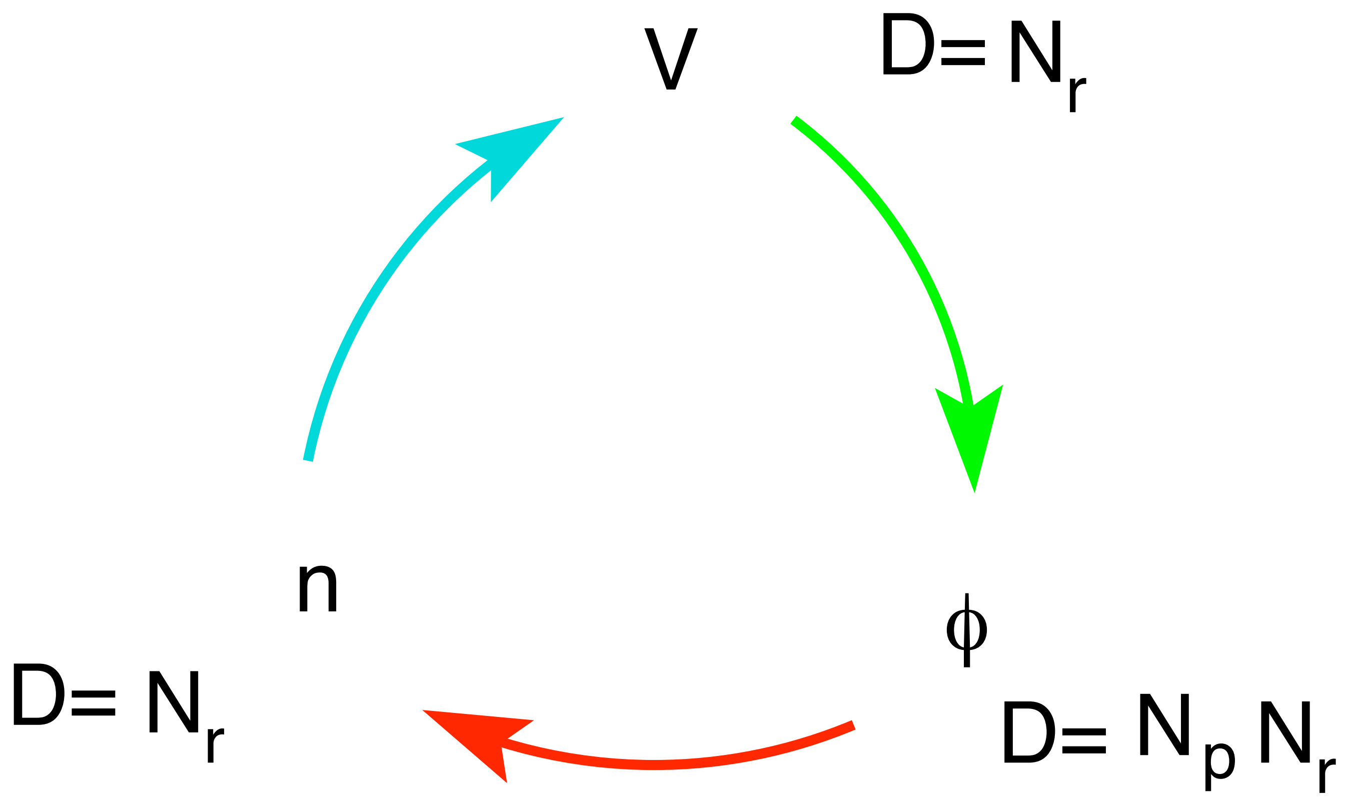
The Self-Consistent Loop



Current Implementation

EV8

```
c     * nxmu                                                        *
c     *         damping factor for the mean-field potential (evolve)  *
c     *         xmu=nxmu/100.; w(n+1)=xmu*w(n+1)+(1.-xmu)*w(n)        *
c     *         if nxmu is read 0, xmu is set to 0.25

      xmu = float(nxmu)/t100
      ymu = one-xmu
          do i=1,2*mv
            rho(i)  = xmu* rho(i)+ymu*rvst(i,1)
            vtau(i) = xmu*vtau(i)+ymu*rvst(i,2)
            vdiv(i) = xmu*vdiv(i)+ymu*rvst(i,3)
            rvst(i,1) =  rho(i)
            rvst(i,2) = vtau(i)
            rvst(i,3) = vdiv(i)
          enddo
          call newpot
```

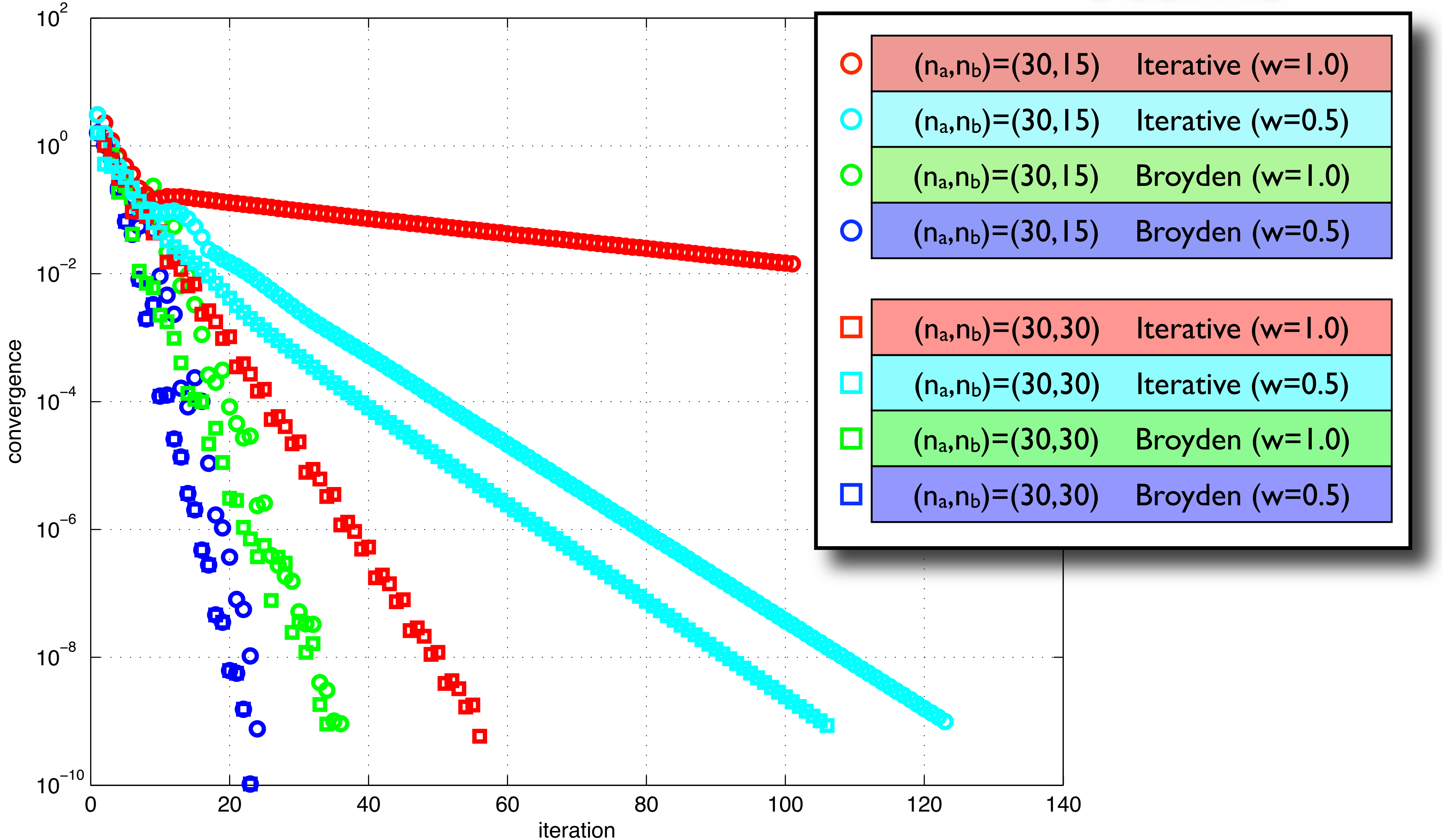
HHODD

```
      SLOWEV=0.500
      XOLDEV=SLOWEV
      XNEWEV=1.00D0-XOLDEV
      DO IX=1,NXHERM
          DO IY=1,NYHERM
             DO IZ=1,NZHERM
               VN_MAS(IX,IY,IZ) = VN_MAS(IX,IY,IZ)*XOLDEV+XNEWEV*VNEUTR
             END DO
          END DO
      END DO
```

Improving self-consistent calculations of Fermion systems

Michael McNeil Forbes and Aurel Bulgac

Improving self-consistent calculations of Fermion systems



Outline

- Structure of self-consistent calculations
- Current codes
- Broyden method to accelerate convergence
  - Very easy to implement
- DVR Basis to improve representation

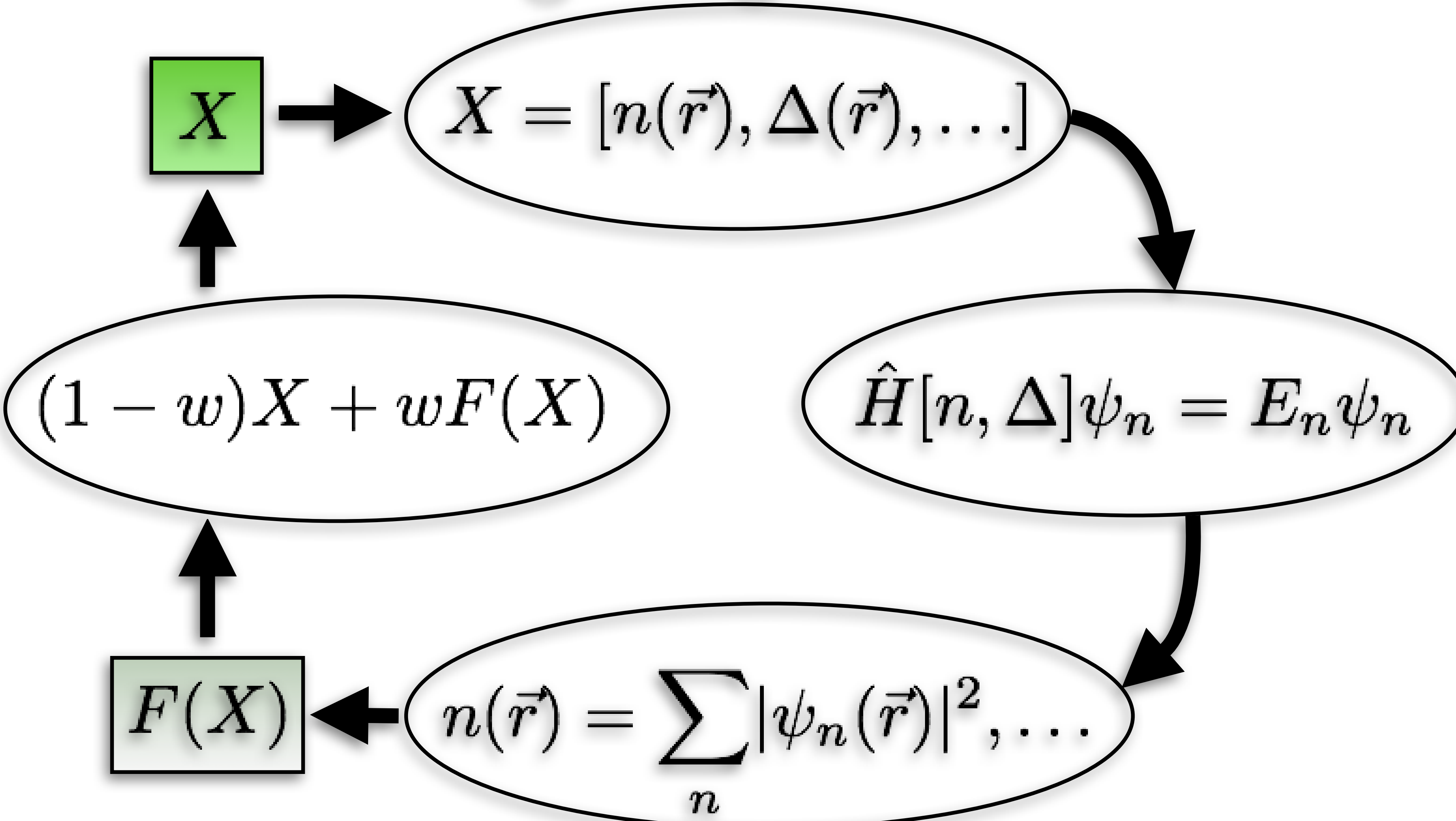
Self-consistent calculations

Find a "fixed-point" in a high dimensional space.

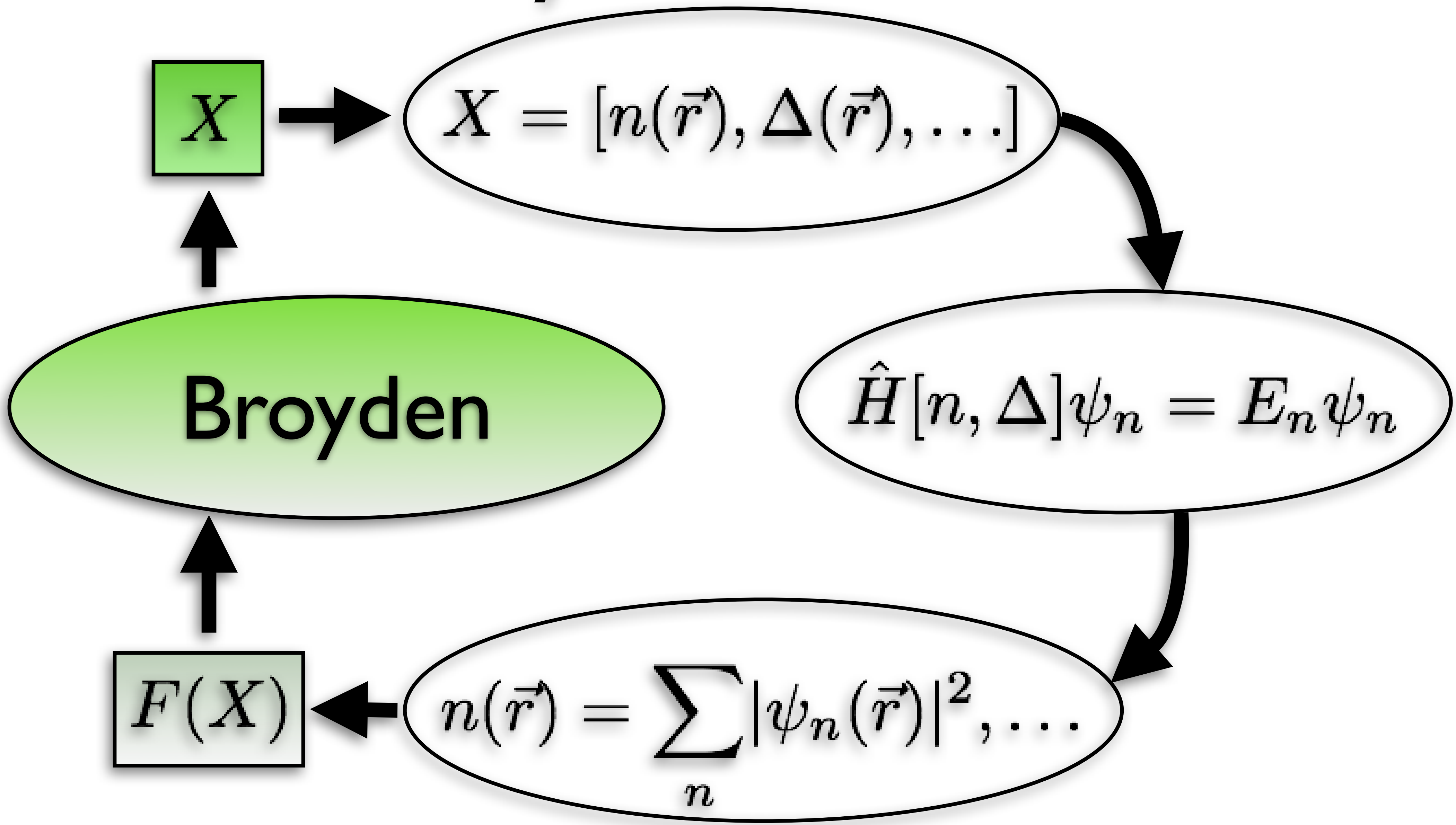
$$X \mapsto F(X)$$

- HFB
- BdG
- DFT (LDA, Kohn)

Self-consistent calculations
Weighting Scheme



Self-consistent calculations Broyden Scheme



Broyden Method

$$G(X) = X - F(X) = 0$$

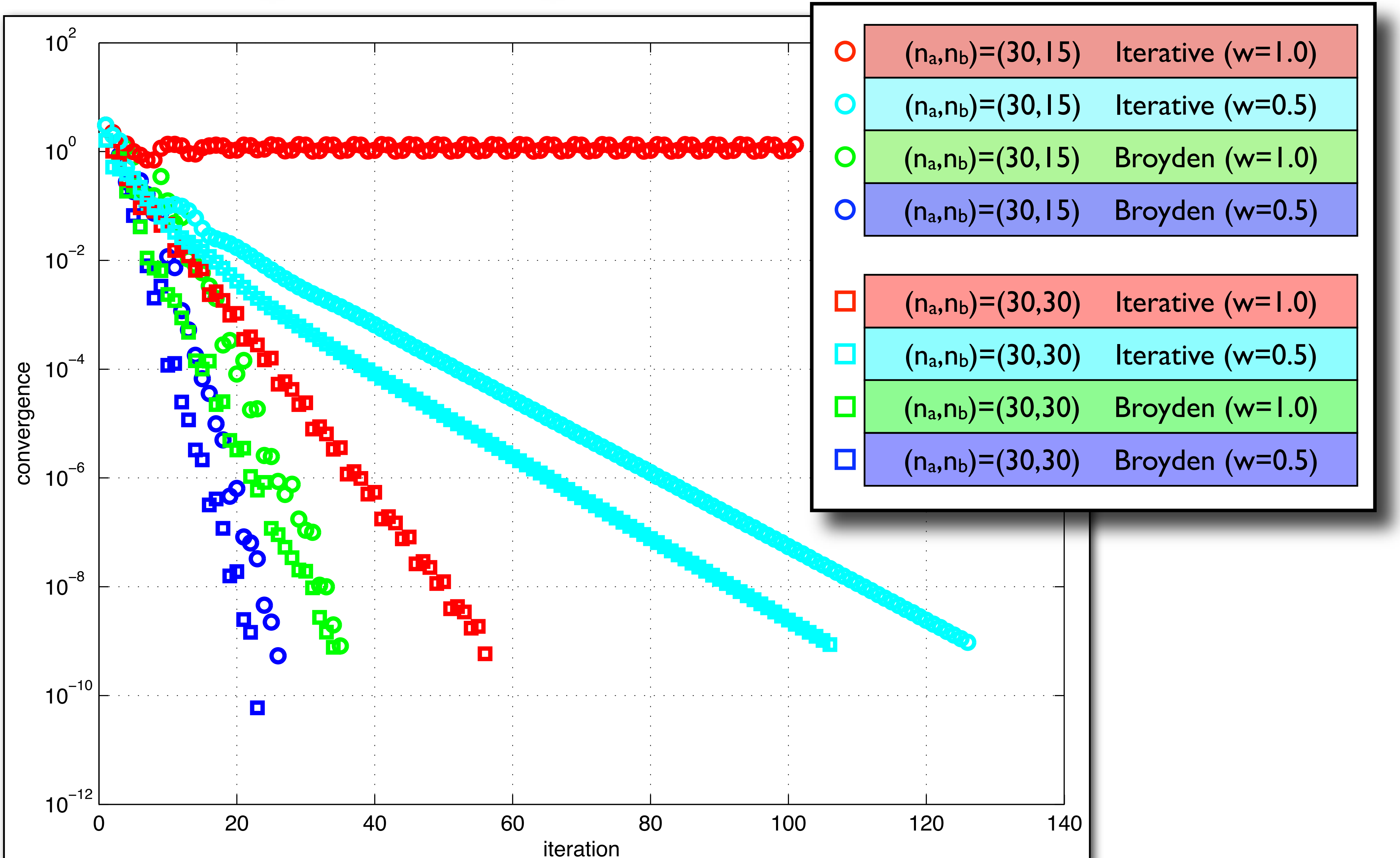
$$\frac{\left(|X_n\rangle,\ |G_n\rangle,\ \mathbf{J}_n^{-1}\right)}{\begin{array}{l} |dX\rangle = -\mathbf{J}_n^{-1} \cdot |G_n\rangle \\ |X_{n+1}\rangle = |X_n\rangle + |dX\rangle \\ |G_{n+1}\rangle = G(|X_{n+1}\rangle) \\ |dG\rangle = |G_{n+1}\rangle - |G_n\rangle \\ \mathbf{J}_{n+1}^{-1} = \mathbf{J}_n^{-1} + \frac{\left(|dX\rangle - \mathbf{J}_n^{-1}|dG\rangle\right)\langle dX|\mathbf{J}_n^{-1}}{\langle dX|\mathbf{J}_n^{-1}|dG\rangle} \end{array}}$$

$$\left(|X_{n+1}\rangle,\ |G_{n+1}\rangle,\ \mathbf{J}_{n+1}^{-1}\right)$$

- Multidimensional Secant method
- Start with $\mathbf{J}_0^{-1} = w$:
  - $X_1 = (\mathbf{1}-w)X_0 + wF(X_0)$
- May keep track of dyadics if space is large
- Hold $\mathbf{J}_n^{-1} = w$ for old method

Described in *Numerical Recipies in* _*_, Press, Teukolsky, Vetterling, Flannery (1992)

Broyden Improves Convergence



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              END DO
          END DO
      END DO
```

Simple Code Modifications

MATLAB Code

```
if iter == 1       % usual step for first iteration or if using usual procedure
   G0    =   x0 - [V_0;D_0;V_1;D_1; mu_a*N_a/N0_a;mu_b*N_b/N0_b];
   Jinv0 =   w    % use weight on initial step or if using usual procedure
   dx    = - Jinv0*G0;
   x0    =   x0 + dx;
elseif iter > 1    % broyden step from second iteration
   G1    =    x0 - [V_0;D_0;V_1;D_1; mu_a*N_a/N0_a;mu_b*N_b/N0_b];
   dG    =    G1 - G0;
   ket   =    dx - Jinv0*dG;
   bra   =    dx'*Jinv0;
   inorm =    1.0/(bra*dG);
   Jinv0 =    Jinv0 + ket*bra*inorm;     % update inverse jacobian here
   dx    =  - Jinv0*G1;
   x0    =    x0  + dx;
   G0    =    G1;
end
```

Broyden Method

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Described in *Numerical Recipies in* <u>*</u>, Press, Teukolsky, Vetterling, Flannery (1992)

Broyden Costs

- Simple: (Maintain and update Jacobian inverse)
  - $O(N^2) \times N_{iter}$
- Dyadic Representation:
  - $O(N \times N_{iter}) \times N_{iter}$

$$\mathbf{J}_{m+1}^{-1} = w\mathbf{1} + \sum_{n=1}^{m} |a_n\rangle \langle b_n|$$

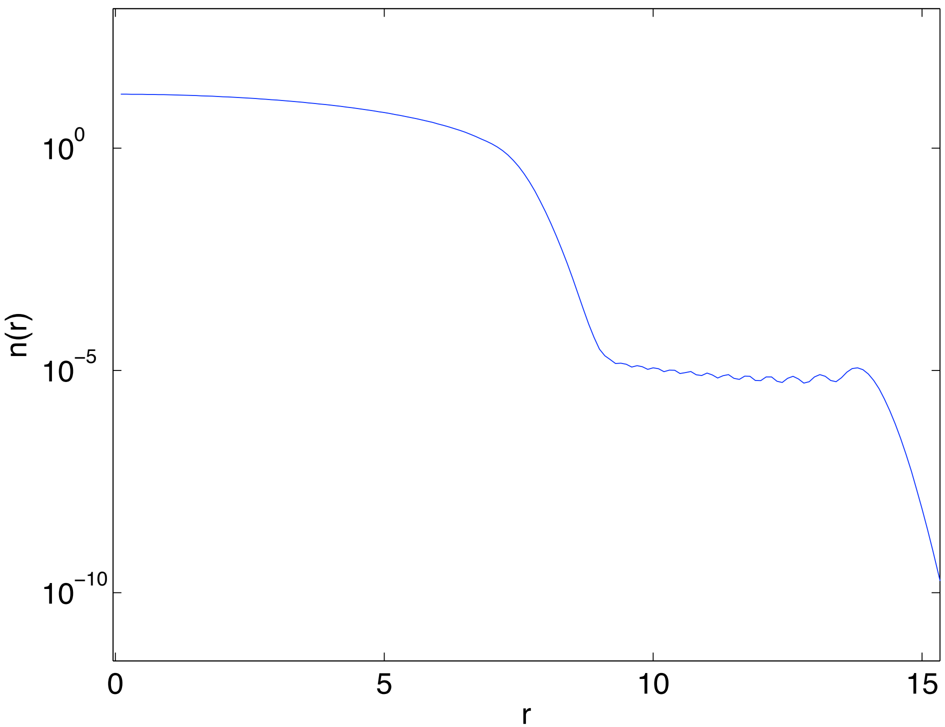
$$|a_n\rangle = |dX_n\rangle - \mathbf{J}_n^{-1} |dG_n\rangle$$

$$\langle b_n| = \frac{\langle dX_n| \mathbf{J}_n^{-1}}{\langle dX_n|\mathbf{J}_n^{-1}|dG_n\rangle}$$

Difficulties with HO Basis

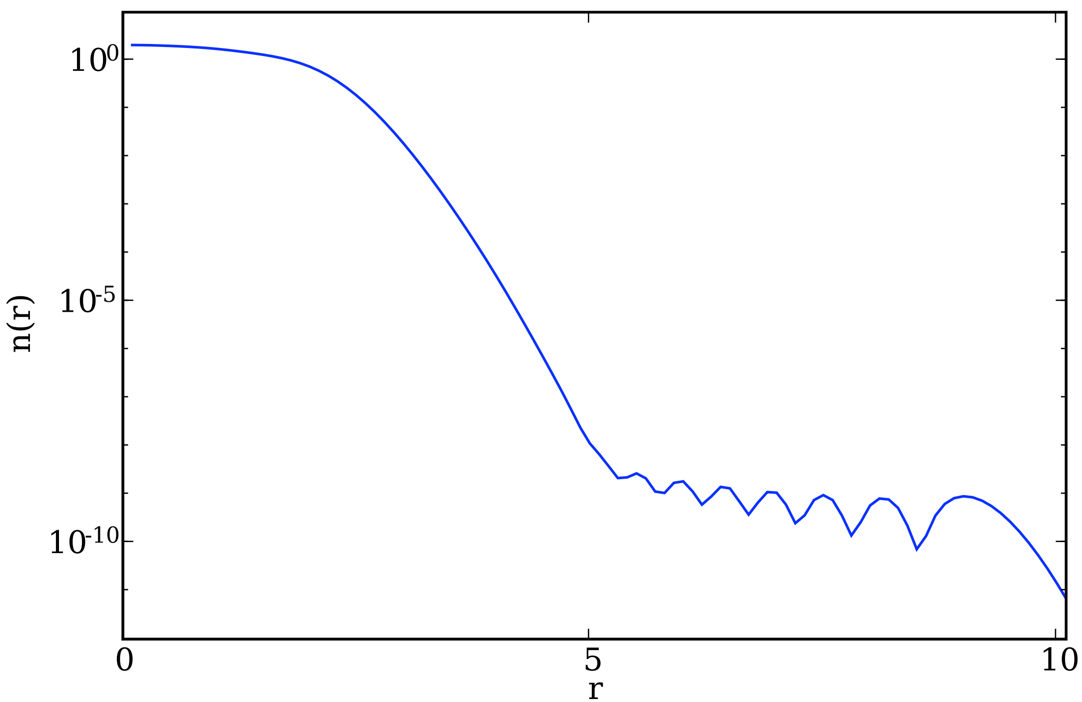
- Large radius behaviour of HO Basis introduces artifacts
- Need large number of states to correct
  - (Requires HO Basis wavefunctions to high precision)

Grasso and Urban, BCS Code

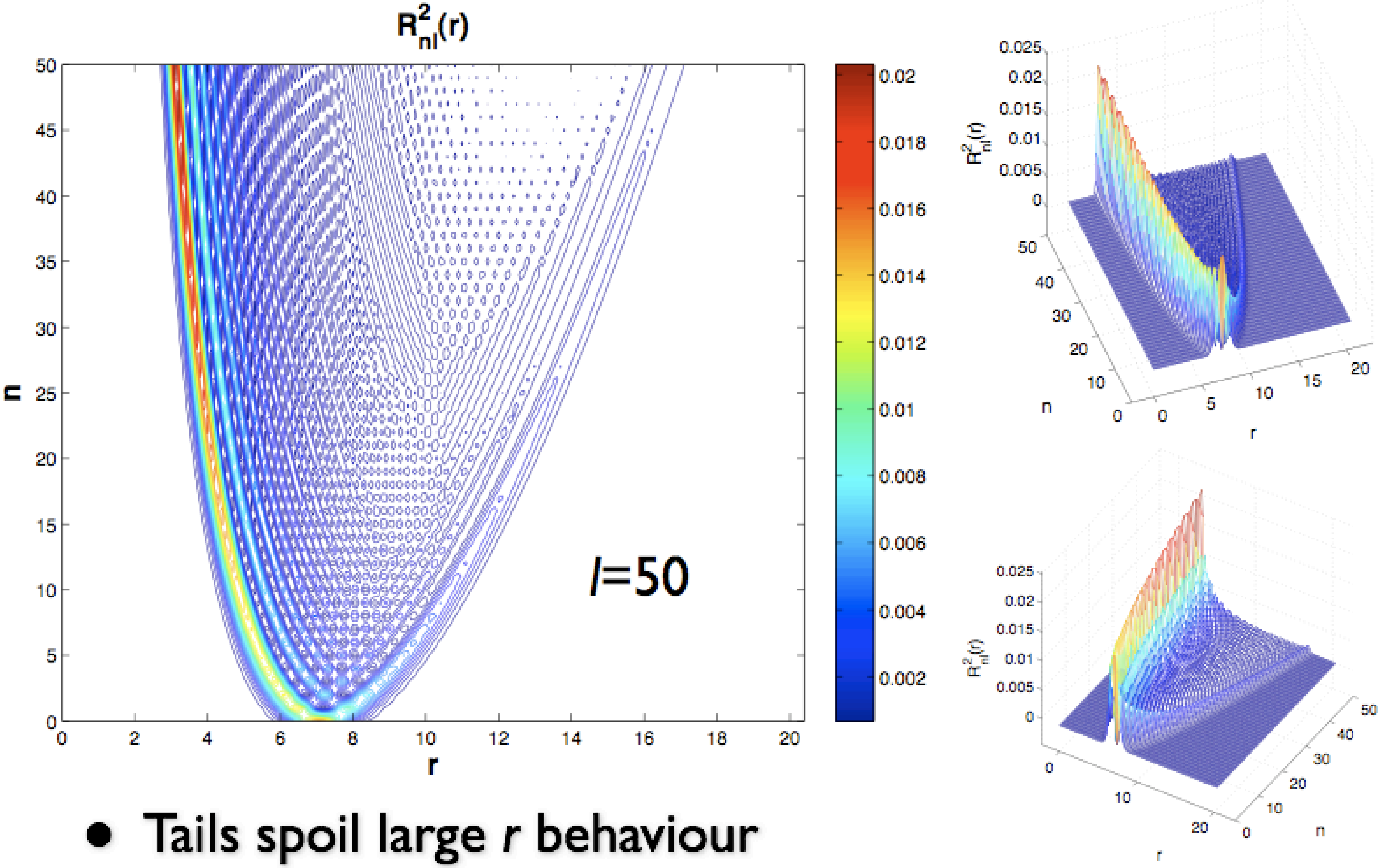


Grasso and Urban, PRA, 68, 033610 (2003)

Our Unitary HO Basis Code



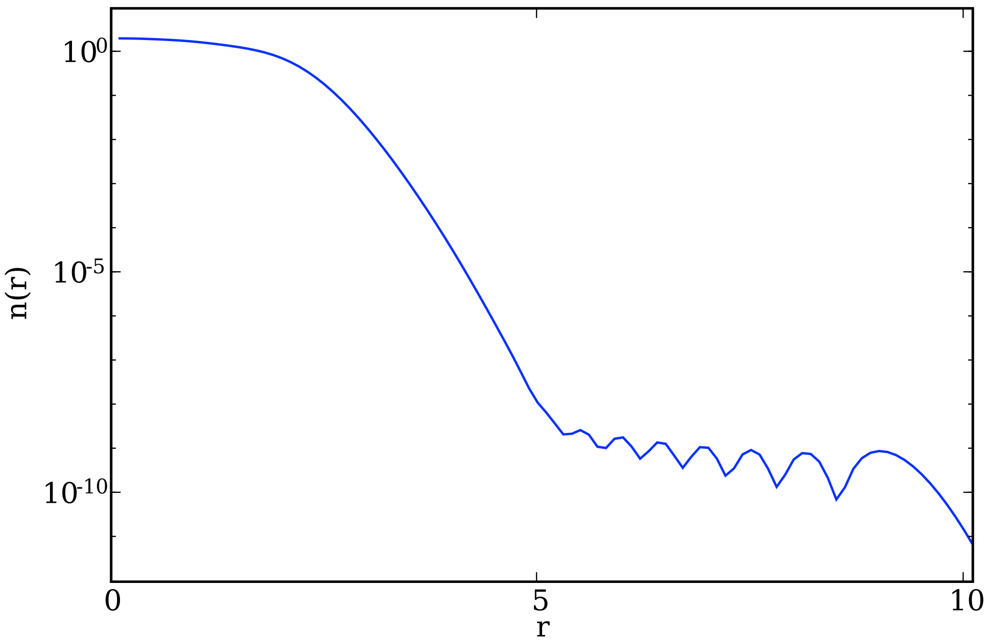
Problem with HO Basis



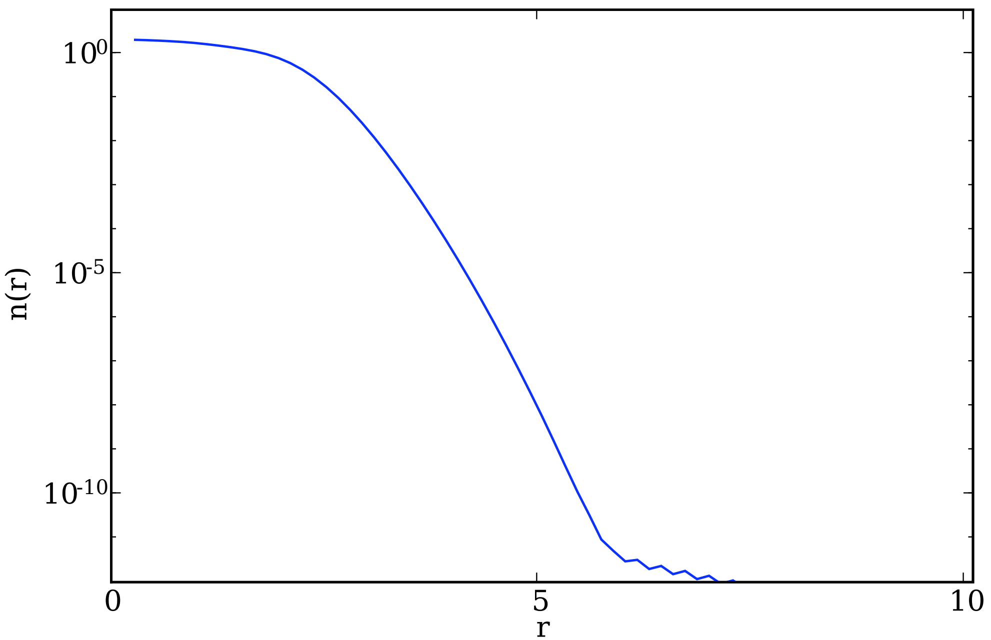
- Tails spoil large *r* behaviour

DVR solves the problem

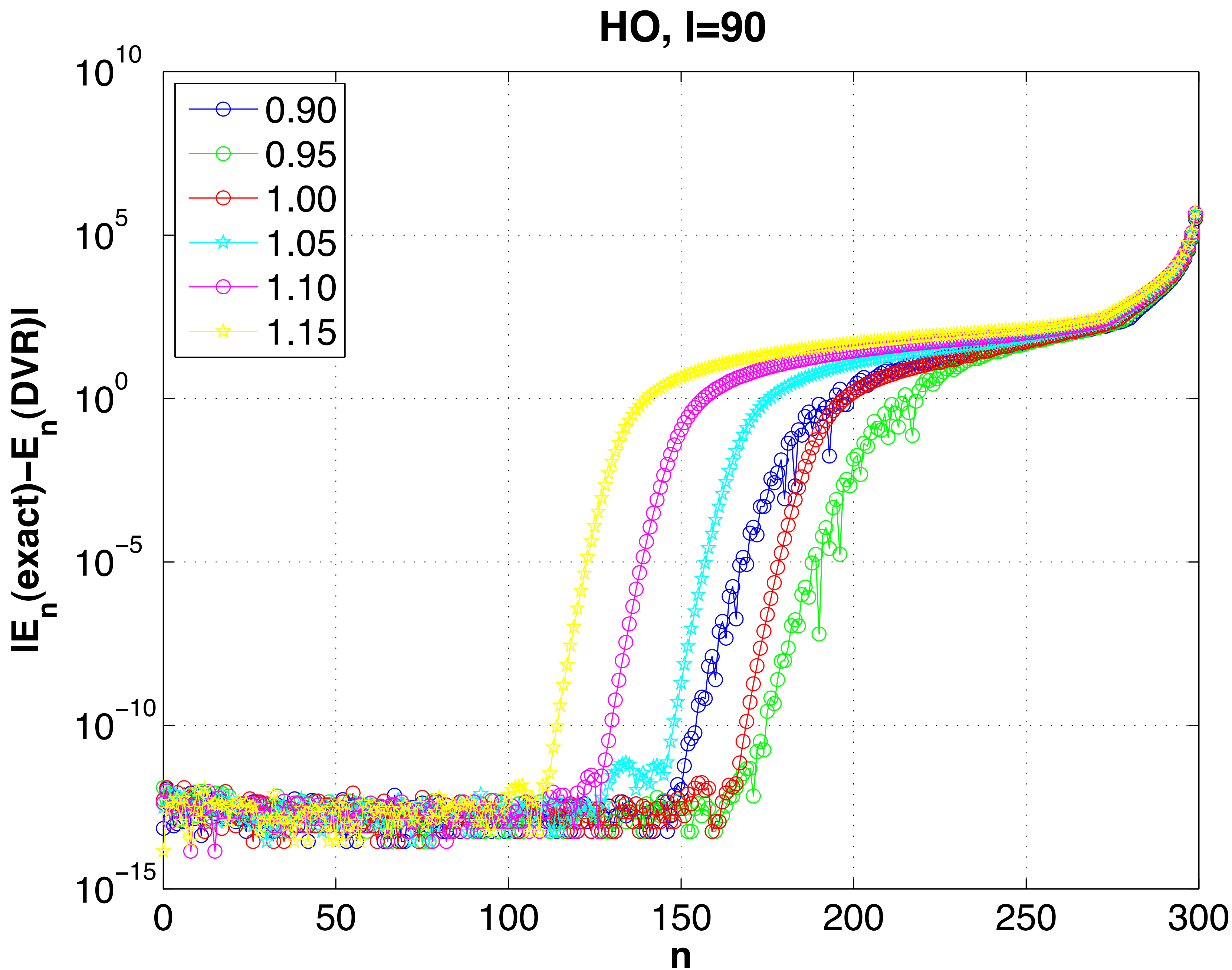
Our code in HO Basis



Our code in DVR basis



HO Spectrum with DVR



DVR Basis in one-dimension

(Higher dimensional generalization is straightforward)

$P^2 = P$ (Projection onto restricted Hilbert space)

$$\langle x|P|y\rangle = \int_{-\pi/l}^{\pi/l} \frac{\mathrm{d}k}{2\pi} e^{ik(x-y)} = \frac{\sin\left(\frac{\pi}{l}(x-y)\right)}{\pi(x-y)},$$

$$\Delta_\alpha = P[\delta(x-x_\alpha)],$$

$$\langle \Delta_\alpha|\Delta_\beta\rangle = \Delta_\alpha(x_\beta) = \Delta_\beta(x_\alpha) = K_\alpha \delta_{\alpha\beta},$$

$$\psi(x) = \sum_{\alpha=1}^{N} c_\alpha \Delta_\alpha + \mathrm{O}(e^{-cN}) \approx \sum_n \psi(nl) \frac{\sin\left[\frac{\pi}{l}(x-nl)\right]}{\frac{\pi}{l}(x-nl)}$$

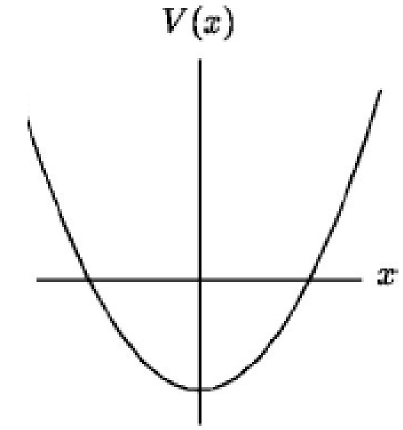
$$c_\alpha = \int \mathrm{d}x \, \frac{1}{K_\alpha} \Delta_\alpha(x)\psi(x) = \frac{1}{K_\alpha}\psi(x_\alpha), \qquad x_\alpha = nl$$

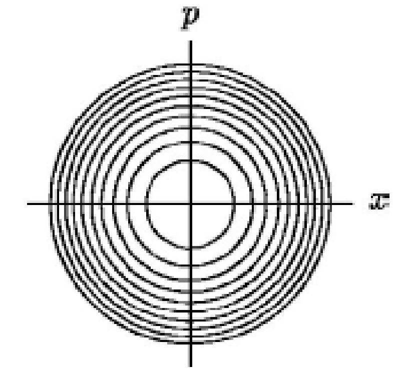
Littlejohn *et al.* J. Chem. Phys. **116**, 8691 (2002)

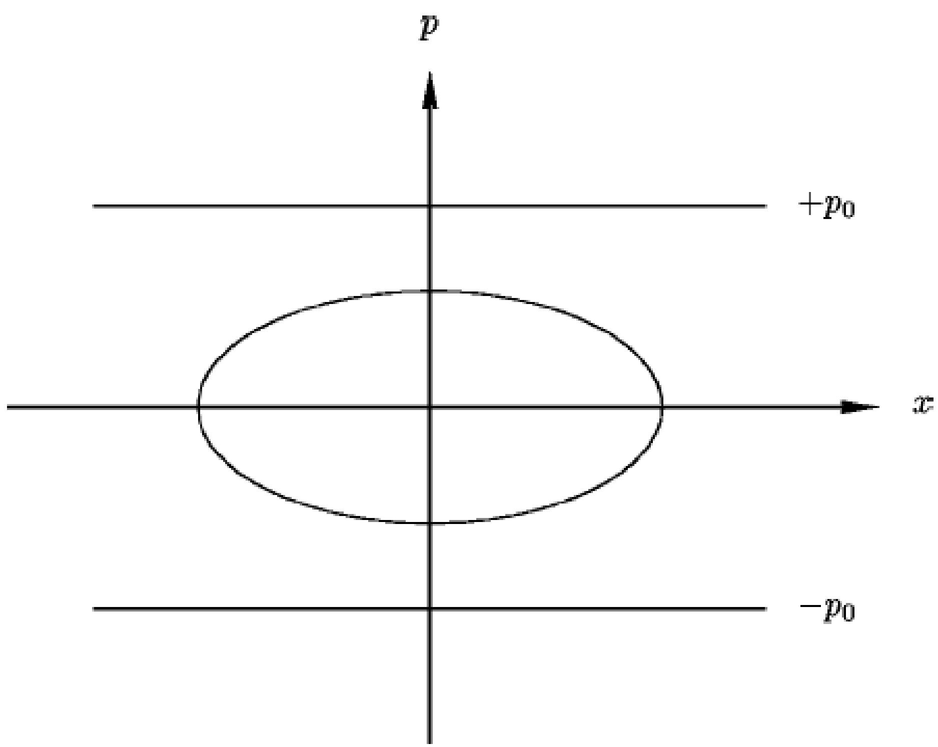
$$\psi(x) = \sum_{\alpha=1}^{N} d_\alpha F_\alpha(x) + \mathrm{O}(e^{-cN}),$$

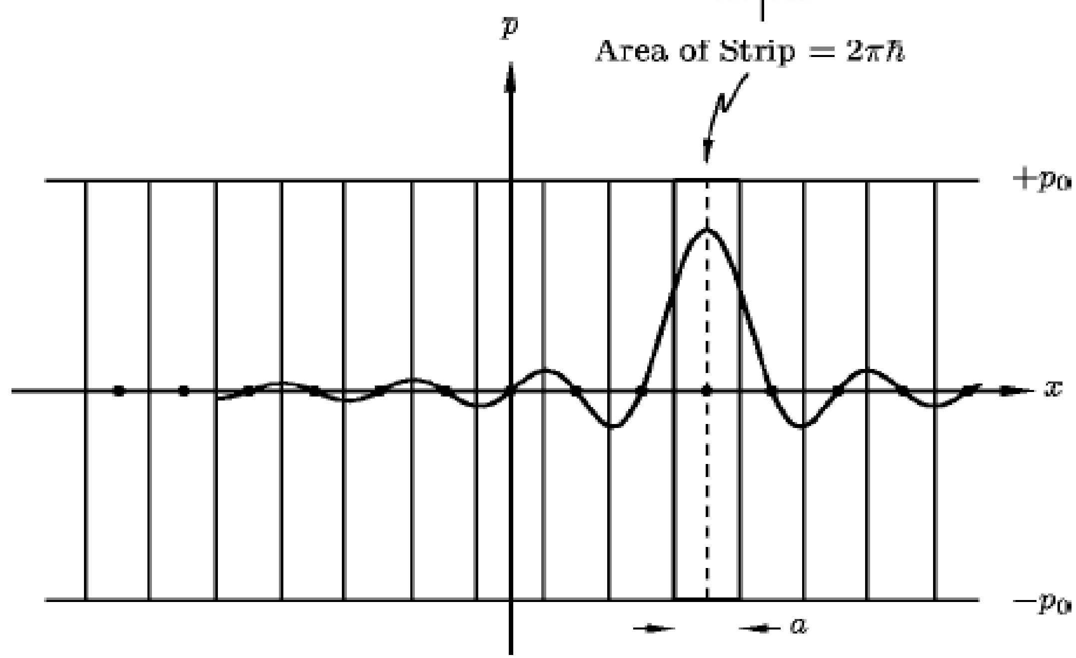
$$F_\alpha = \frac{1}{\sqrt{K_\alpha}} \Delta_\alpha(x), \quad x_\alpha = nl, \quad \langle F_\alpha | F_\beta \rangle = \delta_{\alpha,\beta},$$

$$\sum_\beta \left[\langle F_\alpha | \widehat{\mathbf{T}} | F_\beta \rangle + V(x_\alpha)\delta_{\alpha\beta} \right] d_\beta = E d_\alpha$$









DVR for Radial Equation: Bessel DVR Basis

Littlejohn *et al.* J. Chem. Phys. **117**, 27 (2002)

$$F_{\nu n}(r) = (-1)^{n+1} \frac{K z_{\nu n} \sqrt{2r}}{K^2 r^2 - z_{\nu n}^2} J_\nu(Kr)$$

$$P(r, r') = \int_0^K \mathrm{d}k \ \langle kr | J_\nu \rangle \langle J_\nu | kr' \rangle$$

$$\langle F_{\nu n} | k_r^2 + \frac{\nu^2 - \frac{1}{4}}{r^2} | F_{\nu n'} \rangle$$

$$= \begin{cases} \dfrac{K^2}{3}\left[1 + \dfrac{2(\nu^2 - 1)}{z_{\nu n}^2}\right], & n = n', \\ (-1)^{n-n'} 8K^2 \dfrac{z_{\nu n} z_{\nu n'}}{(z_{\nu n}^2 - z_{\nu n'}^2)^2}, & n \neq n', \end{cases}$$

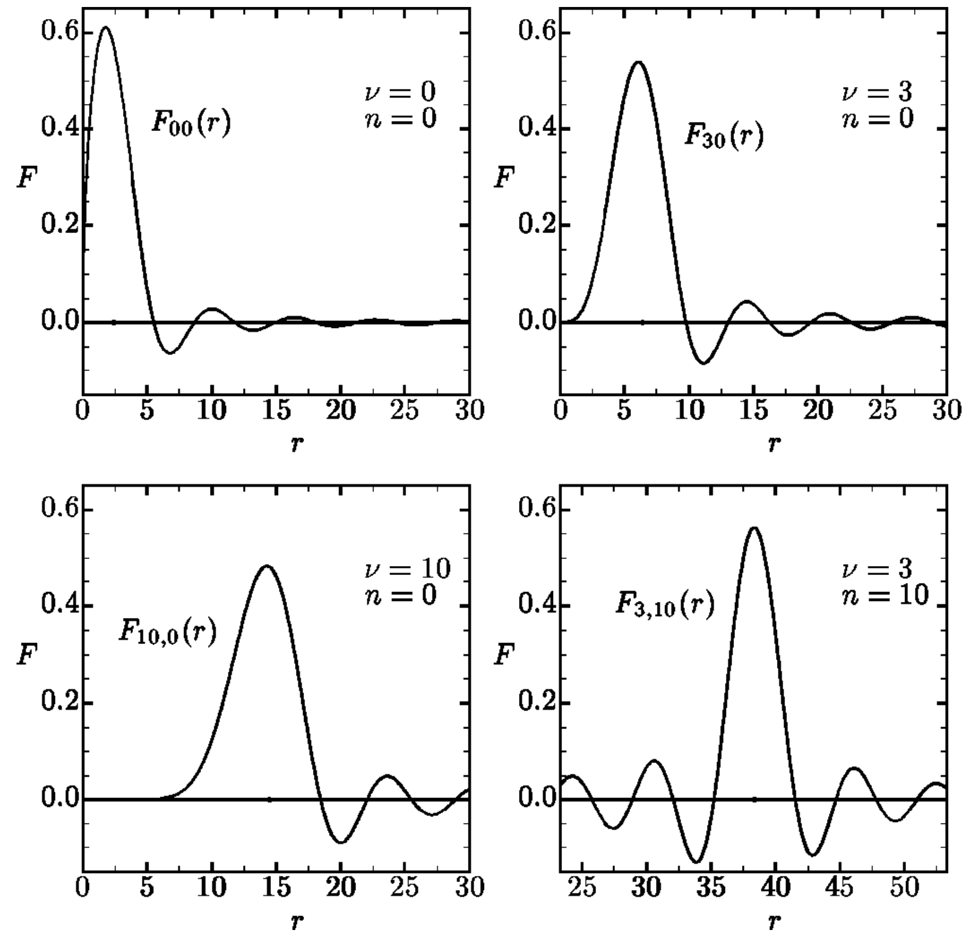
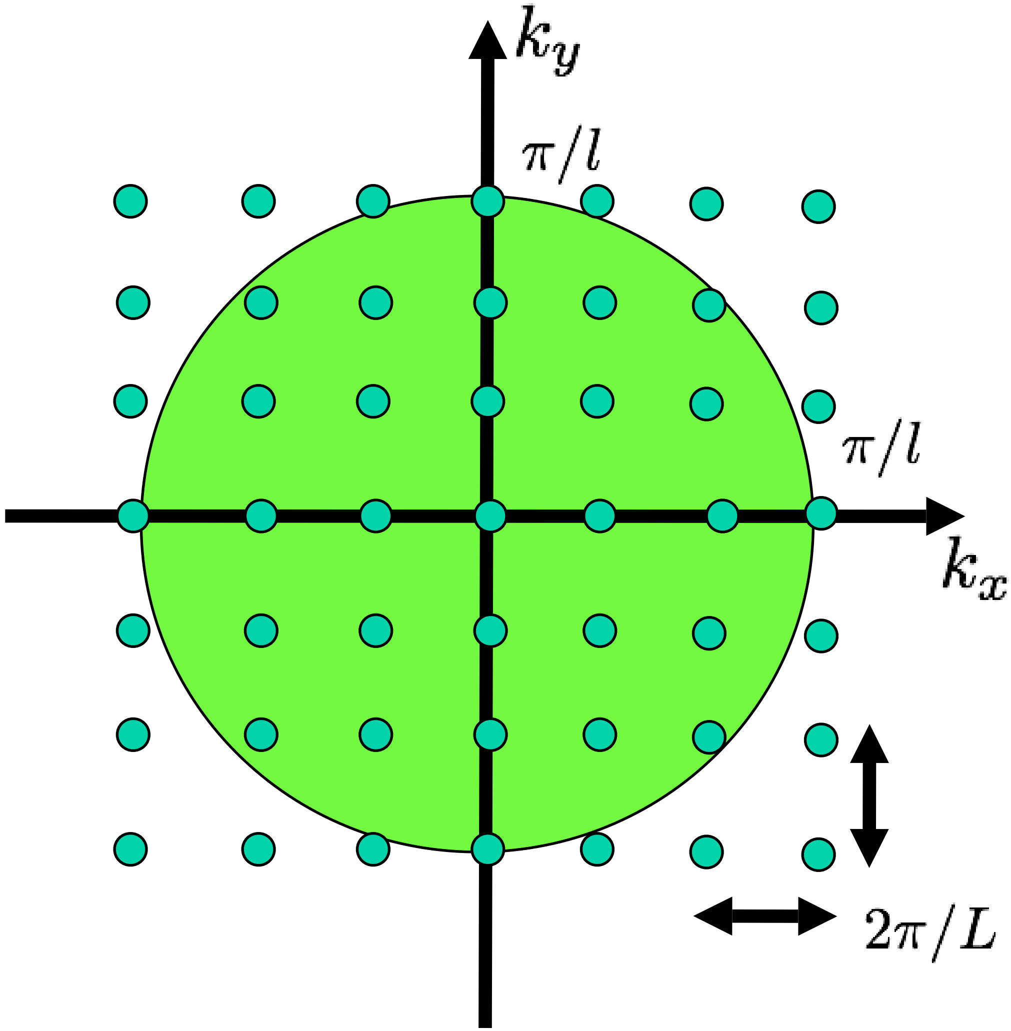


FIG. 2. Plots of the Bessel DVR functions $F_{\nu n}(r)$ for $K = 1$ and for selected values of ν and n.



Momentum Space

$$\varepsilon_F, \quad \Delta, \quad T \ll \frac{\hbar^2\pi^2}{2ml^2},$$

$$\delta\varepsilon > \frac{2\hbar^2\pi^2}{mL^2},$$

$$\varepsilon_F, \quad \Delta T \gg \frac{2\hbar^2\pi^2}{mL^2},$$

$$\xi \ll L = N_s l,$$

$$\delta p > \frac{2\pi\hbar}{L}.$$

Summary

- Broyden Improves Convergence
  - Extremely easy to implement
  - Can be made inexpensive
- HO Basis has problems with large *r* tails
- DVR Basis solves these problems
  - Near optimal phase-space coverage