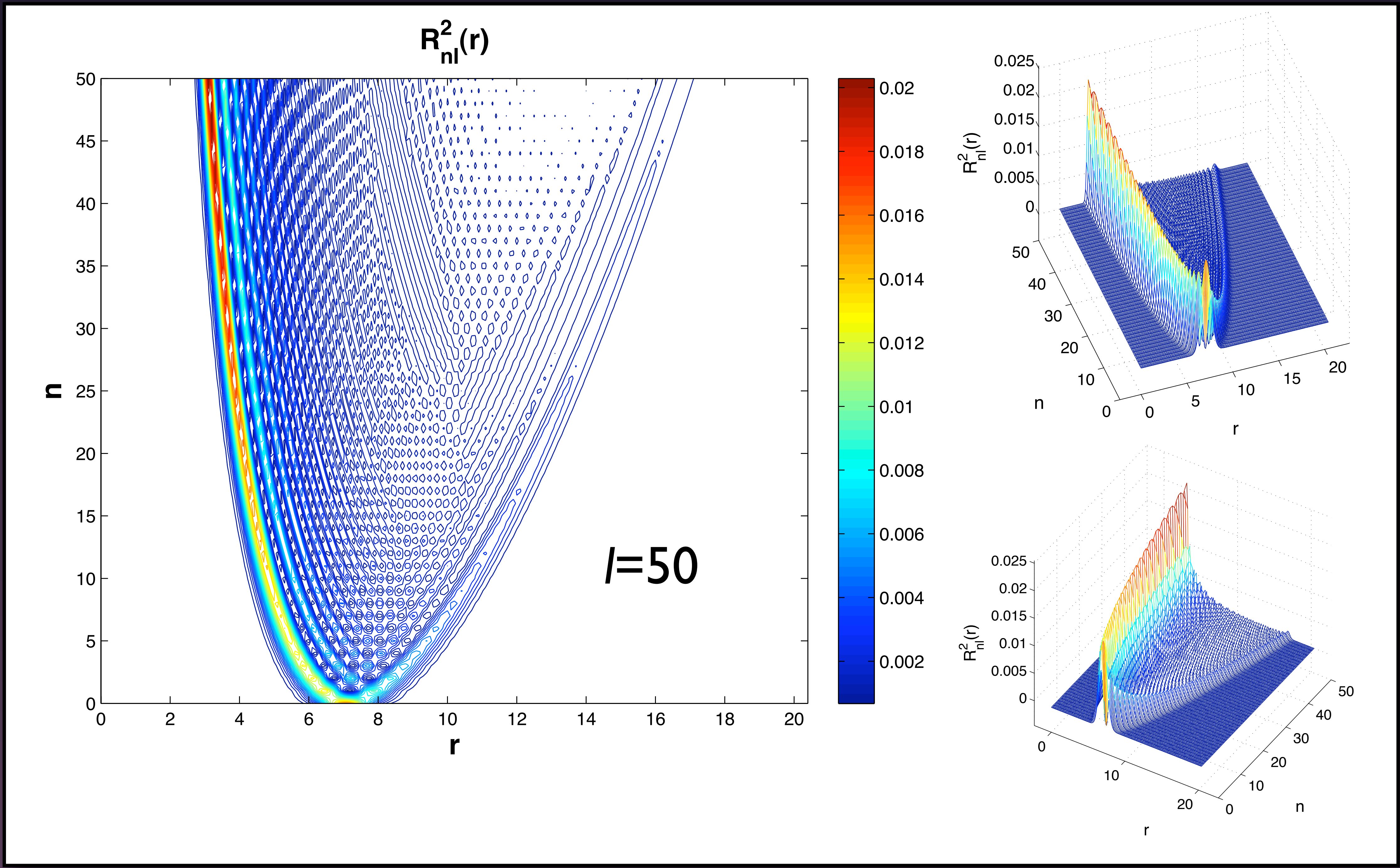
Our Unitary HO Basis Code



Grasso and Urban, PRA, 68, 033610 (2003)

Difficulties with HO Basis

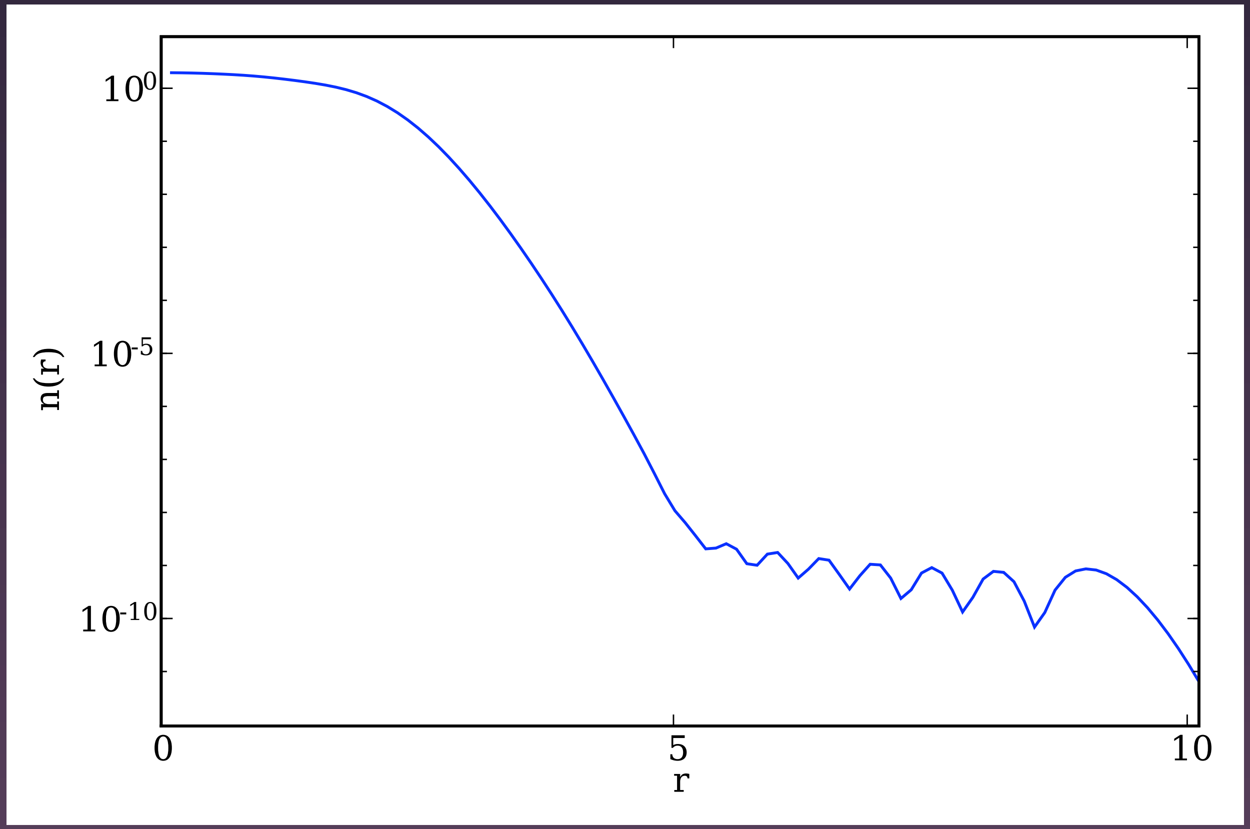
- Tails (turning points) spoil large r behaviour



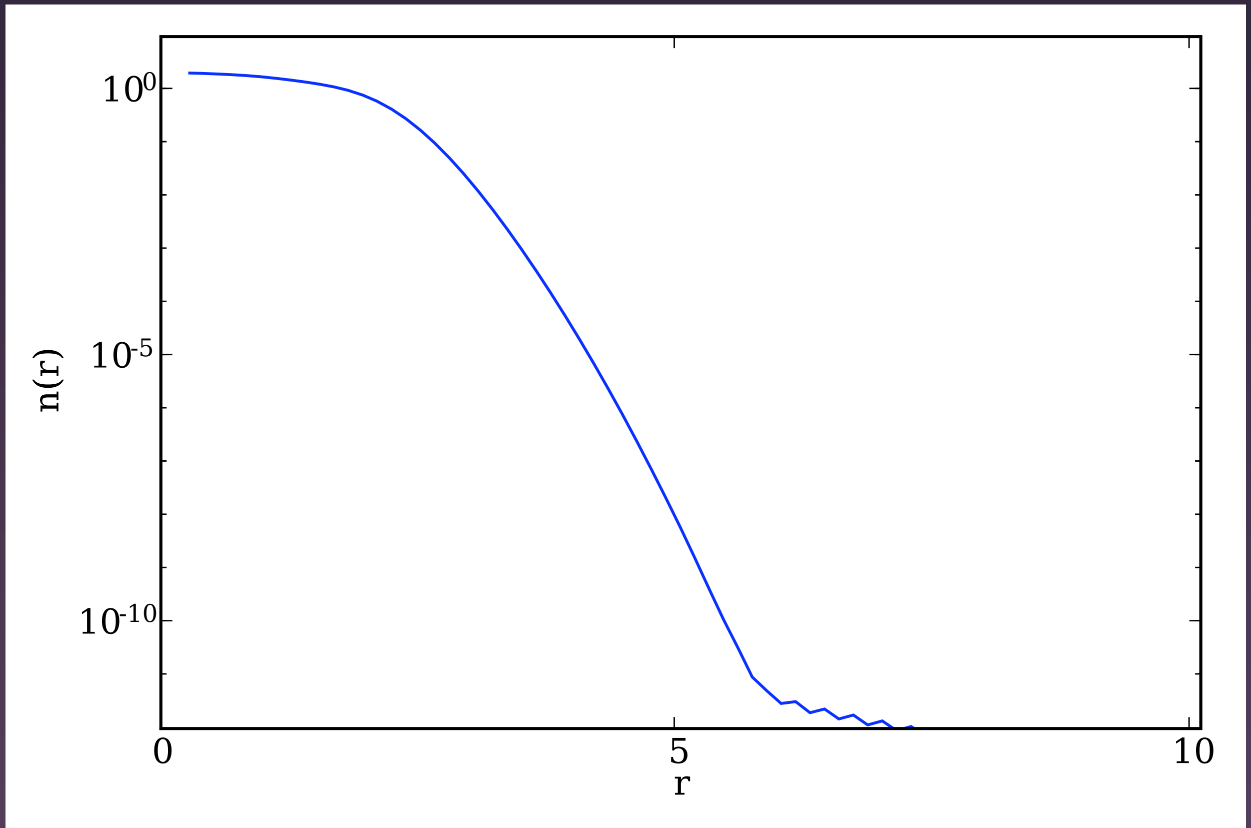
DVR Solves the Problem

- Tails spoil large r behaviour

Our code with HO Basis



Our code with DVR Basis



Difficulties with HO Basis
Complex Convergence

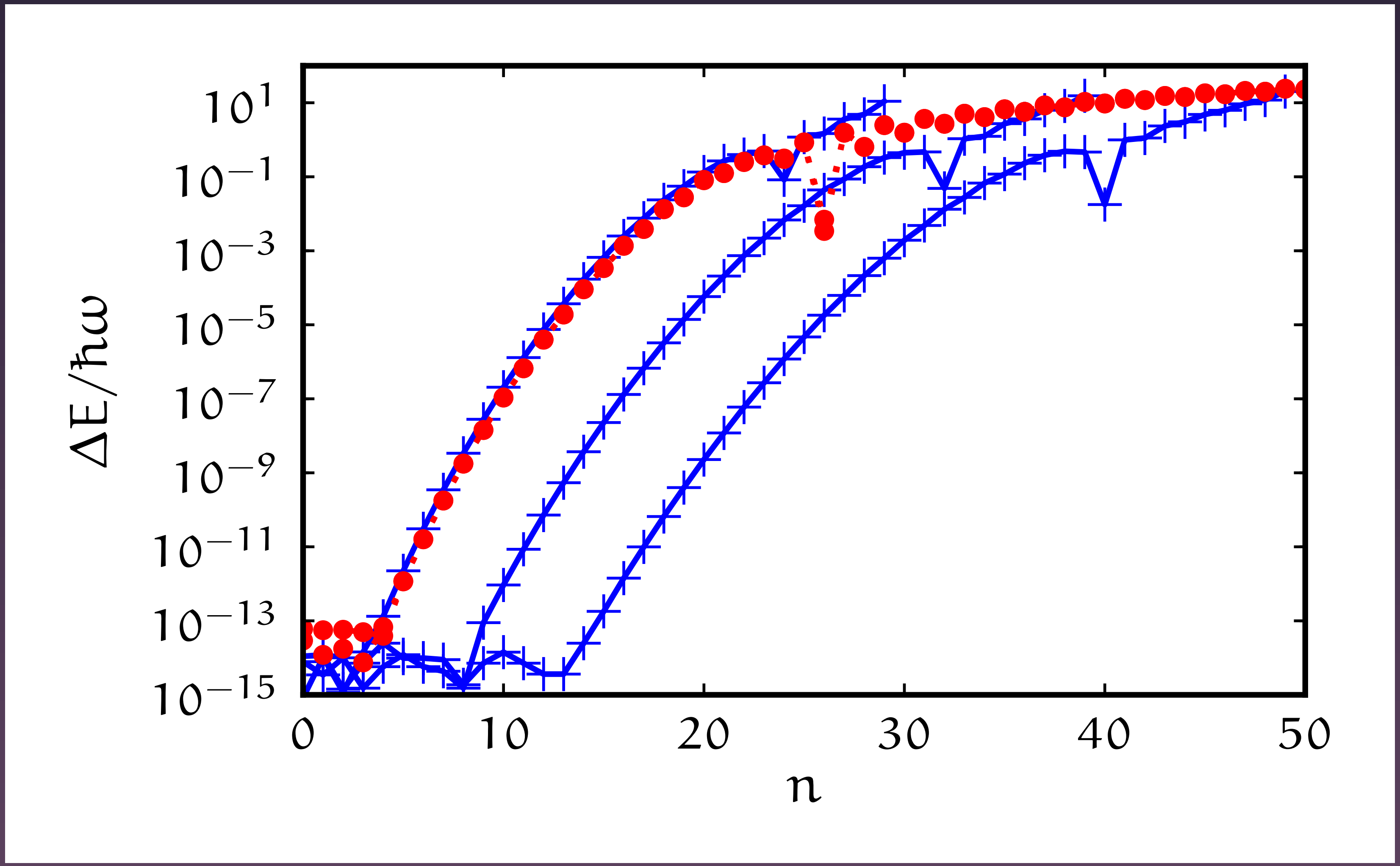
- Subtle convergence issues:
  - IR needs subtle properties of HO wavefunctions

    Furnstahl, Hagen, & Papenbrock PRC 86 (2012) 031301(R)

    More, Ekstrom, Furnstahl, Hagen, & Papenbrock arXiv:1302.3815
  - UV convergence?
    - Emperical: $E(\Lambda_{UV}) = E_\infty + A_0 \exp(-2\Lambda^2_{UV}/\lambda^2)$

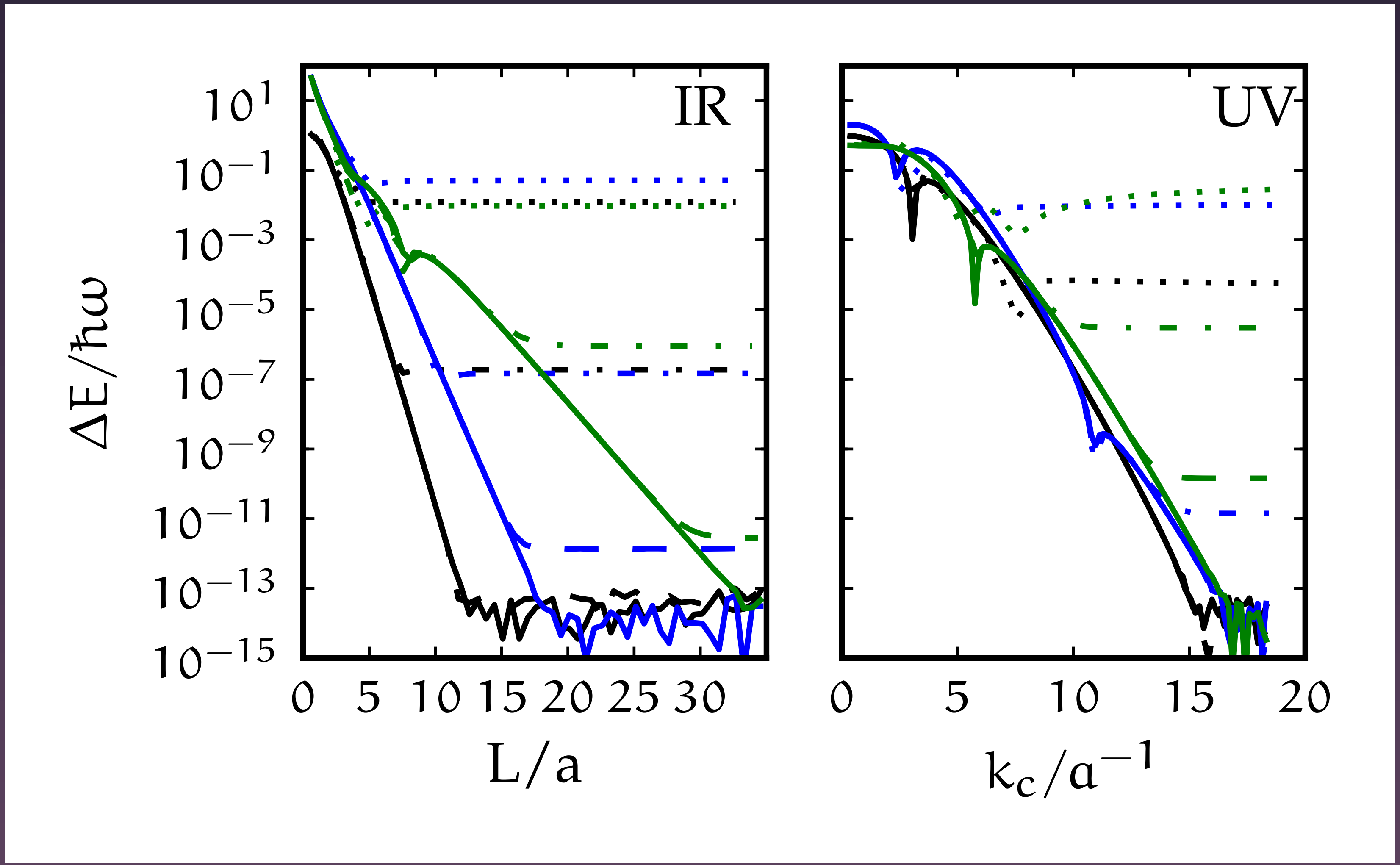
      Furnstahl, Hagen, & Papenbrock PRC 86 (2012) 031301(R)
    - Where does this Gaussian behaviour come from?

HO Eigentstates with DVR basis



Bulgac & Forbes arXiv:1301.7354

Simple Convergence



IR convergence:

- Periodic Box (images)
- Lowest many-body threshold
- Band theory

UV convergence:

- Fourier analysis

Both are simple exponentials

Bulgac & Forbes arXiv:1301.7354

IR Convergence

- Band theory
- Exponential (think "tunneling") with scale set by lowest many-body dissociation threshold
  - e.g. s-wave two-body threshold

$$E(L) = E_\infty + \frac{A\exp(-2\sqrt{2MQ(L)})L/\hbar}{L^2}$$

UV Convergence

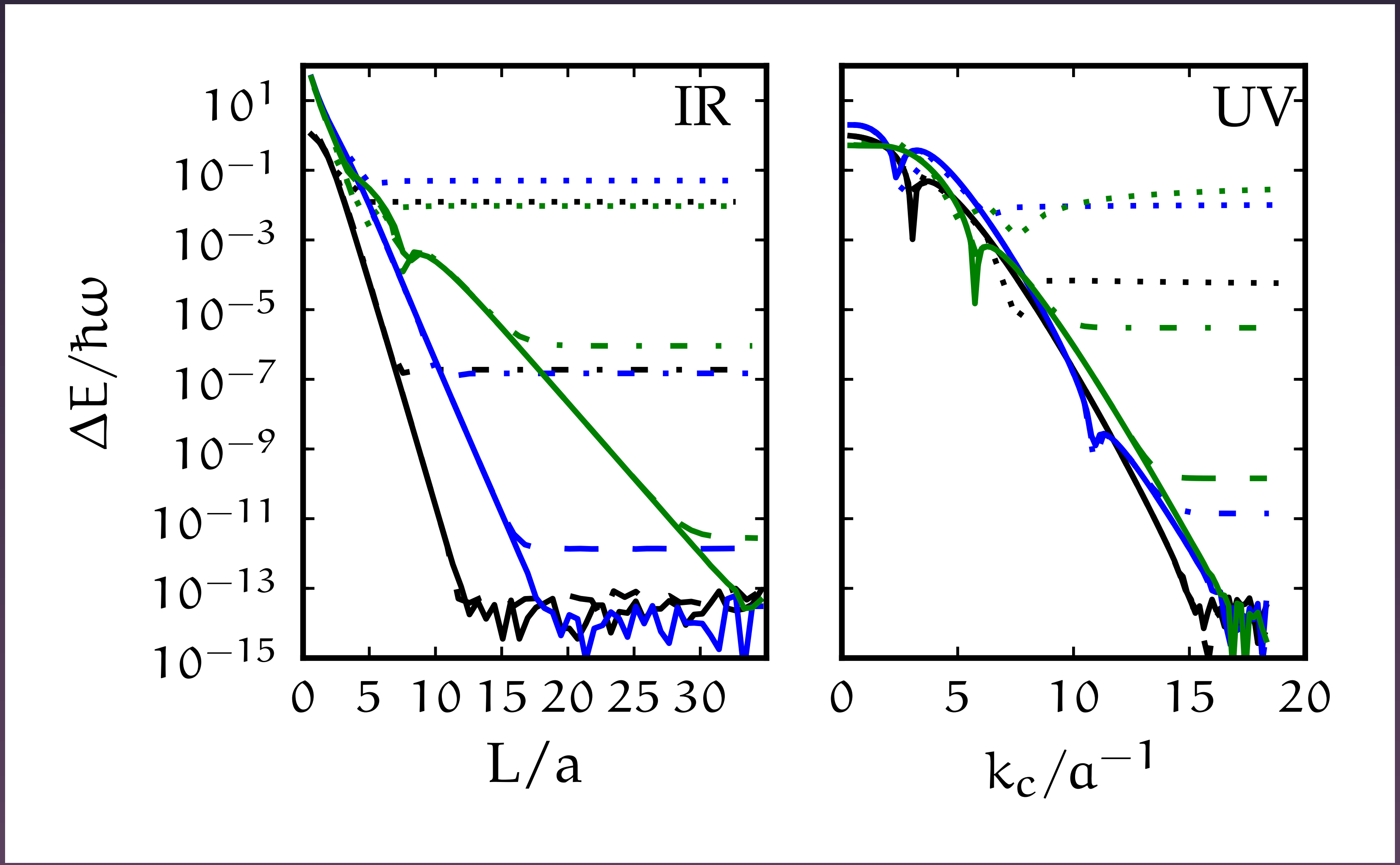
- Follows from Fourier analysis

$$E(k_c) = E_\infty + A \exp(-2k_c r_0)$$

- Exponential (not Gaussian)
    - Recall “emperical” formula for HO basis:

$$E(\Lambda_{UV}) = E_\infty + A \exp(-2\Lambda_{UV}^2/\lambda^2)$$

Simple Convergence



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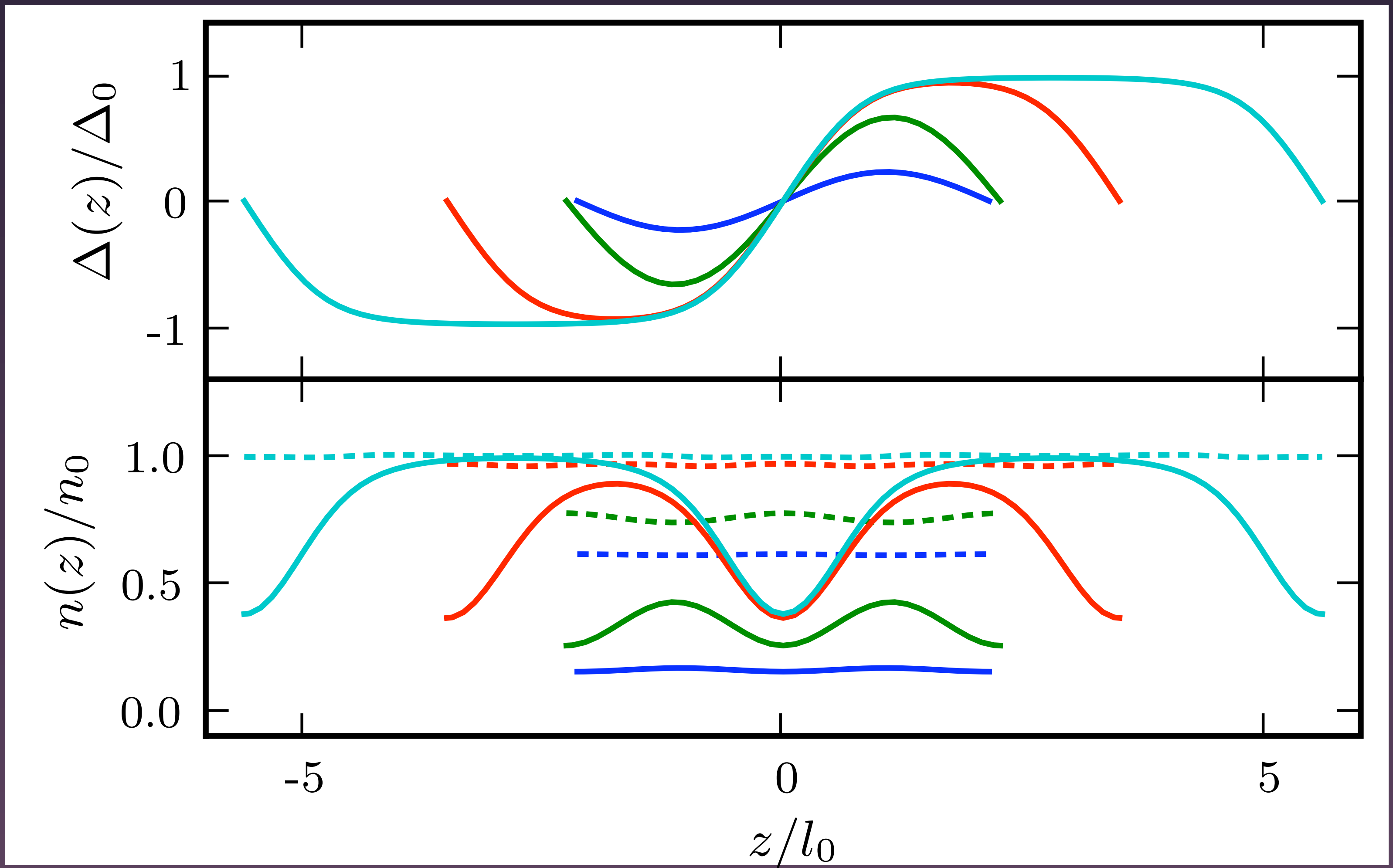
Bulgac & Forbes arXiv:1301.7354

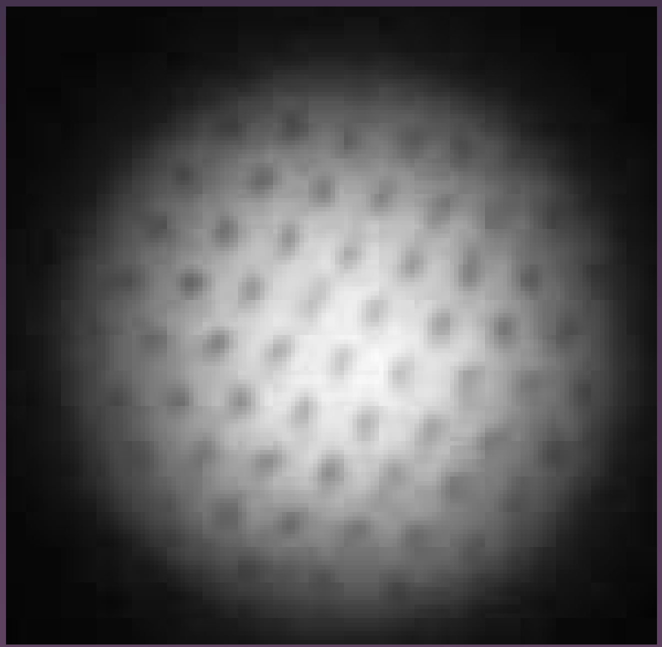
DFT predicts (FF)LO at Unitarity: Supersolid!



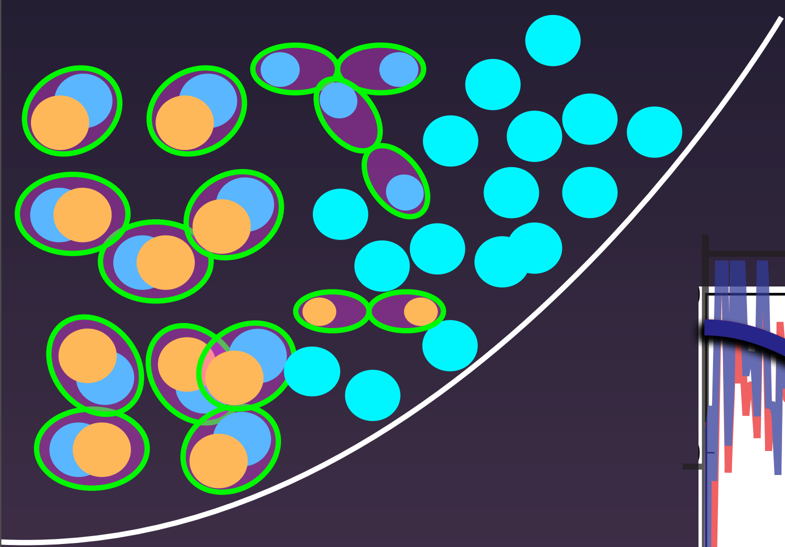
Bulgac and Forbes PRL 101 (2008) 215301

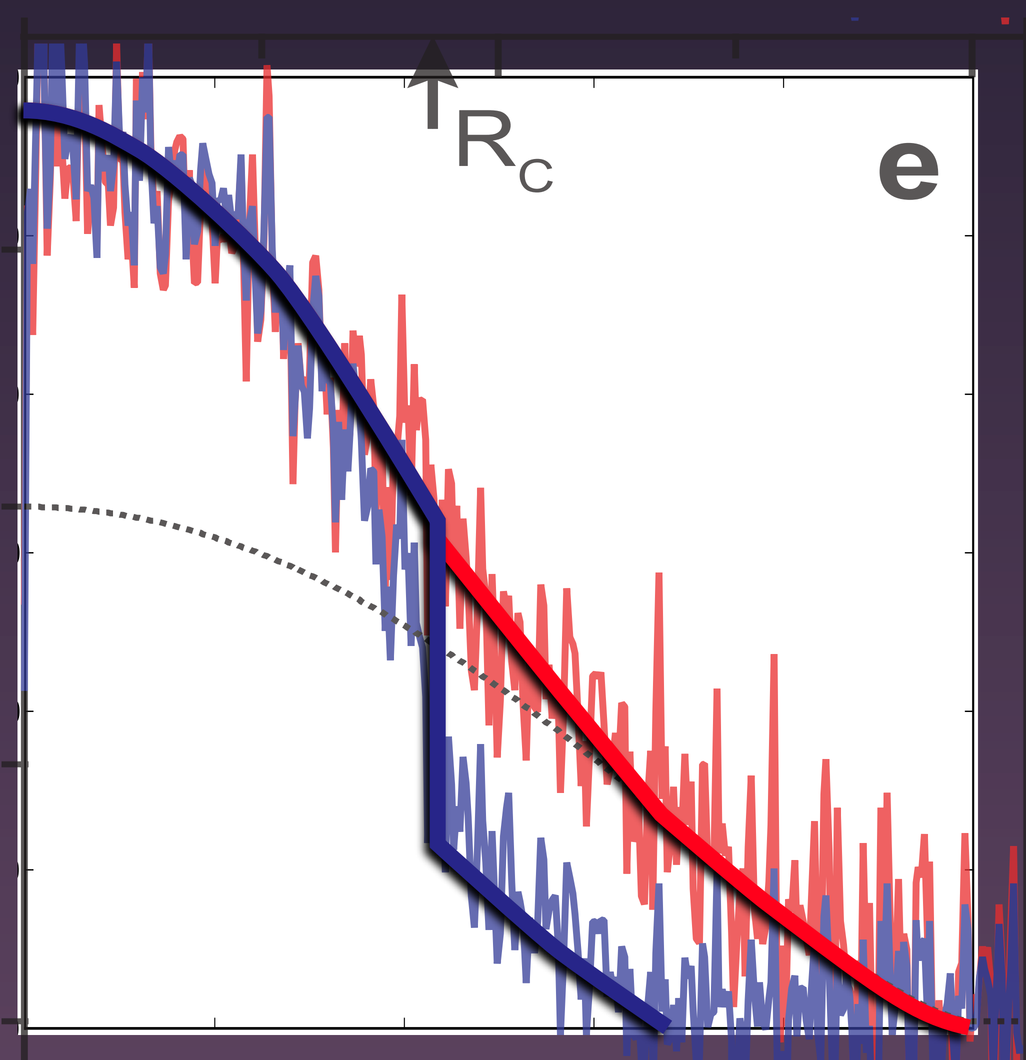
Large density contrast (factor of 2)

Similar to contrast of vortex core



Observations: Nothing?





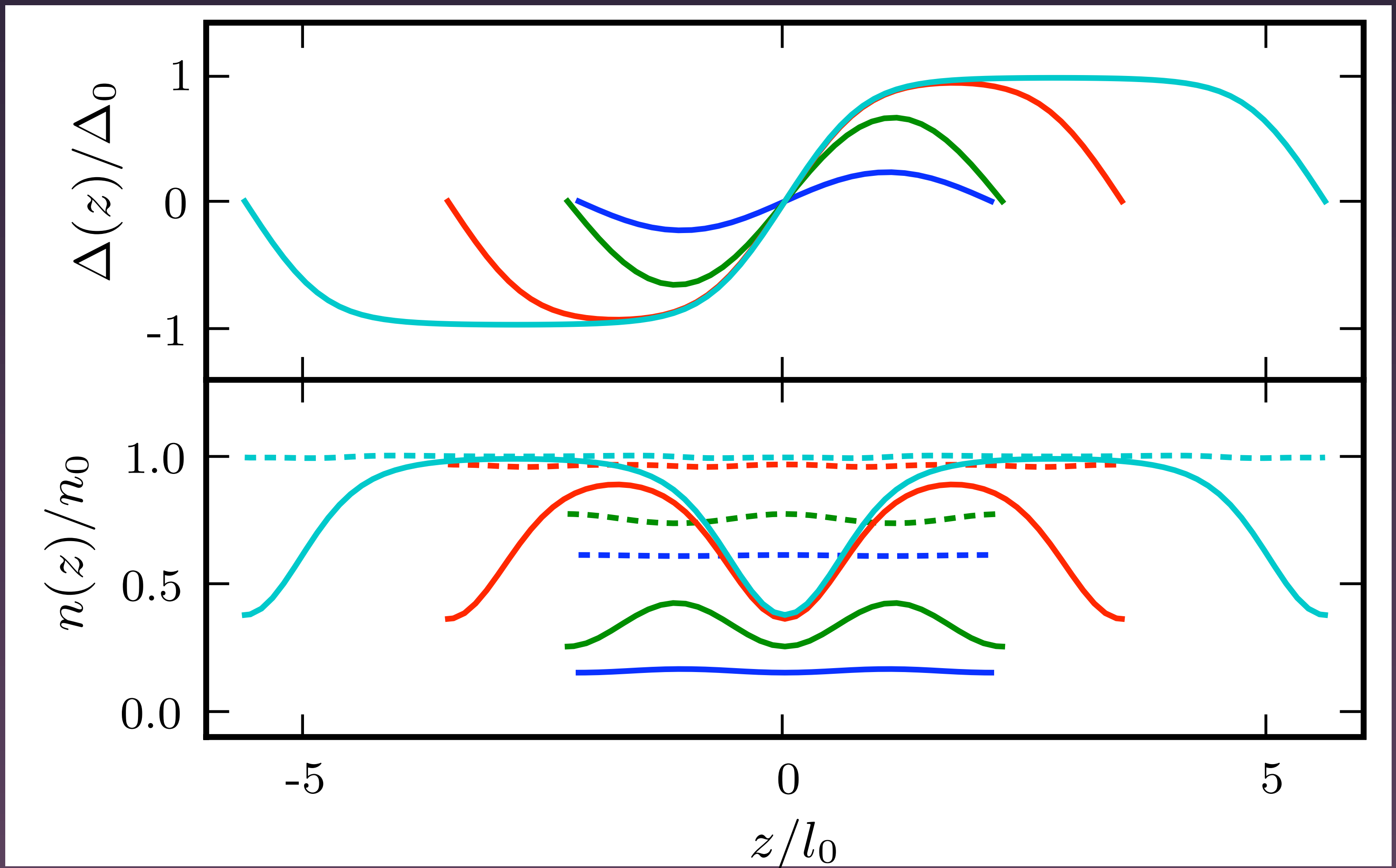
MIT Experimental data from Shin et. al (2008)

Paired core

Polarized wings

Maybe there are no interesting polarized superfluid phases?

DFT predicts (FF)LO at Unitarity: Supersolid!



Bulgac and Forbes PRL 101 (2008) 215301

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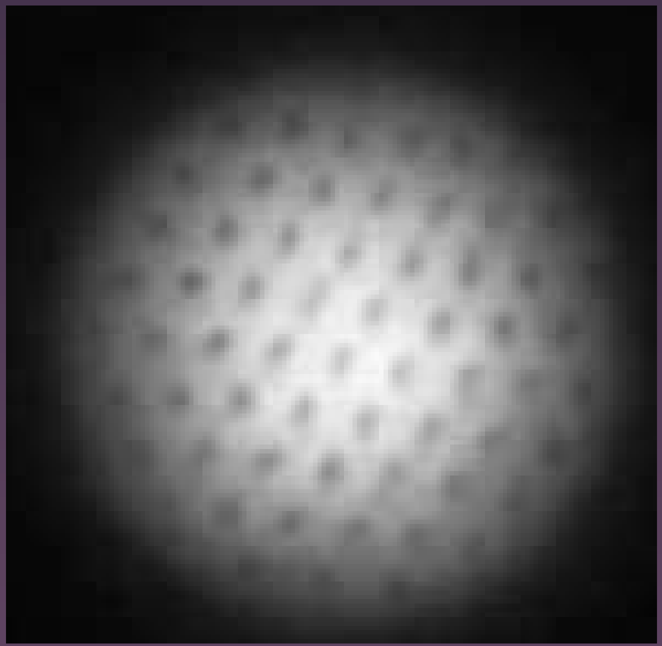
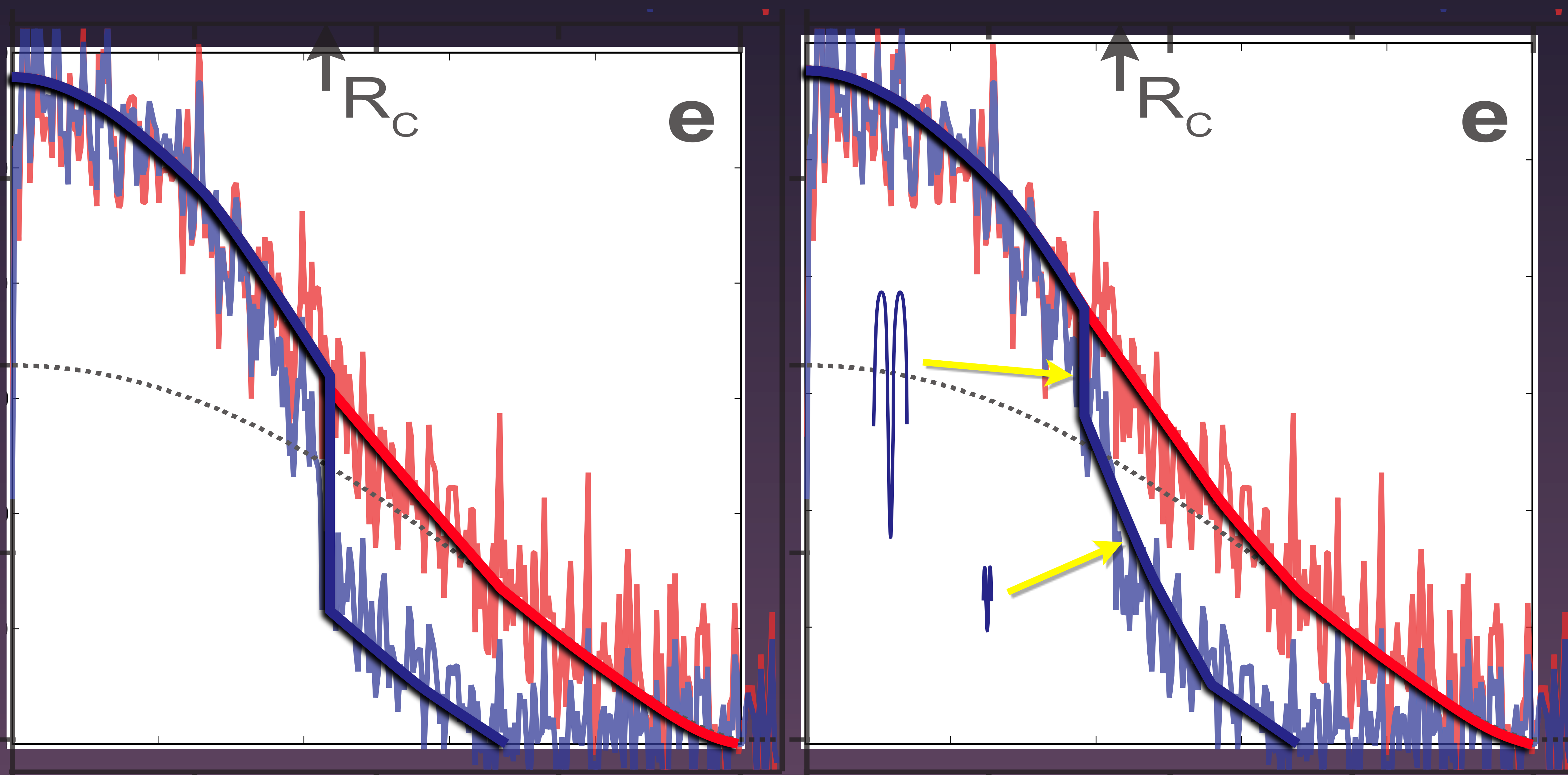


Observations: Inconclusive

- Need detailed structure or novel signature

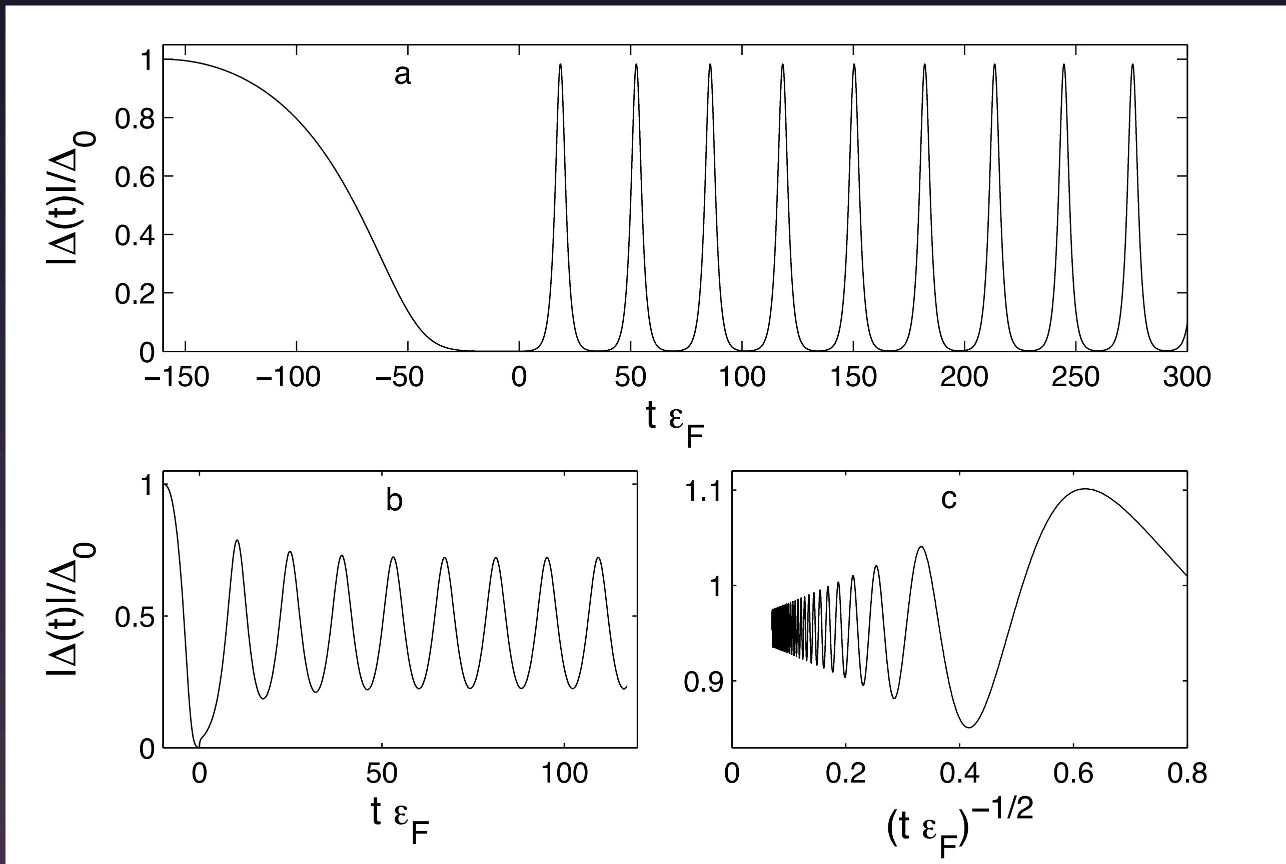


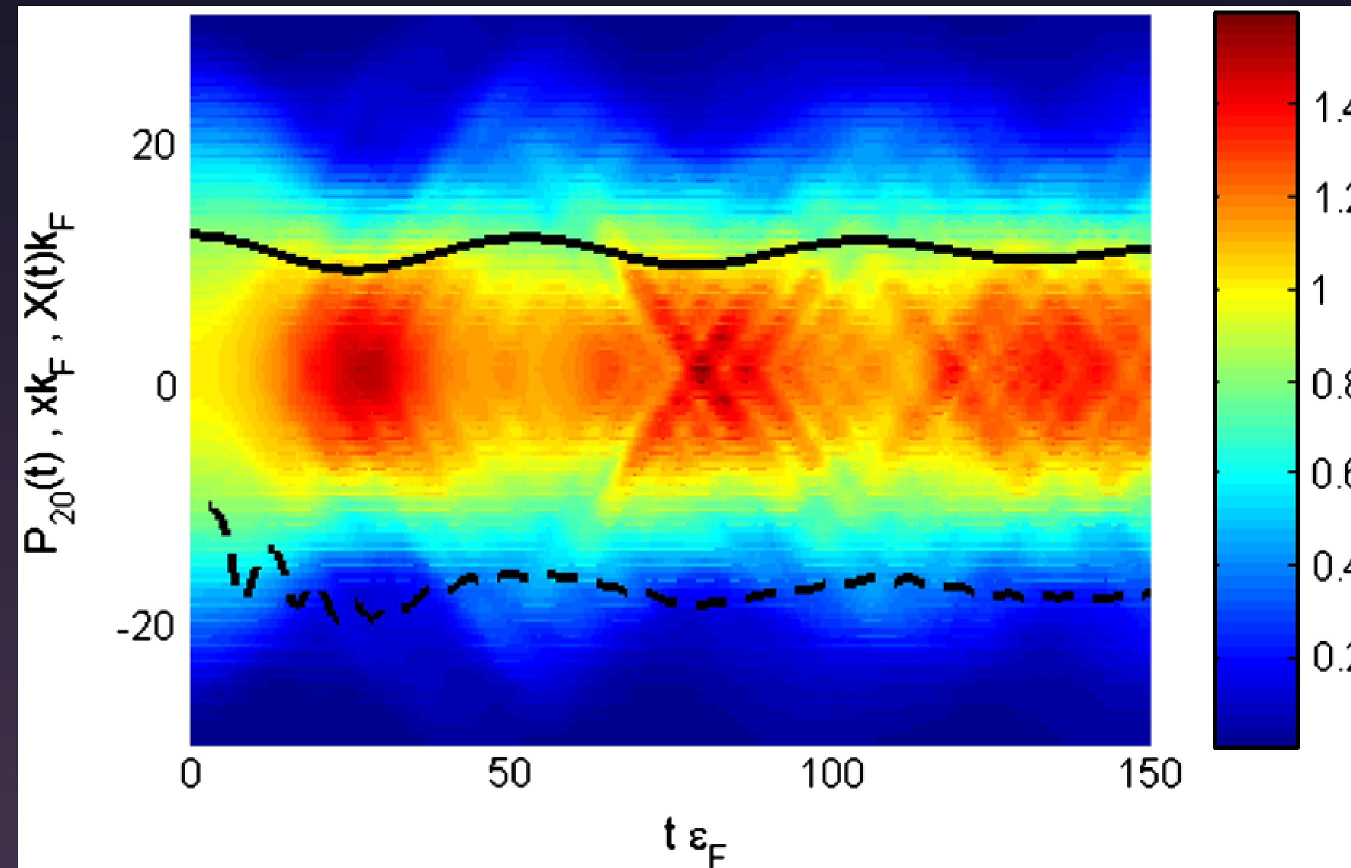
MIT Experimental data from Shin et. al (2008)

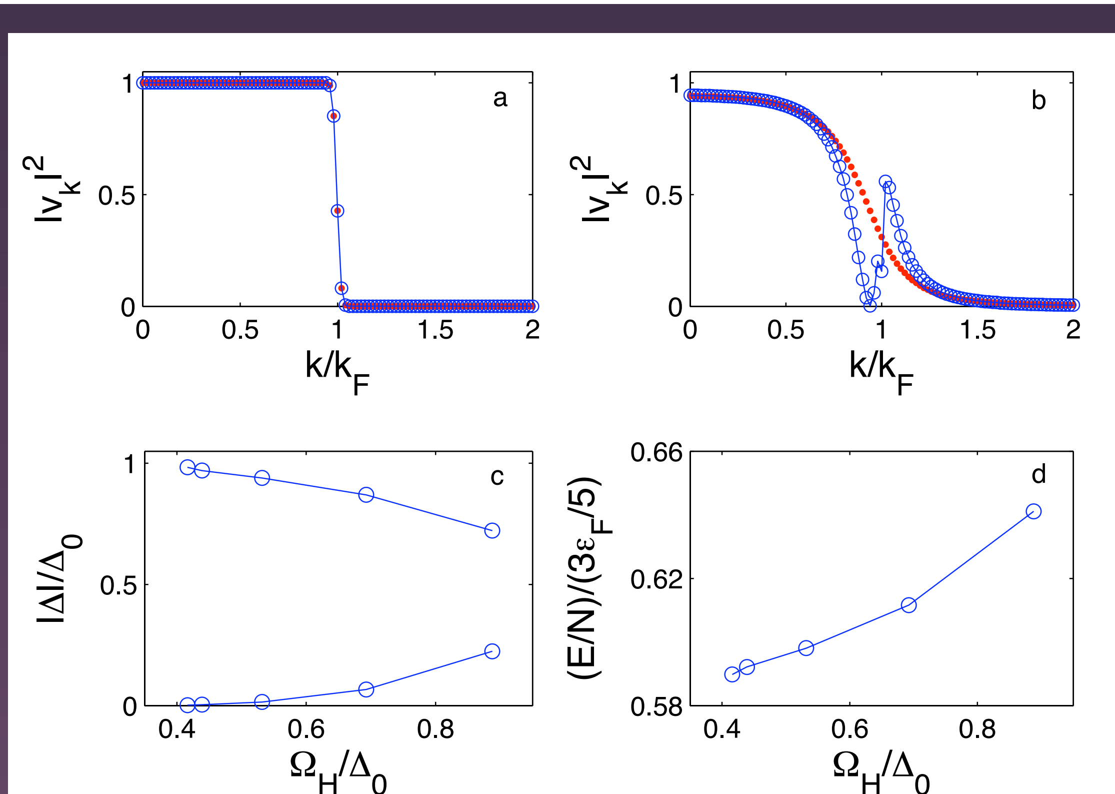
Why FFLO not seen?

- It is not there:
  - Other homogenous phases might be better.
  - T might be too high (fluctuations kill 1D FFLO).
  - Trap frustrates formation (traps are not flat enough).
- It is not seen:
  - Noise washes out signature.
  - Small physical volume for FFLO.
- Need a nice flat trap: Large physical volume of FFLO

TDDFT: Higgs Mode



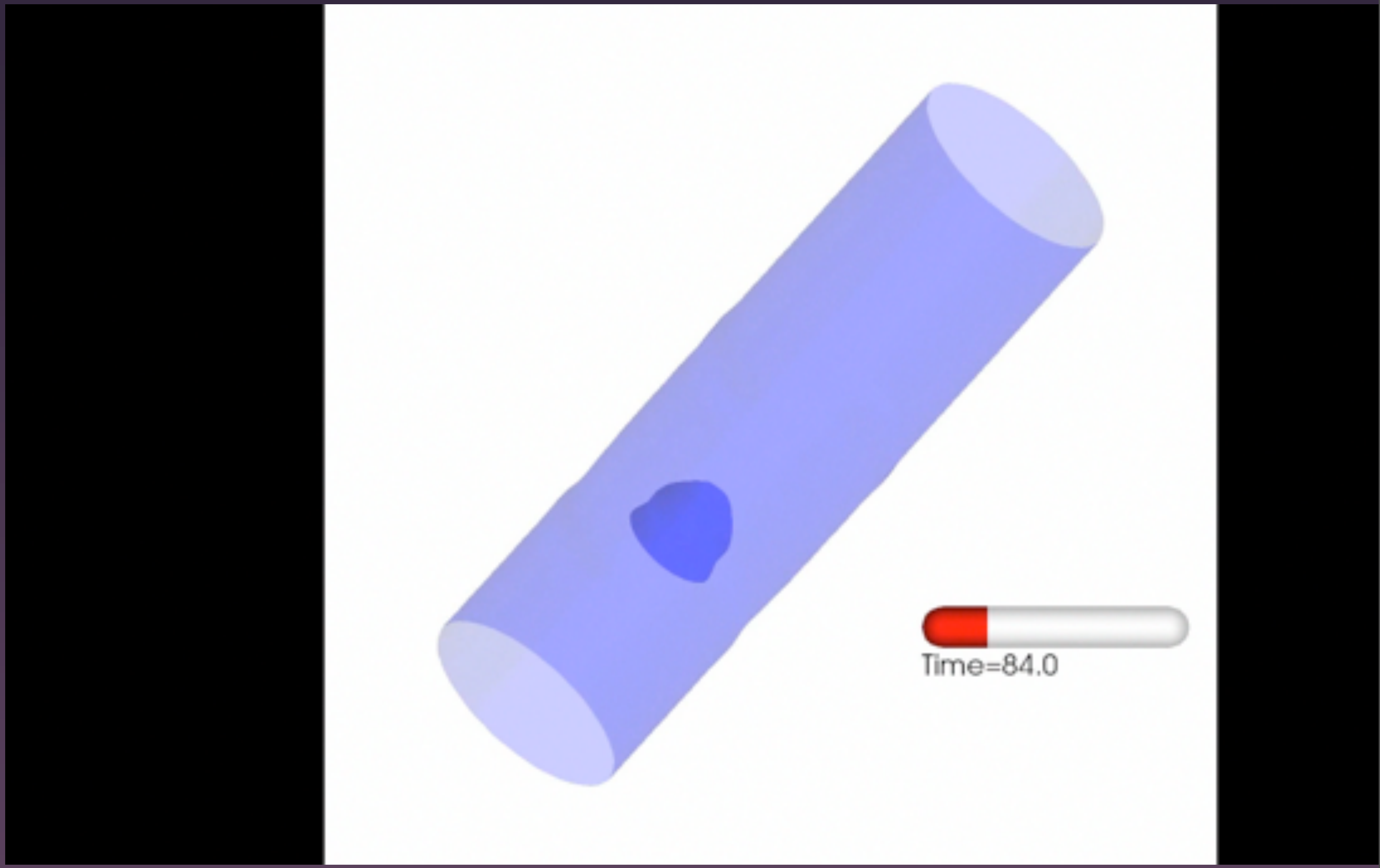




Bulgac and Yoon PRL 102, 085302 (2009)

SLDA TDDFT

$$\imath\partial_t\Psi_n = H[\Psi]\Psi_n = \begin{pmatrix} \frac{-\alpha\nabla^2}{2m} - \mu + U & \Delta^\dagger \\ \Delta & \frac{\alpha\nabla^2}{2m} + \mu - U \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix}$$



Bulgac, Luo, Magierski, Roche, Yu (2011)

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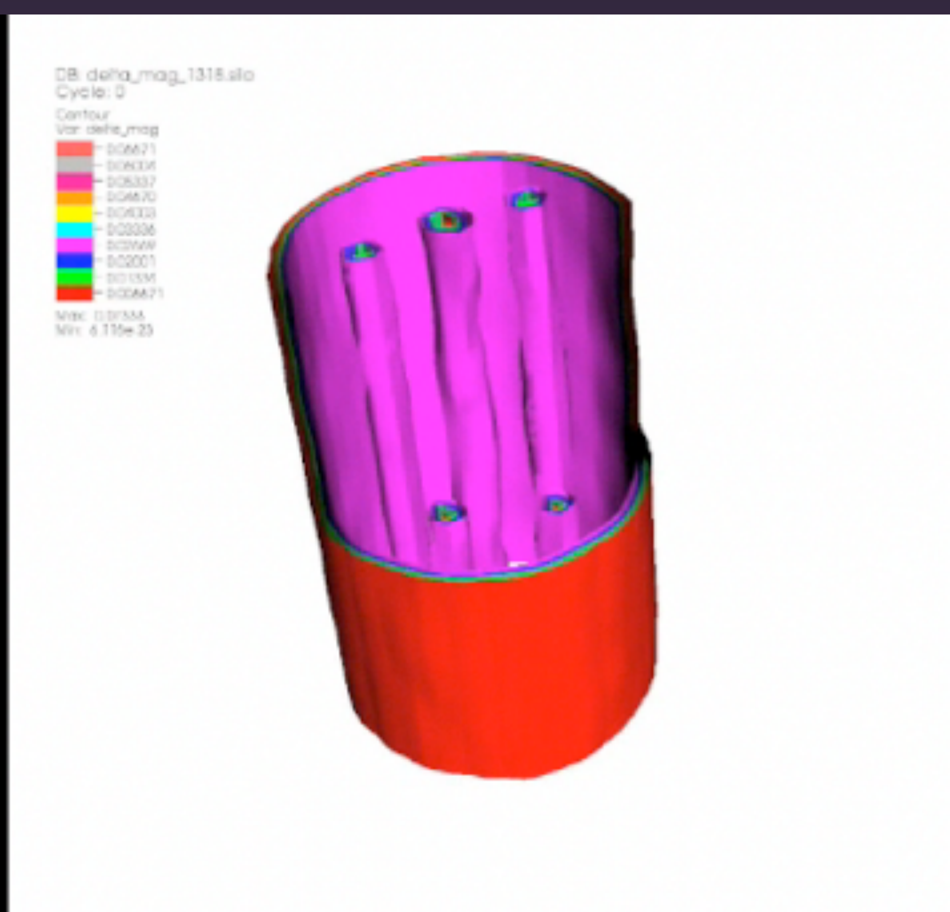
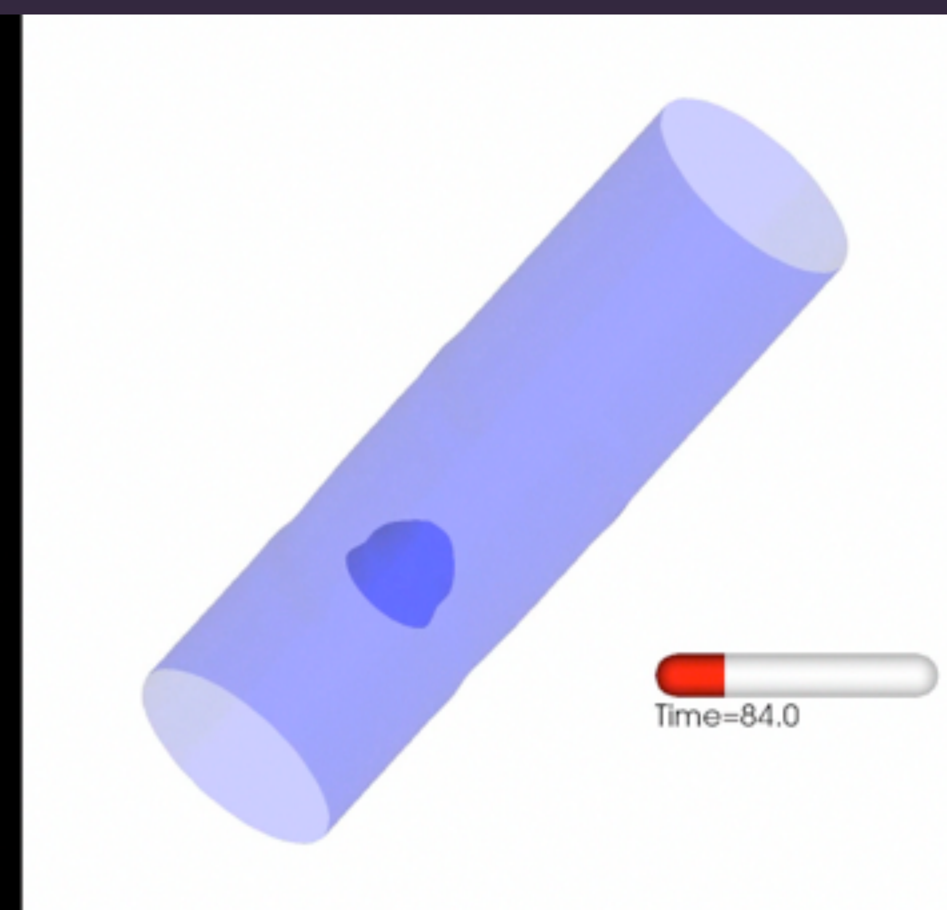


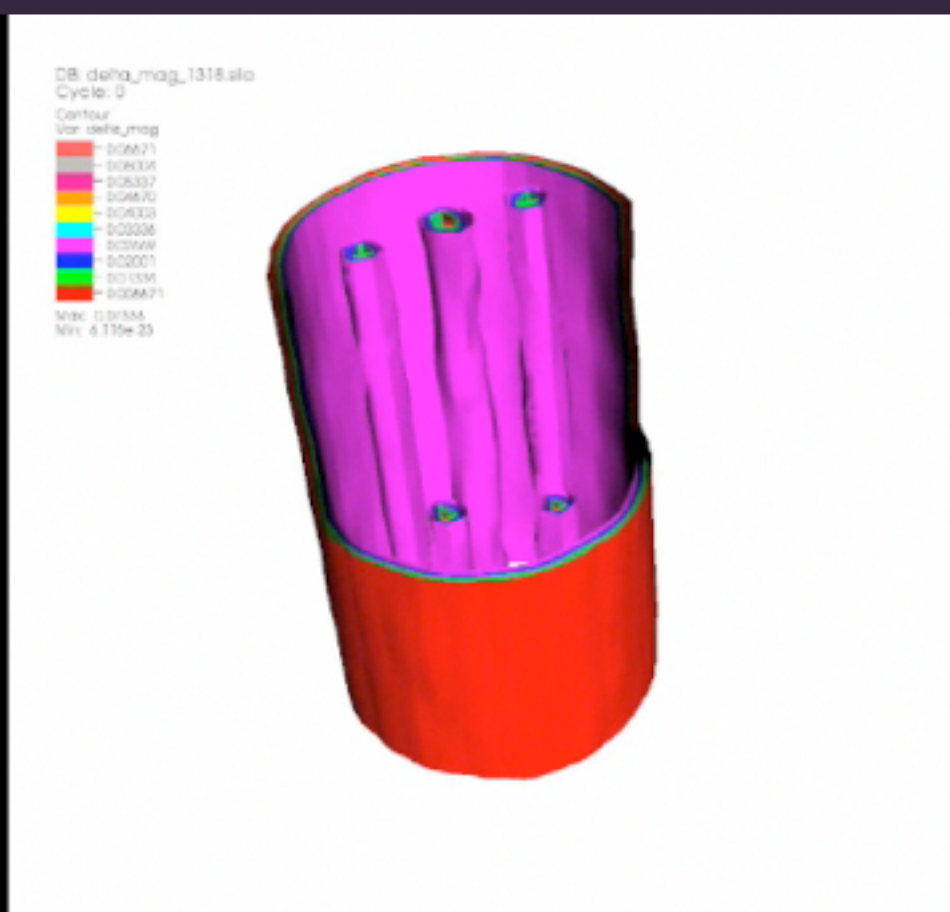


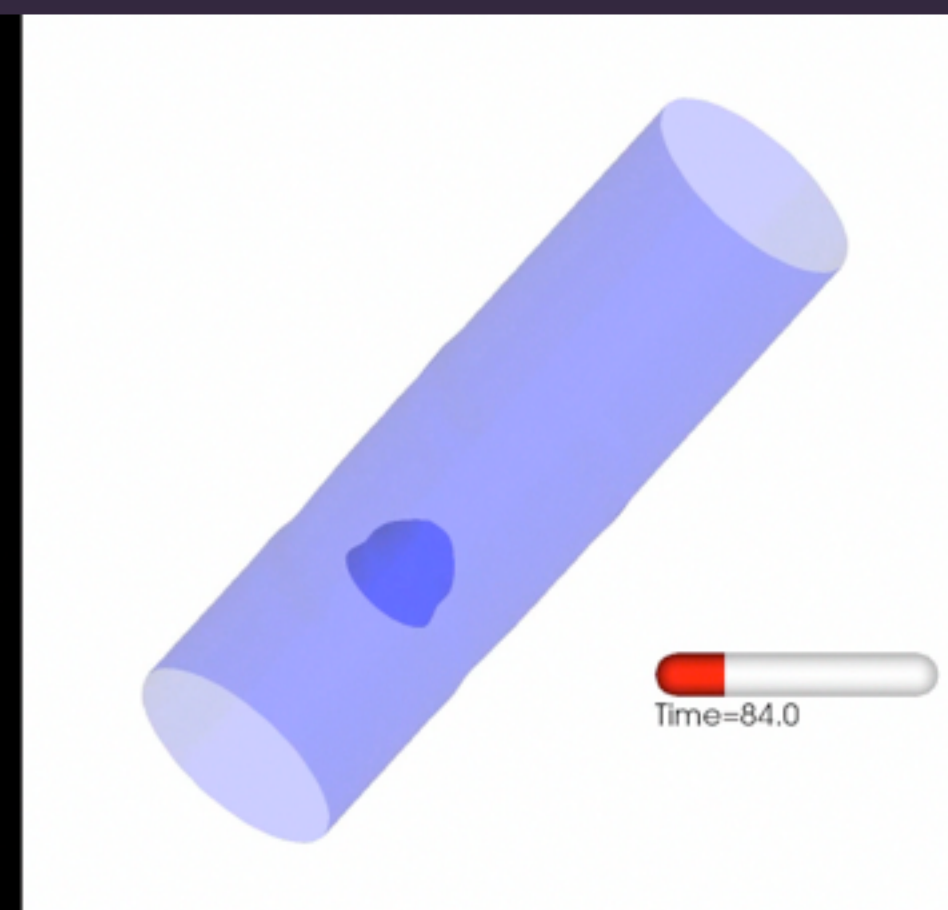
Bulgac, Luo, Magierski, Roche, Yu (2011)

SLDA TDDFT

48^3 and 196×32^2 grids

5×10^5 independent wavefunctions

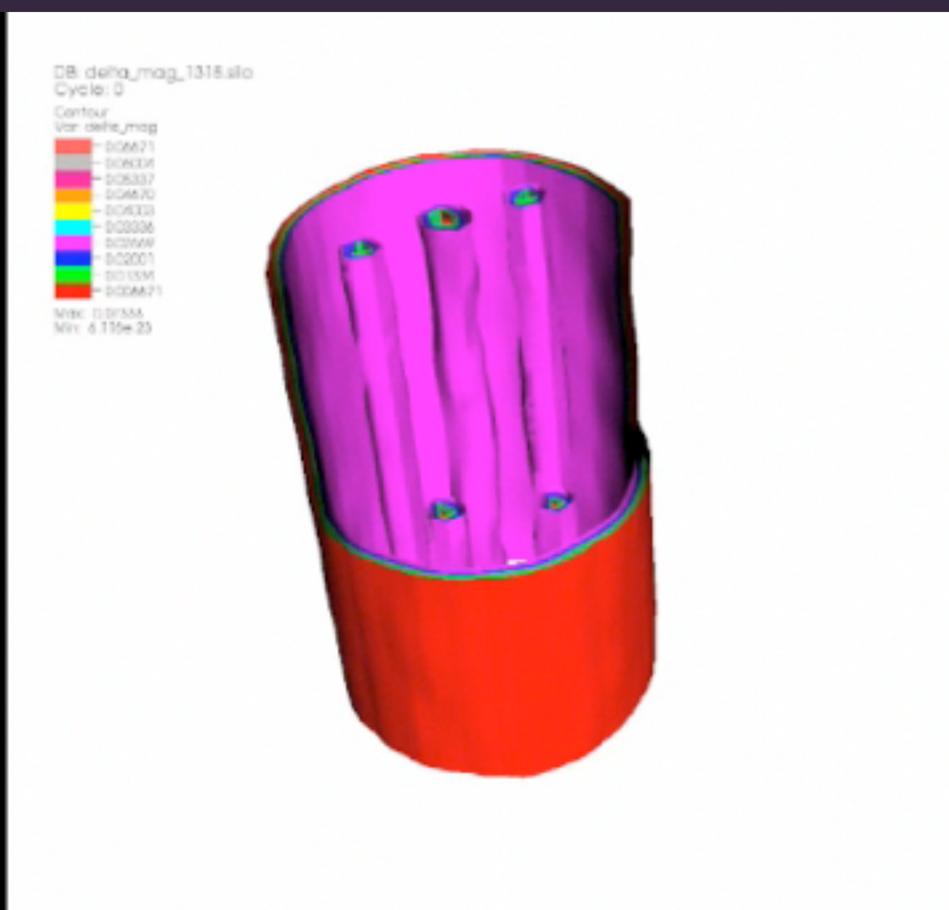


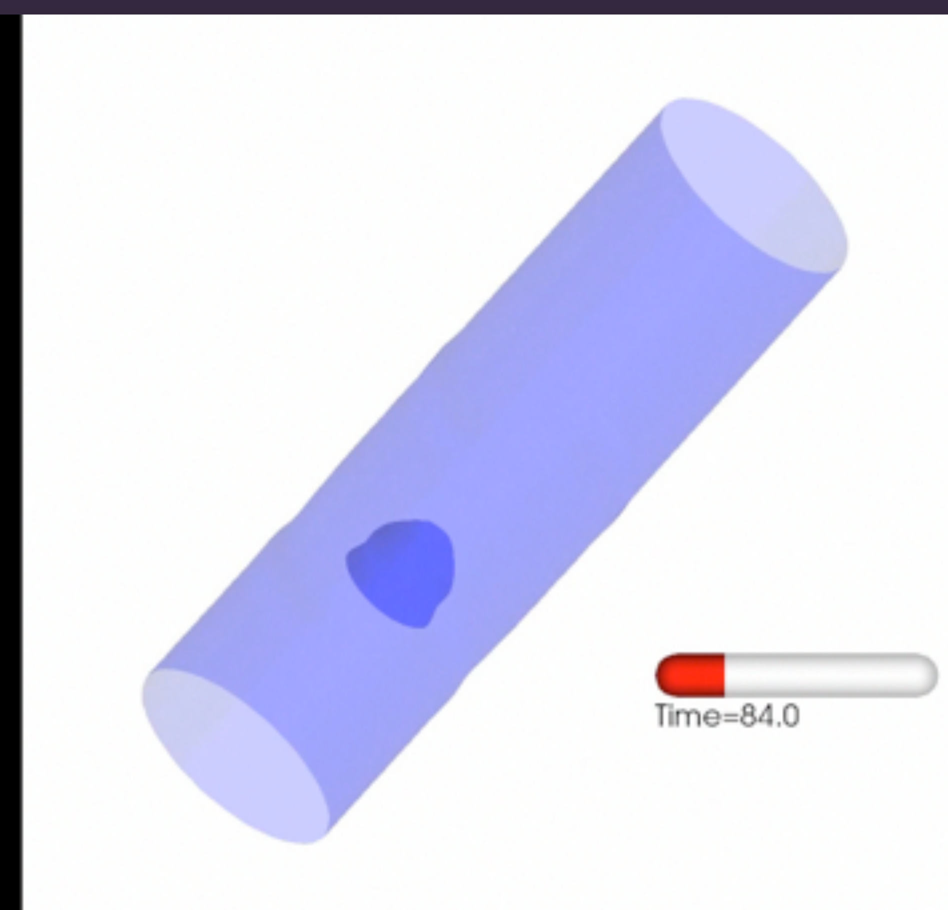


Bulgac, Luo, Magierski, Roche, Yu (2011)

SLDA TDDFT

TDDFT for triaxial GDR with nuclear functionals
Stetcu, Bulgac, Magierski, & Roche, PRC 84, (2011) 051309(R) (2011),





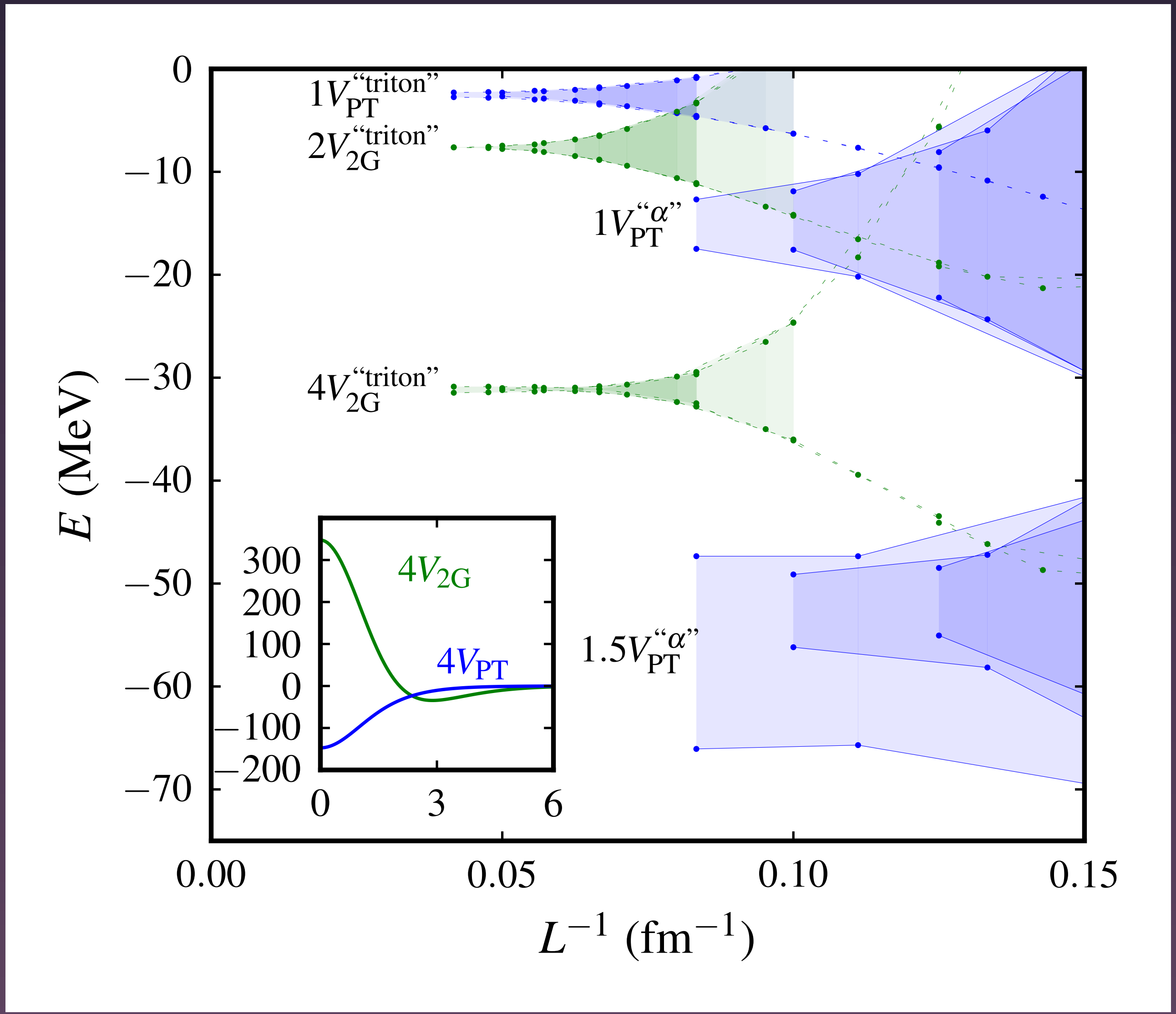
Bulgac, Luo, Magierski, Roche, Yu (2011)

AFQMC

- Unitary Fermi Gas
- Full 3D from $6^3=216$ to $16^3=4096$ grids
  - 20 - 160 particles
  - 5000 steps of imaginary time

Drut, Lähde, Wlazłowski, & Magierski, PRA 85 (2012) 051601
Wlazłowski, Magierski, Drut, Bulgac, & Roche, PRL 110 (2013) 090401

Exact Diagonalization ("Triton" and "Alpha")



Bulgac & Forbes arXiv:1301.7354

Use DVR for relative coords.

Directly solve 6D and 9D Schrödinger Eq.

Lanczos iterations

- No matrices $O(N \ln N)$

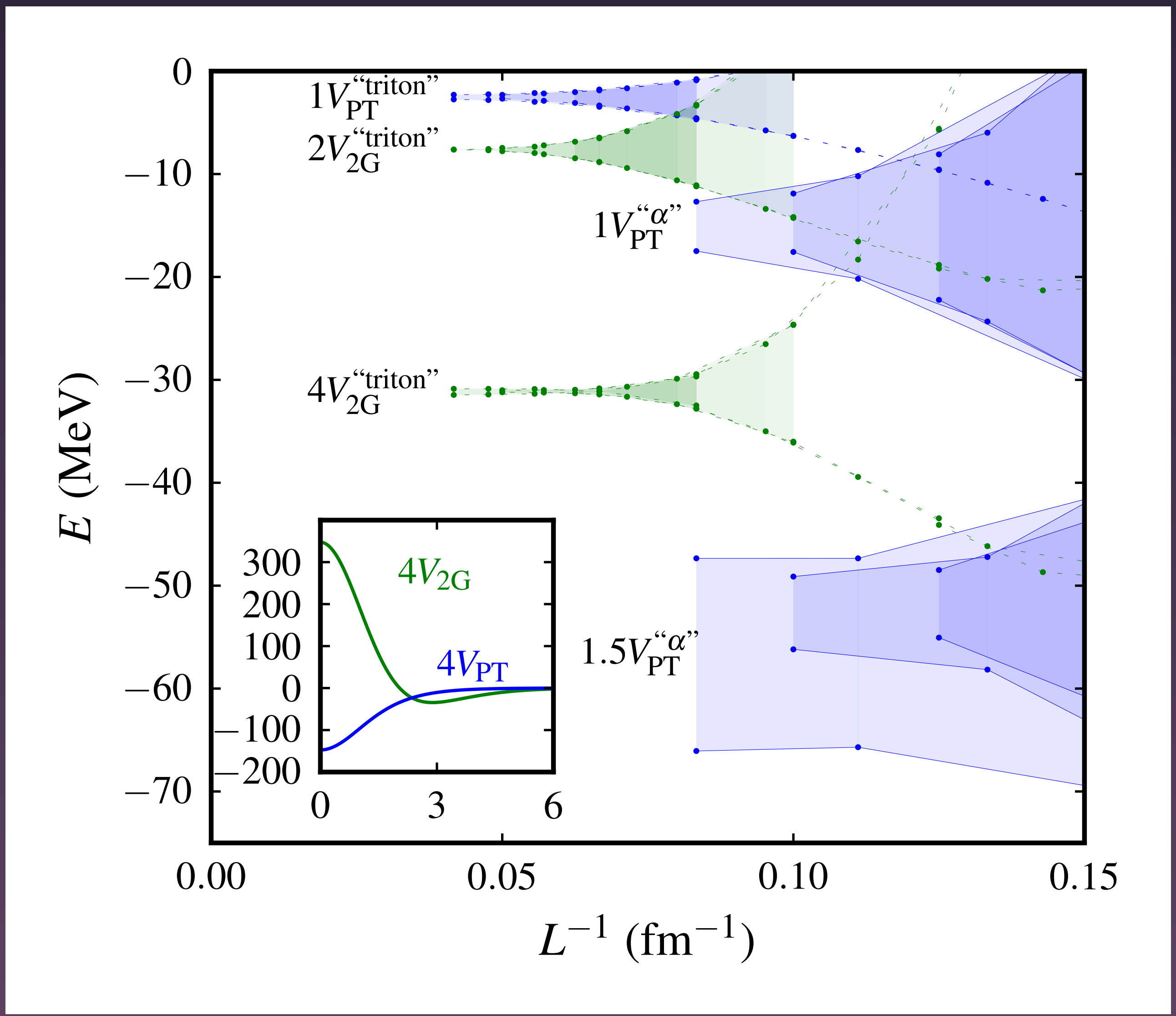
Several minutes on laptop

Hilbert space to $8^9 = 10^8$

- $a = 0.5$ to 1.5 fm
- $\Lambda = 300$ to 930 MeV/c

Monday, April 8, 13

Exact Diagonalization ("Triton" and "Alpha")



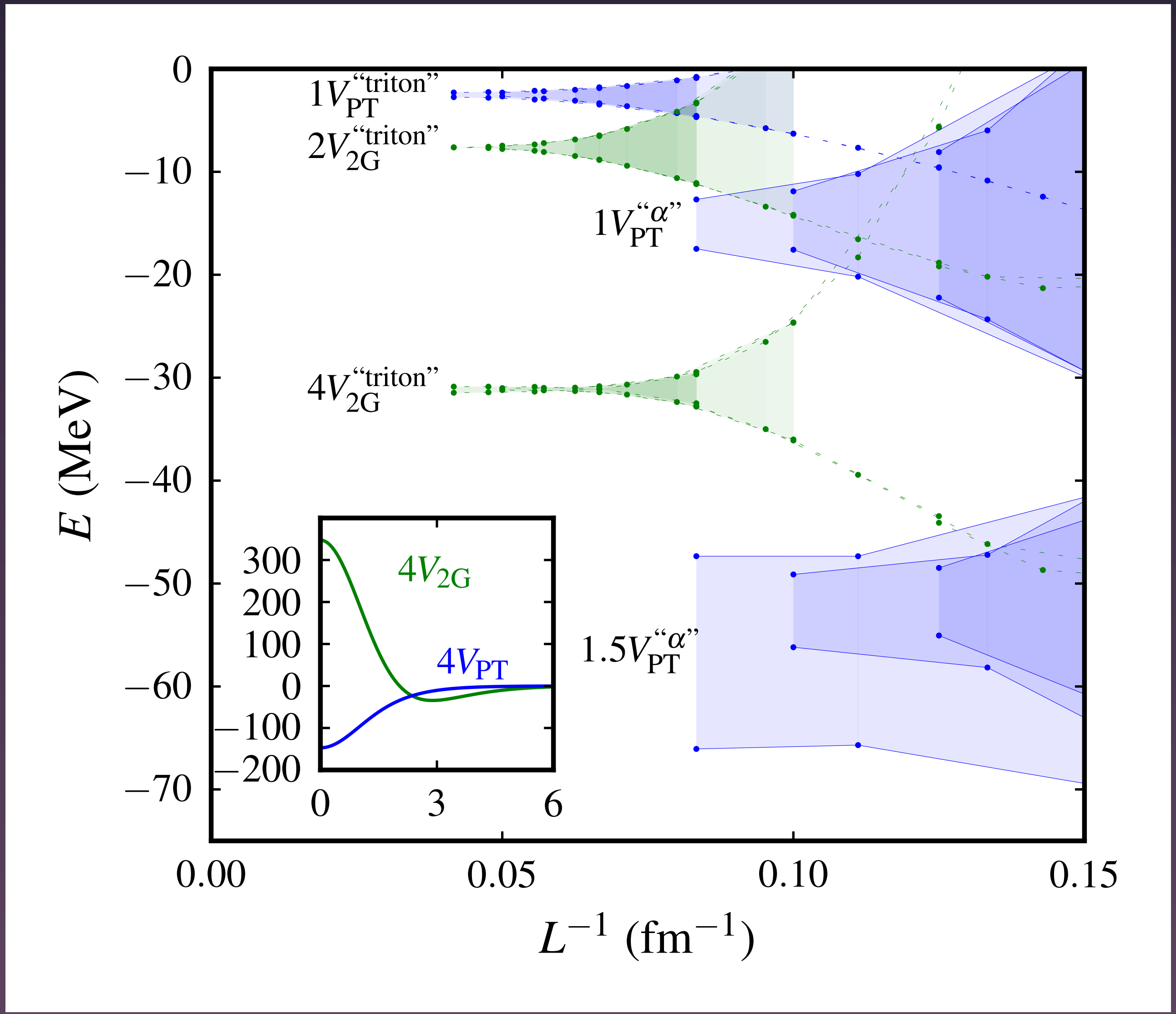
Bulgac & Forbes arXiv:1301.7354

Fourier basis "lower bound"

Band structure lowers energy

- (Tunneling to neighboring cells)

Exact Diagonalization ("Triton" and "Alpha")



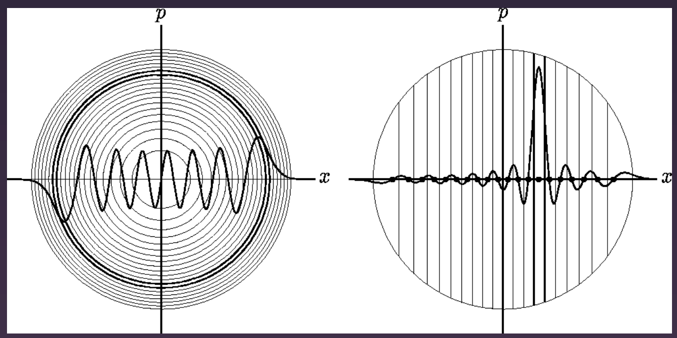
Bulgac & Forbes arXiv:1301.7354

Dirichlet basis "upper bound"

Boundary conditions raises energy

DVR: an Efficient basis

- Quasi-local
  - $\langle F_m | V | F_n \rangle \approx \delta_{mn} V(x_n)$
  - $f_n = f(x_n)/w_n$
- Good phase-space coverage



- Easy to implement
- Straightforward convergence properties
- An efficient alternative to HO basis?