

Nonlinearity of Inverse Scattering Problem and the Resolution Limit: Does Multiple Scattering Provide Subwavelength Information?

Vadim A. Markel

University of Pennsylvania
Department of Radiology
Philadelphia, PA

vmarkel@upenn.edu
<http://whale.seas.upenn.edu/vmarkel>



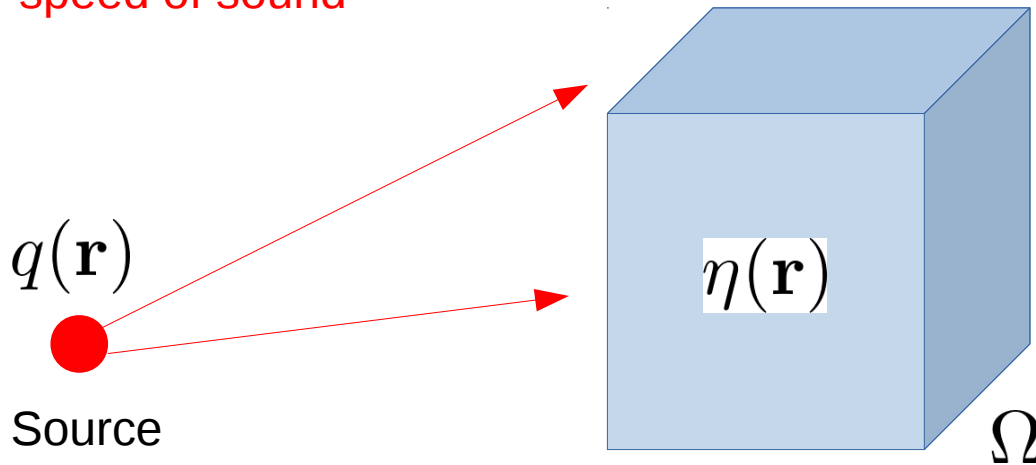
Plan of the talk

1. Inverse scattering problem, Ewald sphere, discretization
2. Toy Problem 1 (3 dof)
3. Toy Problem 2 (4 dof)
4. Toy Problem 3 (N dof)
5. Distorted Born approximation and tangent spaces
6. Model with a realistic interaction and N degrees of freedom ($N=2501$)

1a. Inverse Scattering Problem (Scalar Waves)

This can be relative speed of sound

$$\eta(\mathbf{r}) = 1 \quad \text{for } \mathbf{r} \notin \Omega$$



We work in frequency domain:

$$U(\mathbf{r}, t) = \text{Re}[u(\mathbf{r})e^{-i\omega t}]$$

$$k = \frac{\omega}{c} = \text{const}$$

$$[\nabla^2 + k^2\eta(\mathbf{r})] u(\mathbf{r}) = -4\pi k^2 q(\mathbf{r})$$

← Everywhere in space (and + boundary conditions at infinity)

$$(\nabla^2 + k^2) u(\mathbf{r}) = -4\pi k^2 [V(\mathbf{r})u(\mathbf{r}) + q(\mathbf{r})]$$

← Identical transformation of the previous equation

$$V(\mathbf{r}) \equiv \frac{\eta(\mathbf{r}) - 1}{4\pi}$$

← The "potential" is zero outside of the domain

1b. Inverse Scattering Problem (cont.)

$$(\nabla^2 + k^2) u(\mathbf{r}) = -4\pi k^2 [V(\mathbf{r})u(\mathbf{r}) + q(\mathbf{r})] \quad \leftarrow \text{From previous page}$$

$$u(\mathbf{r}) = u_{\text{inc}}(\mathbf{r}) + \underbrace{\int_{\Omega} G(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') u(\mathbf{r}') d^3 r'}_{\text{Scattered field}} \quad \leftarrow \text{Lippmann-Schwinger equation}$$

Where

Scattered field

$$u_{\text{inc}}(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}') q(\mathbf{r}') d^3 r'$$

This is the incident field; it would be the total field for the given source in the absence of the scatterer.

$$G(\mathbf{r}, \mathbf{r}') = k^2 \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}$$

The free-space Green's function; it satisfies the radiation (Sommerfeld) boundary conditions at infinity.

1c. Inverse Scattering Problem (T-matrix)

Introduce
the “polarization”
field:

$$P(\mathbf{r}) = V(\mathbf{r})u(\mathbf{r}) \quad (\text{vanishes outside of the domain})$$

$$u(\mathbf{r}) = u_{\text{inc}}(\mathbf{r}) + \int_{\Omega} G(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')u(\mathbf{r}')d^3r'$$

↓ Multiply by V

$$P(\mathbf{r}) = V(\mathbf{r})u_{\text{inc}}(\mathbf{r}) + \int_{\Omega} V(\mathbf{r})G(\mathbf{r}, \mathbf{r}')P(\mathbf{r}')d^3r' \quad (\mathbf{r} \in \Omega)$$

↓ From linearity

The T-matrix

$$P(\mathbf{r}) = \int_{\Omega} T(\mathbf{r}, \mathbf{r}')u_{\text{inc}}(\mathbf{r}')d^3r'$$

Higher-order
terms contain
integrals

$$T(\mathbf{r}, \mathbf{r}') = V(\mathbf{r})\delta(\mathbf{r}, \mathbf{r}') + V(\mathbf{r})G(\mathbf{r}, \mathbf{r}')V(\mathbf{r}') + \dots$$

1d. Inverse Scattering Problem (cont.)

$$P(\mathbf{r}) = \int_{\Omega} T(\mathbf{r}, \mathbf{r}') u_{\text{inc}}(\mathbf{r}') d^3 r'$$

$$T = (I - VG)^{-1} V \xrightarrow{\text{(if converges)}} V + VGV + VGVGV + \dots$$

$$\begin{aligned} u_{\text{scatt}}(\mathbf{r}) &= \int_{\Omega} G(\mathbf{r}, \mathbf{r}') P(\mathbf{r}') d^3 r' \\ &= \int_{\Omega} G(\mathbf{r}, \mathbf{r}_1) T(\mathbf{r}_1, \mathbf{r}_2) u_{\text{inc}}(\mathbf{r}_2) d^3 r_1 d^3 r_2 \end{aligned}$$

We will next assume that the incident field is a plane wave and make the far-field approximation for the Green's function

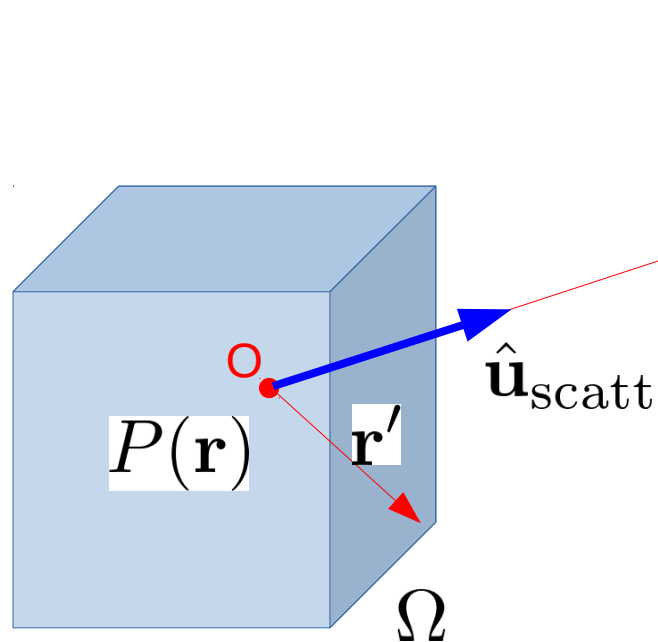
This will lead to loss of high-frequency information about the target

1e. Inverse Scattering Problem (far-field)

Scattered field (from previous page)

$$u_{\text{scatt}}(\mathbf{r}) = \int_{\Omega} G(\mathbf{r}, \mathbf{r}') P(\mathbf{r}') d^3 r'$$

Point of observation
in the far field
of the scatterer:



$$|\mathbf{r}| = R = \text{const}$$

$$kR \gg 1$$

$$G(\mathbf{r}, \mathbf{r}') \simeq \frac{k^2 e^{ikR}}{R} e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}'}$$

$$\mathbf{k}_{\text{scatt}} = k \hat{\mathbf{u}}_{\text{scatt}}$$

Far-field approximation

$$u_{\text{scatt}}(\mathbf{r}) = \frac{k^2 e^{ikR}}{R} \int_{\Omega} e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}} P(\mathbf{r}) d^3 r$$

Not a regular Fourier transform of the
polarization field; can not be inverted.....

1f. Inverse Scattering Problem (scattering amplitude)

recall that
$$P(\mathbf{r}) = \int_{\Omega} T(\mathbf{r}, \mathbf{r}') u_{\text{inc}}(\mathbf{r}') d^3 r'$$

... and let
$$u_{\text{inc}}(\mathbf{r}) = e^{i\mathbf{k}_{\text{inc}} \cdot \mathbf{r}}$$

$$\begin{aligned} u_{\text{scatt}}(\mathbf{r}) &= \frac{k^2 e^{ikR}}{R} \int_{\Omega} e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}} P(\mathbf{r}) d^3 r \\ &= \frac{k^2 e^{ikR}}{R} \int_{\Omega} e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}_1} T(\mathbf{r}_1, \mathbf{r}_2) e^{i\mathbf{k}_{\text{inc}} \cdot \mathbf{r}_2} d^3 r_1 d^3 r_2 \end{aligned}$$

$$f(\mathbf{k}_{\text{scatt}}, \mathbf{k}_{\text{inc}}) = \int_{\Omega} T(\mathbf{r}_1, \mathbf{r}_2) e^{i(\mathbf{k}_{\text{inc}} \cdot \mathbf{r}_2 - \mathbf{k}_{\text{scatt}} \cdot \mathbf{r}_1)} d^3 r_1 d^3 r_2$$

Scattering amplitude
(measurable quantity)

T-matrix (uniquely defined by V)

ISP: Given measurements of scattering amplitude, reconstruct V

1g. Inverse Scattering Problem (linear regime)

$$T(\mathbf{r}_1, \mathbf{r}_2) \approx V(\mathbf{r}_1)\delta(\mathbf{r}_1 - \mathbf{r}_2)$$

This is approximately true in the weak scattering regime when V is in some sense small

$$f(\mathbf{k}_{\text{scatt}}, \mathbf{k}_{\text{inc}}) = \int_{\Omega} V(\mathbf{r}) e^{i(\mathbf{k}_{\text{inc}} - \mathbf{k}_{\text{scatt}}) \cdot \mathbf{r}} d^3r$$

$$|\mathbf{k}_{\text{inc}} - \mathbf{k}_{\text{scatt}}| \leq 2k = \frac{2\omega}{c}$$

Ewald sphere radius

Resolution limit in 3D? Sphere is not a cube!

$$\Delta > \lambda/4, \quad \lambda = 2\pi/k$$

(because a circumscribed cube with side $4k$ contains the Ewald sphere but has some empty corners (we do not know Fourier data in these regions))

$$\Delta < \sqrt{3}\lambda/4, \quad \lambda = 2\pi/k$$

(because we know Fourier data every where in a cube inscribed inside the Ewald sphere plus some additional data outside of the cube.)

1h. Inverse Scattering Problem (nonlinear regime)

$$f(\mathbf{k}_{\text{inc}}, \mathbf{k}_{\text{scatt}}) = \int e^{i\mathbf{k}_{\text{inc}} \cdot \mathbf{r}} V(\mathbf{r}) e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}} d^3 r \\ + \int e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}_1} V(\mathbf{r}_1) G(\mathbf{r}_1, \mathbf{r}_2) V(\mathbf{r}_2) e^{i\mathbf{k}_{\text{inc}} \cdot \mathbf{r}_2} d^3 r_1 d^3 r_2 + \dots$$

We can write this expansion in terms of the Fourier transform of the Potential:

$$G(\mathbf{r}, \mathbf{r}') = \int g(\mathbf{q}) e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} d^3 q$$

$$f(\mathbf{k}_{\text{inc}}, \mathbf{k}_{\text{scatt}}) = \tilde{V}(\mathbf{k}_{\text{inc}} - \mathbf{k}_{\text{scatt}}) \\ + \int \tilde{V}(\mathbf{k}_{\text{inc}} - \mathbf{q}) g(\mathbf{q}) \tilde{V}(\mathbf{q} - \mathbf{k}_{\text{scatt}}) d^3 q + \dots$$

Here we already have Fourier wave vectors outside of the Ewald sphere

1i. Some History

The idea to use nonlinearity of ISP to achieve super-resolution, although in a somewhat implicit form (Chew and coo-authors)

- * M. Moghaddam, W. C. Chew, and M. Oristaglio, Int. J. Imaging Syst. Technol. 3, 318, 1991
- * M. Moghaddam, W. C. Chew, IEEE Trans. Geosci. Remote Sensing 30, 147, 1992.
- * F.-C. Chen and W. C. Chew, Appl. Phys. Lett. 72, 3080, 1998
- * T. J. Cui, W. C. Chew, X. X. Yin, and W. Hong, IEEE Trans. Ant. Propag. 52, 1398, 2004.

More explicit claims:

- * F. Simonetti, Phys. Rev. E 73, 036619, 2006
- * K. Belkebir, P. C. Chaumet, and A. Sentenac, J. Opt. Soc. Am. A 23, 586, 2006
- * G. Maire et al., Phys. Rev. Lett. 102, 213905, 2009
- * C. Gilmore et al., IEEE Antennas Wireless Propagation Lett. 9, 393, 2010
- * T. Zhang et al., Optica 3, 609, 2016 ← Experimental demonstration of resolution $\lambda/10$ (but with strong a priori constraints)

A review article in which the super-resolution in nonlinear ISP is presented as a fact:

M. T. Testorf and M. A. Fiddy, "Superresolution imaging – Revisited," Adv. Imaging Electron Phys. 163, 165, 2010

1j. Discretization

$$\int_{\Omega} \underbrace{e^{-i\mathbf{k}_{\text{scatt}} \cdot \mathbf{r}_1}}_A \underbrace{T(\mathbf{r}_1, \mathbf{r}_2)}_T \underbrace{e^{i\mathbf{k}_{\text{inc}} \cdot \mathbf{r}_2}}_B d^3 r_1 d^3 r_2 = \underbrace{f(\mathbf{k}_{\text{scatt}}, \mathbf{k}_{\text{inc}})}_{\Phi \text{ Data matrix}}$$

$$AT[V]B = \Phi$$

This is the algebraic statement of the nonlinear ISP. Namely, given

- the data matrix Φ
- the measurement matrices A,B
- the algebraic relation between T and V

find all elements of the diagonal matrix V

Number of voxels

Number of incidence directions

$N_s \times N$ matrix: $A_{ln} = e^{i\mathbf{k}_l^{(\text{inc})} \cdot \mathbf{r}_n}$

$N \times N_d$ matrix: $B_{nm} = e^{-i\mathbf{k}_m^{(\text{scatt})} \cdot \mathbf{r}_n}$

$N_s \times N_d$ matrix: $\Phi_{lm} = f(\mathbf{k}_l^{(\text{scatt})}, \mathbf{k}_m^{(\text{inc})})$

$N \times N$ matrices: T, G, V (V is diagonal)

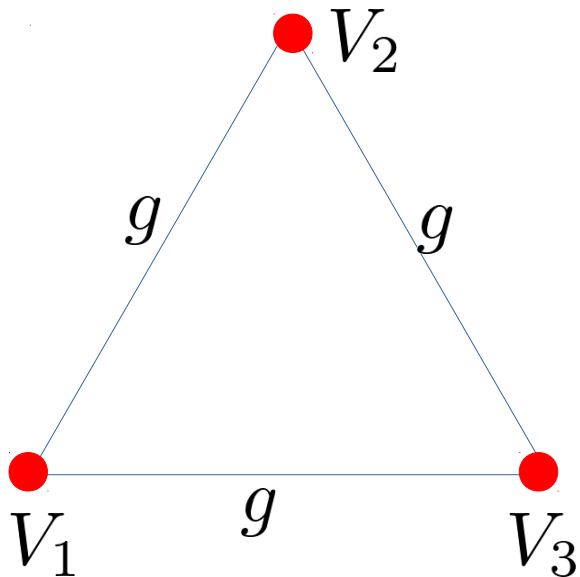
Number of detection directions

2a. Toy Problem 1 with 3 degrees of freedom

$$\mathbf{G} = \begin{bmatrix} 0 & g & g \\ g & 0 & g \\ g & g & 0 \end{bmatrix}$$

$$T_{nm} = V_n \delta_{nm} + g \frac{\kappa_n \kappa_m}{1 - gS}$$

$$\kappa_n = \frac{V_n}{1 + gV_n}, \quad S = \sum_{n=1}^3 \kappa_n.$$



We will construct the measurement matrices A and B from the following three orthogonal basis vectors:

$$\mathbf{u}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

2b. Toy Problem 1

(a) Band-limited measurement (u_1 and u_2)

$$A = \begin{bmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \end{bmatrix}, \quad B = [\mathbf{u}_1 \quad \mathbf{u}_2] = \begin{bmatrix} 1 & 1 \\ 1 & -2 \\ 1 & 1 \end{bmatrix}.$$

(a.i) Linear regime $g=0$

$$\begin{bmatrix} V_1 + V_2 + V_3 & V_1 - 2V_2 + V_3 \\ V_1 - 2V_2 + V_3 & V_1 + 4V_2 + V_3 \end{bmatrix} = \begin{bmatrix} \phi_{11} & \phi_{12} \\ \phi_{21} & \phi_{22} \end{bmatrix}$$

$$\phi_{12} = \phi_{21} \quad \text{AND} \quad \phi_{22} = 2\phi_{11} - \phi_{12}$$

Condition of physical admissibility of data

If satisfied

$$V_1 + V_2 + V_3 = \phi_{11}$$

$$V_1 - 2V_2 + V_3 = \phi_{12}$$

Two independent equations for three unknowns, hence, the IP is "band-limited"

2c. Toy Problem 1

(a.ii) Non-linear regime $g \neq 0$

$$\begin{bmatrix} \frac{\kappa_1 + \kappa_2 + \kappa_3}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} & \frac{\kappa_1 - 2\kappa_2 + \kappa_3}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} \\ \frac{\kappa_1 - 2\kappa_2 + \kappa_3}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} & \kappa_1 + 4\kappa_2 + \kappa_3 + \frac{g(\kappa_1 - 2\kappa_2 + \kappa_3)^2}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} \end{bmatrix} = \begin{bmatrix} \phi_{11} & \phi_{12} \\ \phi_{21} & \phi_{22} \end{bmatrix}$$

Consistency requires that

$$\kappa_n = \frac{V_n}{1 + gV_n}$$

$$\phi_{12} = \phi_{21} \quad \text{AND} \quad \phi_{22} = \frac{2\phi_{11} - \phi_{12} + g\phi_{12}^2}{1 + g\phi_{11}}$$

If satisfied

Condition of physical admissibility of data

$$\frac{V_1}{1 + gV_1} + \frac{V_3}{1 + gV_3} = \frac{1}{3} \frac{2\phi_{11} + \phi_{12}}{1 + g\phi_{11}}$$

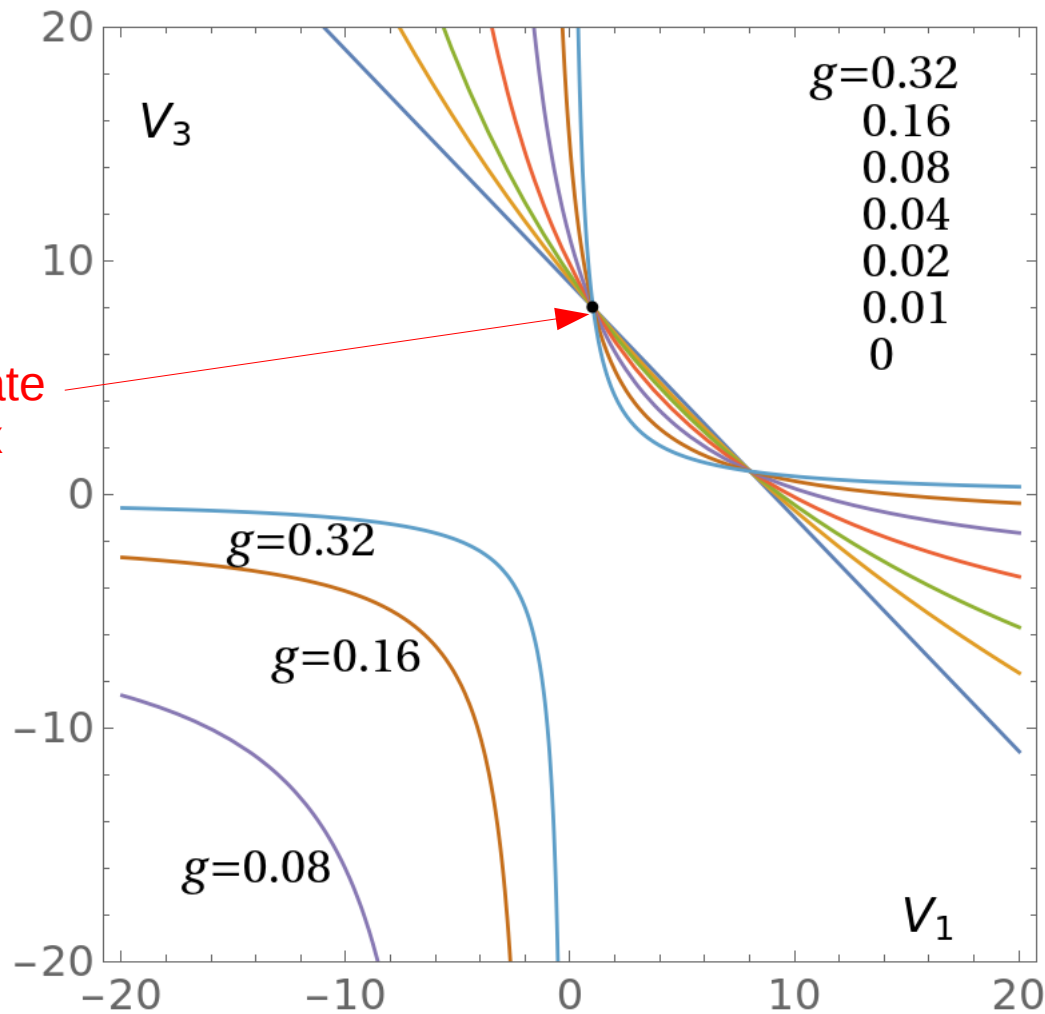
Still only two independent equations for three unknowns.

$$V_2 = \frac{\phi_{11} - \phi_{12}}{3 + g(2\phi_{11} + \phi_{12})}$$

Nonlinearity in the ISP did not force uniqueness

2d. Toy Problem 1

Solutions in the case of band-limited measurements



Loci of all points in the (V_1, V_3) plane that satisfy the nonlinear equations, assuming the data is physically-admissible (in range of the forward operator) for various values of the interaction parameter g .

The data were generated in each case using the same model shown by a circular dot in the plot.


2e. Toy Problem 1

(b) Non-band-limited measurements (u_1, u_3)

$$A = \begin{bmatrix} u_1 \\ u_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \end{bmatrix}, \quad B = [u_1 \quad u_3] = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

(b.i) Linear regime $g=0$

$$\begin{bmatrix} V_1 + V_2 + V_3 & V_1 - V_3 \\ V_1 - V_3 & V_1 + V_3 \end{bmatrix} = \begin{bmatrix} \phi_{11} & \phi_{12} \\ \phi_{21} & \phi_{22} \end{bmatrix}$$


$$\phi_{12} = \phi_{21}$$

If satisfied



$$V_1^{\text{inv}} = (\phi_{22} + \phi_{12})/2$$

$$V_2^{\text{inv}} = \phi_{11} - \phi_{22}$$

$$V_3^{\text{inv}} = (\phi_{22} - \phi_{12})/2$$

This is the only physical admissibility condition. Data matrix must be symmetric (reciprocity)

This is the unique inverse solution

2f. Toy Problem 1

(b.ii) Non-linear regime $g \neq 0$

$$\begin{bmatrix} \frac{\kappa_1 + \kappa_2 + \kappa_3}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} & \frac{\kappa_1 - \kappa_3}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} \\ \frac{\kappa_1 - \kappa_3}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} & \kappa_1 + \kappa_3 + \frac{g(\kappa_1 - \kappa_3)^2}{1 - g(\kappa_1 + \kappa_2 + \kappa_3)} \end{bmatrix} = \begin{bmatrix} \phi_{11} & \phi_{12} \\ \phi_{21} & \phi_{22} \end{bmatrix}$$

↓

$$\phi_{12} = \phi_{21}$$

↓ If satisfied

This condition must still be satisfied (reciprocity)

$$\kappa_1^{\text{inv}} = \frac{1}{2} \left(\phi_{22} + \phi_{12} \frac{1 - g\phi_{12}}{1 + g\phi_{11}} \right)$$

$$\kappa_2^{\text{inv}} = -\phi_{22} + \frac{\phi_{11} + g\phi_{12}^2}{1 + g\phi_{11}}$$

$$\kappa_3^{\text{inv}} = \frac{1}{2} \left(\phi_{22} - \phi_{12} \frac{1 + g\phi_{12}}{1 + g\phi_{11}} \right)$$

$$V_n^{(\text{inv})} = \kappa_n^{\text{inv}} / (1 - g\kappa_n^{\text{inv}})$$

This is the unique nonlinear inverse solution

2g. Toy Problem 1 Solutions in the case of non-band-limited measurements

$$g = 0.1$$

$$\phi_{12} \approx 2.5$$

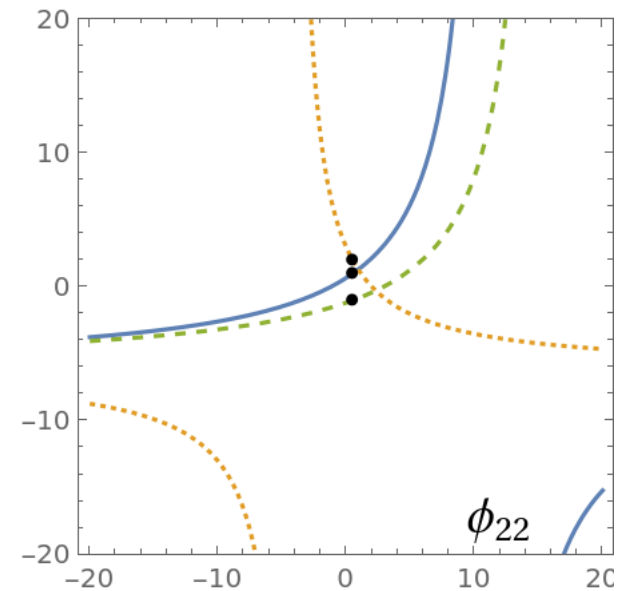
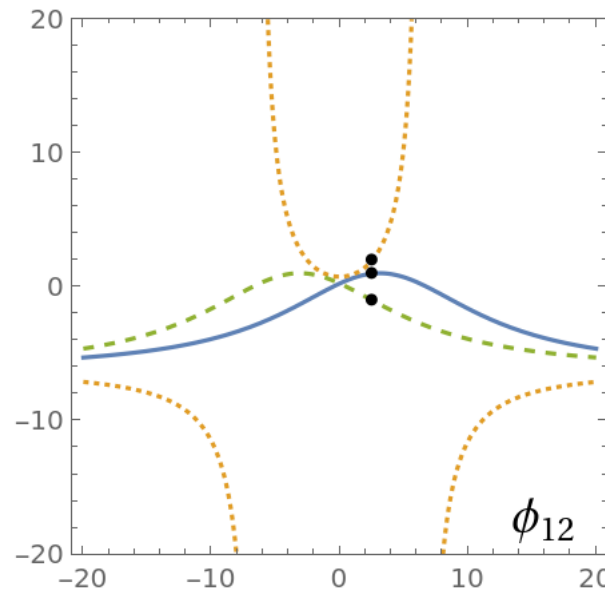
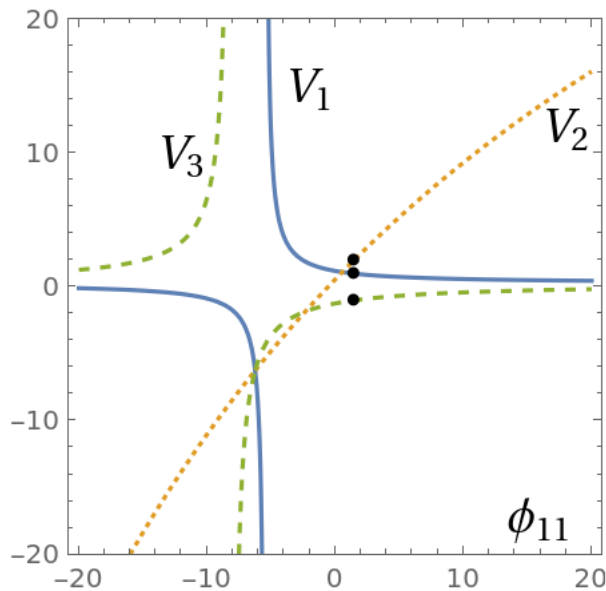
$$\phi_{11} \approx 1.5$$

$$\phi_{11} \approx 1.5$$

$$\phi_{22} \approx 0.5$$

$$\phi_{22} \approx 0.5$$

$$\phi_{12} \approx 2.5$$



$$(\phi_{11}, \phi_{12}, \phi_{22}) \approx (1.5, 2.5, 0.5) \iff (V_1, V_2, V_2) = (1, 2, -1)$$

2h. Toy Problem 1 Why the first measurement scheme was band-limited and the second was not? Select a pair u 's and form Hadamard products:

u_1 and u_2
(band-limited
scheme):

$$\mathbf{u}_1 \circ \mathbf{u}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{u}_1 \circ \mathbf{u}_2 = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 \circ \mathbf{u}_2 = \begin{bmatrix} 1 \\ 4 \\ 1 \end{bmatrix}$$

Two of these vectors are linearly-independent

u_1 and u_3
(not a
band-limited
scheme):

$$\mathbf{u}_1 \circ \mathbf{u}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{u}_1 \circ \mathbf{u}_3 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}, \quad \mathbf{u}_3 \circ \mathbf{u}_3 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

All three vectors are linearly-independent 20 / 51

In General:

$$\text{rank}[\mathbf{A} * \mathbf{B}] < N$$



Linear inverse problem is
band-limited
(under-determined)

$$\text{rank}[\mathbf{A} * \mathbf{B}] \geq N$$



Linear inverse problem is
not band-limited
(exactly determined or
over-determined)

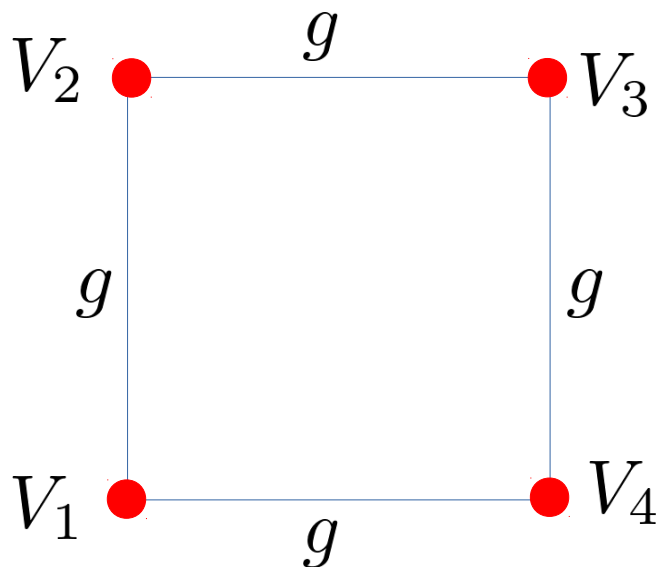
↑
Khatri-Rao product assuming each
matrix consists of just one block

$$A_{in} B_{nj} = (\mathbf{A} * \mathbf{B})_{(ij),n}$$

3a. Toy Problem 2 with 4 degrees of freedom

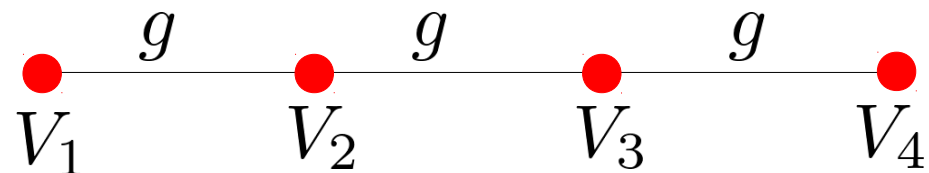
a) Cyclic tight-binding model

$$\mathbf{G} = \begin{bmatrix} 0 & g & 0 & g \\ g & 0 & g & 0 \\ 0 & g & 0 & g \\ g & 0 & g & 0 \end{bmatrix}$$



b) Chain tight-binding model

$$\mathbf{G} = \begin{bmatrix} 0 & g & 0 & 0 \\ g & 0 & g & 0 \\ 0 & g & 0 & g \\ 0 & 0 & g & 0 \end{bmatrix}$$



3b. Toy Problem 2. Measurement matrices

$$\mathbf{u}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 1 & -1 \\ 1 & -1 & 0 \end{bmatrix}$$

$$\text{rank}[\mathbf{A} * \mathbf{B}] = 3 < N = 4$$

The linear inverse problem is under-determined:
3 linearly-independent equations and 4 unknowns

3c. Toy Problem 2. Linear solution ($g=0$)

The data matrix is 3x3 and therefore has 9 elements. Physical admissibility conditions are:

$$\phi_{ij} = \phi_{ji} \leftarrow \text{Reciprocity}$$

$$\phi_{13} = \phi_{23} , \quad \phi_{12} + \phi_{22} = 2\phi_{33} , \quad \phi_{11} = \phi_{22} \leftarrow \text{Additional conditions}$$

So, only 3 data matrix elements are independent.



If conditions hold

$$V_1^{\text{inv}} = \frac{1}{2} (\phi_{33} + \phi_{23})$$

$$V_3^{\text{inv}} = \frac{1}{2} (\phi_{33} - \phi_{23})$$

$$V_2^{\text{inv}} + V_4^{\text{inv}} = \phi_{22} - \phi_{33}$$

So, the linearized solution is indeed non-unique

3d. Toy Problem 2.

Nonlinear solution – Cyclic interaction

$$\frac{\phi_{13}}{\phi_{23}} = \frac{1 + g(\phi_{22} - 3\phi_{33}) + g^2(\phi_{22}\phi_{33} - \phi_{23}^2)}{1 - g\phi_{22} - g^2\phi_{23}^2 - g\phi_{33} + g^2\phi_{22}\phi_{33}}$$

$$\phi_{12} = \frac{2\phi_{33} - \phi_{22} + g(\phi_{23}^2 - \phi_{22}\phi_{33} - \phi_{13}\phi_{23})}{1 - g\phi_{33}}$$

$$\phi_{11}(\phi_{22} - \phi_{33}) = \phi_{12}^2 - \phi_{13}^2 + \phi_{23}(2\phi_{13} - \phi_{23}) + \phi_{33}(\phi_{22} - 2\phi_{12})$$



$$V_1^{\text{inv}} = \frac{1}{2} \frac{(\phi_{12} + \phi_{22})\phi_{33} - (\phi_{13} + \phi_{23})\phi_{23}}{\phi_{12} + \phi_{22} - 2\phi_{33}}$$

$$V_3^{\text{inv}} = \frac{1}{2} \frac{(\phi_{12} + \phi_{22})\phi_{33} - (\phi_{13} + \phi_{23})\phi_{23}}{\phi_{12} + \phi_{22} + 2\phi_{33}}$$

$$V_2^{\text{inv}} + V_4^{\text{inv}} = \frac{\phi_{13}(\phi_{22} - \phi_{23}) + \phi_{23}(\phi_{23} - \phi_{12}) + \phi_{33}(\phi_{12} - \phi_{22})}{\phi_{12} + \phi_{13} + \phi_{22} - 4\phi_{33} + 2g(\phi_{22}\phi_{33} - \phi_{23}^3)}$$

Admissibility conditions
(in addition to reciprocity)

Nonlinear inverse solution
is still non-unique

3e. Toy problem 2.

Nonlinear solution - Tight-binding in a chain

$$V_n^{\text{inv}} = \frac{\mathcal{N}_n}{g\mathcal{D}_n}, \quad n = 1, 2, 3, 4$$

$$\mathcal{N}_n = a_n + b_n g + c_n g^2 + d_n g^3 + e_n g^4$$

$$\mathcal{D}_n = p_n + q_n g + r_n g^2 + s_n g^3 + t_n g^4$$

The coefficients are combinations of rational functions and square root and some also depend on g .

Formulas are quite lengthy...

$$a_1 = 2(1 - R) ;$$

$$b_1 = 2[\phi_{11} + 8\phi_{23} + 7\phi_{33} - 2\phi_{22} + (3\phi_{33} - \phi_{23})R] ;$$

$$c_1 = \phi_{11}(6\phi_{23} - \phi_{22} - \phi_{33}) + \phi_{22}(\phi_{22} - 12\phi_{23} - 19\phi_{33}) + 28\phi_{23}^2 \\ + 2\phi_{33}(5\phi_{23} - 6\phi_{33}) + 2[\phi_{23}(2\phi_{33} + \phi_{23}) - \phi_{33}(2\phi_{33} + \phi_{22})]R ;$$

$$d_1 = 2[\phi_{11}(3\phi_{23}^2 - \phi_{22}\phi_{23} - \phi_{22}\phi_{33} - \phi_{23}\phi_{33}) + \phi_{23}(8\phi_{23}^2 - 3\phi_{23}\phi_{33} - 2\phi_{33}^2) \\ + \phi_{22}(\phi_{22}\phi_{23} + 4\phi_{22}\phi_{33} + 7\phi_{33}^2 - 9\phi_{23}\phi_{33} - 6\phi_{23}^2) \\ + (\phi_{22}\phi_{33}^2 + \phi_{23}^3 - \phi_{23}^2\phi_{33} - \phi_{22}\phi_{23}\phi_{33})R] ;$$

$$e_1 = \phi_{11}\phi_{22}(\phi_{33}^2 + \phi_{22}\phi_{33} - 2\phi_{23}\phi_{33} - \phi_{23}^2) + \phi_{23}\phi_{33}(4\phi_{22}^2 - \phi_{11}\phi_{23} - 2\phi_{23}^2) \\ + \phi_{22}\phi_{23}(\phi_{23}\phi_{33} + 2\phi_{33}^2 + \phi_{22}\phi_{23} - 4\phi_{23}^2) - \phi_{22}^2\phi_{33}(3\phi_{33} + \phi_{22}) \\ + 2\phi_{23}^3(\phi_{11} + \phi_{23}) ;$$

$$p_1 = 32 ;$$

$$q_1 = 8(\phi_{11} + 8\phi_{23} - 4\phi_{33} - 5\phi_{22}) ;$$

$$r_1 = 8(\phi_{33} + 2\phi_{22} - 2\phi_{23} - \phi_{11})(\phi_{22} + \phi_{33} - 2\phi_{23}) ;$$

$$s_1 = 2(\phi_{11} - \phi_{22})(\phi_{22} + \phi_{33} - 2\phi_{23})^2 ;$$

$$t_1 = 0$$

$$a_2 = 2[\phi_{11} - \phi_{22} + 2(\phi_{23} + \phi_{33}) - 2(\phi_{23} + \phi_{33})R] ;$$

$$b_2 = \phi_{11}(6\phi_{23} - \phi_{22} - \phi_{33}) + \phi_{22}(\phi_{22} - 6\phi_{23} - 11\phi_{33}) + 8\phi_{33}^2 + 4\phi_{23}^2 \\ + 4(\phi_{33}^2 + \phi_{22}\phi_{33} - 2\phi_{23}^2)R ;$$

$$c_2 = 2[\phi_{11}(3\phi_{23}^2 - \phi_{22}\phi_{23} - \phi_{22}\phi_{33} - \phi_{23}\phi_{33}) + \phi_{22}(\phi_{22}\phi_{23} + 3\phi_{22}\phi_{33} \\ - 3\phi_{23}^2 - 3\phi_{23}\phi_{33}) + 2\phi_{23}(\phi_{23}\phi_{33} + 3\phi_{33}^2 - \phi_{23}^2) - 4\phi_{33}^3 \\ + 2(\phi_{33} - \phi_{23})(\phi_{23}^2 - \phi_{22}\phi_{33})R] ;$$

$$d_2 = (\phi_{22}\phi_{33} - \phi_{23}^2) \\ \times [4(\phi_{23} - \phi_{33})^2 + \phi_{22}(2\phi_{23} - \phi_{33}) + \phi_{11}(\phi_{22} - 2\phi_{23} + \phi_{33}) - \phi_{22}^2] ;$$

$$e_2 = 0 ;$$

$$p_2 = \phi_{11} - \phi_{22} + 4(\phi_{23} + \phi_{33}) ;$$

$$q_2 = 4\phi_{23}(\phi_{11} + 4\phi_{23} - \phi_{22}) + 8(3\phi_{23} - \phi_{22})\phi_{33} + 16\phi_{33}^2 ;$$

$$r_2 = 2[3\phi_{23}^2(\phi_{11} + 4\phi_{23} - \phi_{22}) + \phi_{33}(\phi_{22}^2 - \phi_{11}\phi_{22} + 16\phi_{23}^2 - 12\phi_{22}\phi_{23}) \\ - 8\phi_{33}^2(\phi_{22} + \phi_{33})] ;$$

$$s_2 = 4(\phi_{23}^2 - \phi_{22}\phi_{33})[\phi_{23}(\phi_{11} + 4\phi_{23} - \phi_{22}) + 2\phi_{33}(\phi_{23} - \phi_{22}) - 4\phi_{33}^2] ;$$

$$t_2 = (\phi_{11} - \phi_{22} + 4\phi_{23} - 4\phi_{33})(\phi_{23}^2 - \phi_{22}\phi_{33})^2$$

$$a_3 = 2(R - 1) ;$$

$$b_3 = \phi_{11} + \phi_{22} - 2\phi_{23} ;$$

$$c_3 = d_3 = e_3 = 0 ;$$

$$p_3 = 8 ;$$

$$q_3 = 2(\phi_{11} - \phi_{22}) ;$$

$$r_3 = s_3 = t_3 = 0$$

$$a_4 = 2[\phi_{22} - \phi_{11} - 2(\phi_{23} + \phi_{33}) + 2(\phi_{23} + \phi_{33})R] ;$$

$$b_4 = 2[\phi_{11}(\phi_{22} - 2\phi_{23} + \phi_{33}) + \phi_{22}(4\phi_{23} - \phi_{22}) + \phi_{33}(7\phi_{22} + 2\phi_{23} - 4\phi_{33}) + 2(\phi_{23}^2 - 2\phi_{33}^2 - \phi_{33}(\phi_{22} + 2\phi_{23}))R] ;$$

$$c_4 = 4[\phi_{11}\phi_{23}(\phi_{22} + \phi_{33}) + \phi_{22}(3\phi_{23}^2 + 3\phi_{23}\phi_{33} + 3\phi_{33}^2) - \phi_{22}^2(\phi_{23} + 3\phi_{33}) \\ + \phi_{23}(2\phi_{23}^2 - 3\phi_{23}\phi_{33} - 6\phi_{33}^2) + (\phi_{22}\phi_{33}(\phi_{23} + 3\phi_{33}) - \phi_{23}^2(\phi_{23} + 3\phi_{33}))R] ;$$

$$d_4 = 2[(\phi_{22}\phi_{33} - \phi_{23}^2)(\phi_{22}^2 - \phi_{11}(\phi_{22} + 2\phi_{23} + \phi_{33}) + 10\phi_{23}\phi_{33} - \phi_{22}(4\phi_{23} + 3\phi_{33}) + 2(\phi_{23}^2 - \phi_{22}\phi_{33})R)] ;$$

$$e_4 = 2(\phi_{11} + \phi_{22} - 2\phi_{23})(\phi_{23}^2 - \phi_{22}\phi_{33})^2 ;$$

$$p_4 = \phi_{11} - \phi_{22} + 4(\phi_{23} + \phi_{33}) ;$$

$$q_4 = 4(\phi_{23}(\phi_{11} - \phi_{22} + 4\phi_{23}) - 2(\phi_{22} - 3\phi_{23})\phi_{33} + 4\phi_{33}^2) ;$$

$$r_4 = 2[3\phi_{23}^2(\phi_{11} + 4\phi_{23} - \phi_{22}) + \phi_{33}(16\phi_{23}^2 + \phi_{22}^2) - \phi_{22}\phi_{33}(12\phi_{23} + \phi_{11}) - 8\phi_{33}^2(\phi_{22} + \phi_{33})] ;$$

$$s_4 = 4(\phi_{23}^2 - \phi_{22}\phi_{33})[\phi_{23}(\phi_{11} - \phi_{22} + 4\phi_{23}) + 2\phi_{33}(\phi_{23} - \phi_{22}) - 4\phi_{33}^2] ;$$

$$t_4 = (\phi_{11} - \phi_{22} + 4\phi_{23} - 4\phi_{33})(\phi_{23}^2 - \phi_{22}\phi_{33})^2$$

$$R = \sqrt{1 - 2g(\phi_{11} + \phi_{23} - 2\phi_{33}) + g^2(\phi_{23}^2 - \phi_{22}\phi_{33} + \phi_{11}\phi_{22} - 2\phi_{11}\phi_{23} + \phi_{11}\phi_{33})}$$

3f. Toy Problem 2.

Nonlinear solution – Tight-binding interaction in a chain Expansion in powers of g

$$V_1^{\text{inv}} = \frac{\phi_{11} - \phi_{22}}{8} + \frac{\phi_{33} + \phi_{23}}{2} + O(g)$$

$$V_3^{\text{inv}} = \frac{\phi_{22} - \phi_{11}}{8} + \frac{\phi_{33} - \phi_{23}}{2} + O(g)$$

$$V_2^{\text{inv}} = \frac{2}{g} \frac{\phi_{11} - \phi_{22}}{\phi_{11} - \phi_{22} + 4(\phi_{23} + \phi_{33})} + \frac{\phi_{11} - \phi_{22} + 4(\phi_{23} - \phi_{33})}{(\phi_{11} - \phi_{22} + 4(\phi_{23} + \phi_{33}))^2} \left[\phi_{22}^2 + \phi_{22}(2\phi_{23} + \phi_{33}) \right. \\ \left. - \phi_{11}(\phi_{22} - 2\phi_{23} - 3\phi_{33}) - 4\phi_{33}(\phi_{23} + \phi_{33}) \right] + O(g^1)$$

$$V_4^{\text{inv}} = \frac{2}{g} \frac{\phi_{22} - \phi_{11}}{\phi_{11} - \phi_{22} + 4(\phi_{23} + \phi_{33})} + \frac{2}{(\phi_{11} - \phi_{22} + 4(\phi_{23} + \phi_{33}))^2} \\ \times \left[\phi_{22}(\phi_{11} - \phi_{22})(\phi_{11} - \phi_{22} + 4\phi_{23}) + 4\phi_{23}\phi_{33} \times (\phi_{11} + 3\phi_{22}) \right. \\ \left. + 8\phi_{33}^2(\phi_{11} + \phi_{22} - 2(\phi_{23} + \phi_{33})) - \phi_{33}(\phi_{11} - \phi_{22})^2 \right] + O(g^1)$$

Now the solution
is unique if $g \neq 0$

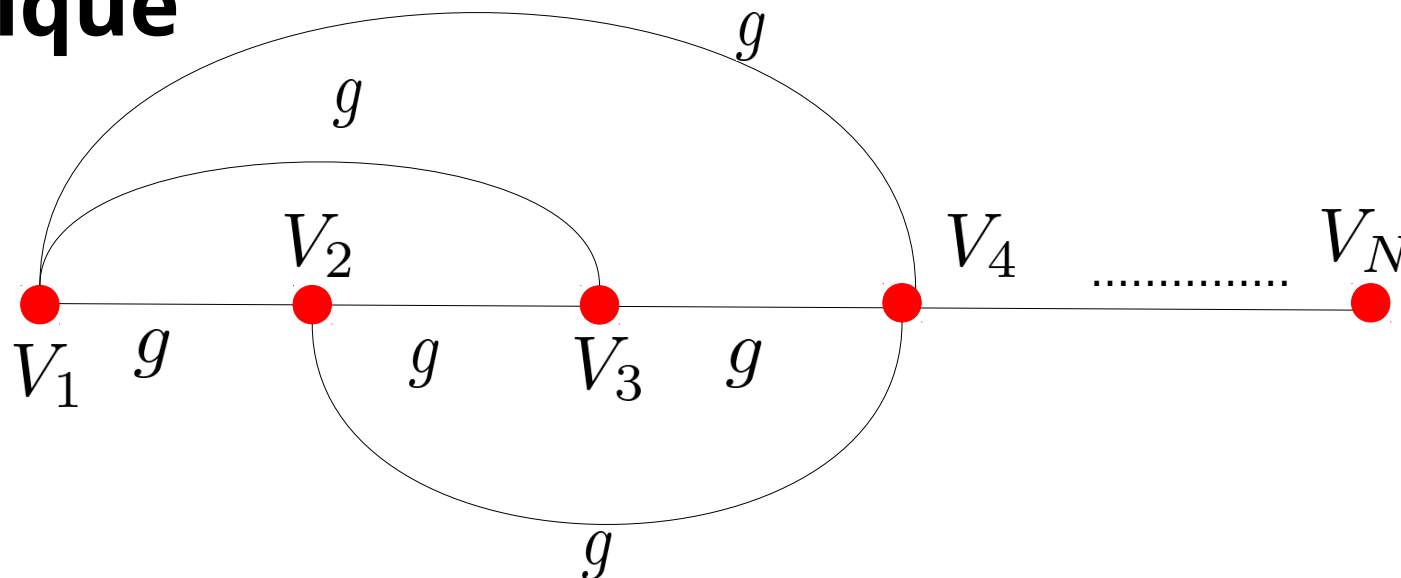
4a. Toy Problem 3.

Linear chain with N degrees of freedom;

Interaction on a fully-connected graph;

The “chain” geometry is only important for measurement matrix definition;

Inverse problem on a fully connected graph can be analytically solved if the solution is unique



4b. Toy Problem 3.

$$G_{nn'} = g(1 - \delta_{nn'})$$

$$T_{nn'} = \kappa_n \delta_{nn'} + g \frac{\kappa_n \kappa_{n'}}{1 - gS}, \quad 1 \leq n, n' \leq N$$

$$\kappa_n = \frac{V_n}{1 + gV_n}, \quad S = \sum_{n=1}^N \kappa_n$$

$$A_{ln} = e^{-i\frac{2\pi}{N}ln}, \quad B_{nl} = e^{i\frac{2\pi}{N}nl}, \quad -L \leq l \leq L$$

We send plane waves with the wave number $k = 2\pi L/Nh$ at different angles to the chain. Here h is the spacing in the chain. The wavelength is $\lambda = Nh/L$.

4c. Toy Problem 3. Linear Regime $g=0$.

$$T_{nn'} = V_n \delta_{nn'}$$

$$\sum_{n=1}^N A_{ln} V_n B_{nm} = \phi_{lm}, \quad -L \leq l, m \leq L$$

$$\sum_{n=1}^N e^{-i\frac{2\pi}{N}ln} V_n e^{i\frac{2\pi}{N}mn} = \phi_{lm}$$

$$\tilde{V}_{m-l} = \phi_{lm} \quad \text{where} \quad \tilde{V}_m = \sum_{n=1}^N V_n e^{i\frac{2\pi}{N}nm}$$

$(2L + 1)^2$ equations, but not all are independent

So, we know from data all discrete Fourier coefficients of V_n in the band $-2L \leq m \leq 2L$. If $2L \geq M = (N - 1)/2$ (assuming N is odd), then we know all DFT coefficients and can invert the DFT uniquely. If $2L < M$, some DFT coefficients of V_n are fundamentally unknown. The minimum- L_2 norm solution is low-band pass-filtered version of V_n :

Minimum norm inverse solution $\rightarrow V_n^{\text{inv}} = \frac{1}{N} \sum_{m=-2L}^{2L} \tilde{V}_m e^{-i\frac{2\pi}{N}nm}$

4d. Toy Problem 3. Nonlinear Regime $g \neq 0$.

$$\tilde{\kappa}_m^{\text{inv}} = \begin{cases} \frac{\phi_{0m}}{1 + g\phi_{00}} & , \quad -L \leq m \leq L \\ \phi_{-L, m-L} - g \frac{\phi_{0L} \phi_{0, m-L}}{1 + g\phi_{00}} & , \quad L < m \leq 2L \\ \phi_{L, m+L} - g \frac{\phi_{0, -L} \phi_{0, m+L}}{1 + g\phi_{00}} & , \quad -2L \leq m < -L \\ \text{Unknown} & , \quad m > |2L| \end{cases}$$

Here $\tilde{\kappa}_m = \sum_{n=1}^N \kappa_n e^{i \frac{2\pi}{N} nm}$, $\kappa_n = \frac{V_n}{1 + gV_n}$

If all $\tilde{\kappa}_m$ are known with $|m| \leq M = (N - 1)/2$

$$\kappa_n^{\text{inv}} = \frac{1}{N} \sum_{m=-M}^M \tilde{\kappa}_m e^{-i \frac{2\pi}{N} nm} , \quad V_n^{\text{inv}} = \frac{\kappa_n^{\text{inv}}}{1 - g\kappa_n^{\text{inv}}}$$

4d. Toy Problem 3. Nonlinear Regime $g \neq 0$ (cont.)

If NOT all $\tilde{\kappa}_m$ are known with $|m| \leq M = (N - 1)/2$
we must make some guess about the coefficients that are unknown:

- Zero
- Random
- See solution so the norm of V is minimized (more difficult)

If we set the unknown DFT coefficients to 0, then

$$\kappa_n^{\text{inv}} = \frac{1}{N} \sum_{m=-2L}^{2L} \tilde{\kappa}_m e^{-i\frac{2\pi}{N}nm}, \quad V_n^{\text{inv}} = \frac{\kappa_n^{\text{inv}}}{1 - g\kappa_n^{\text{inv}}}$$

If we do this, here is what would happen:

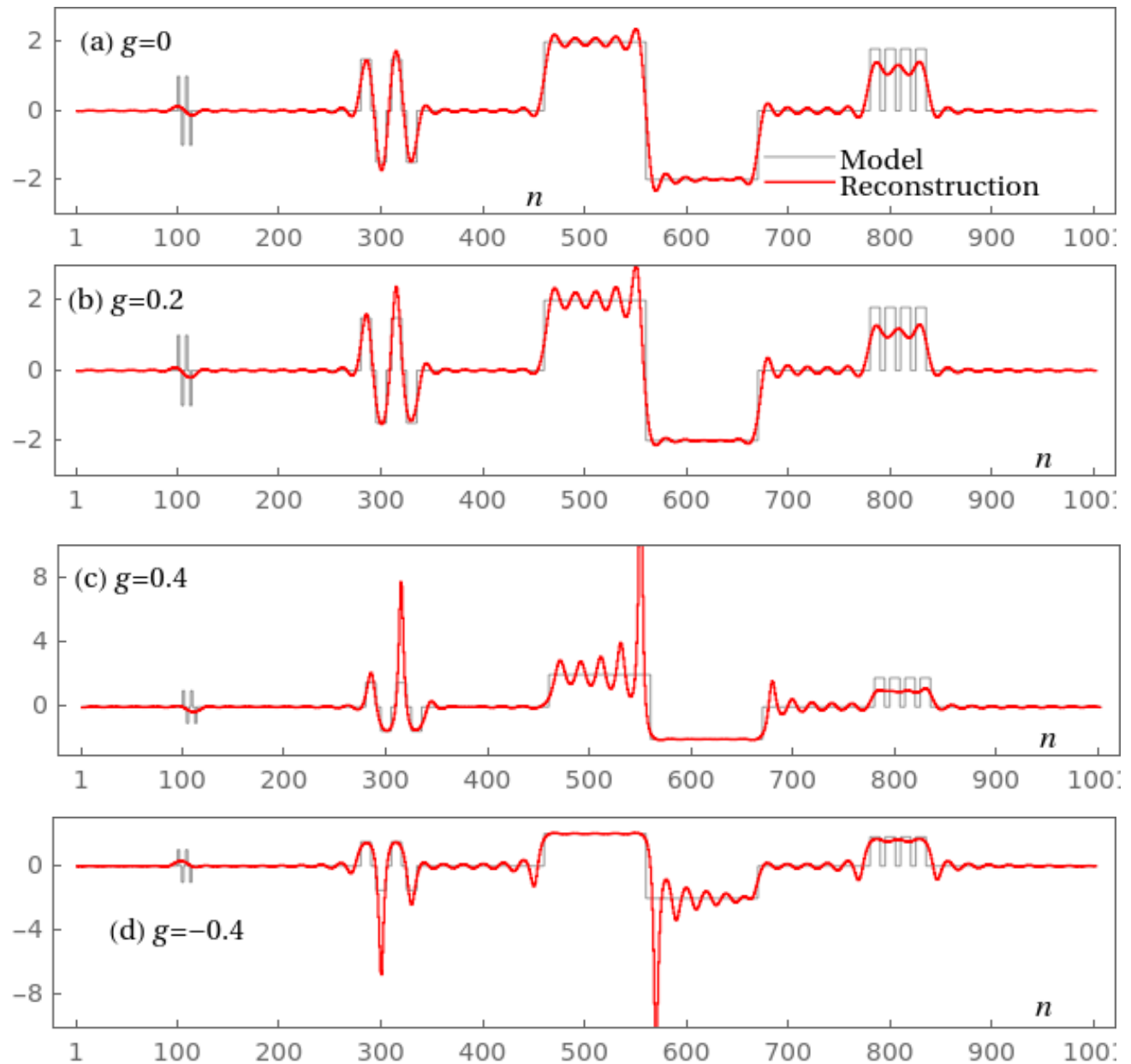
$$N = 1,001$$

$$M = \frac{N - 1}{2} = 500$$

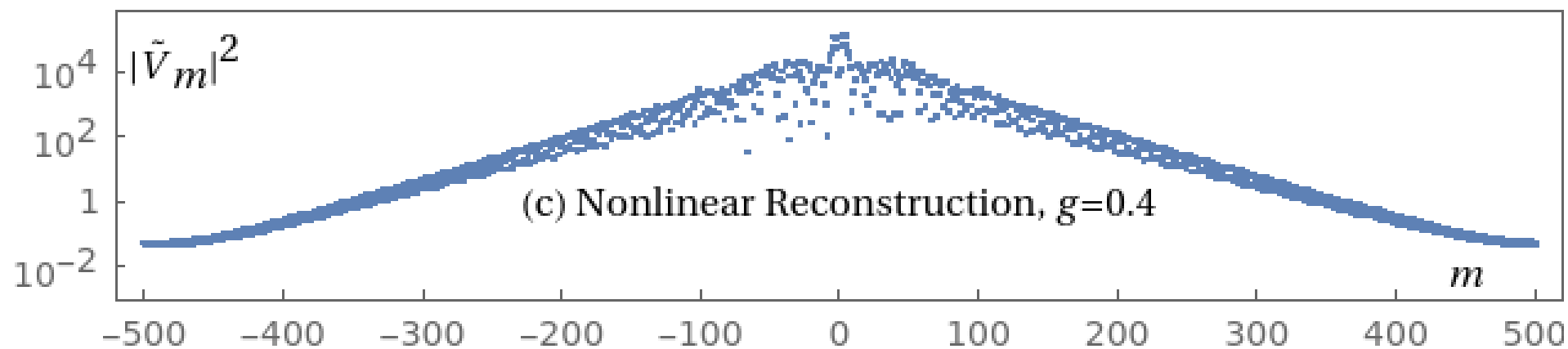
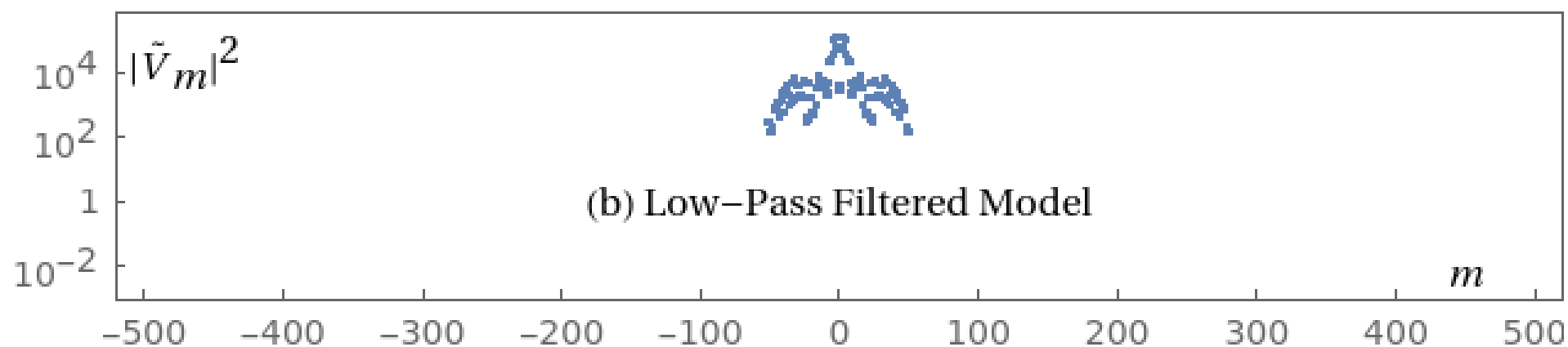
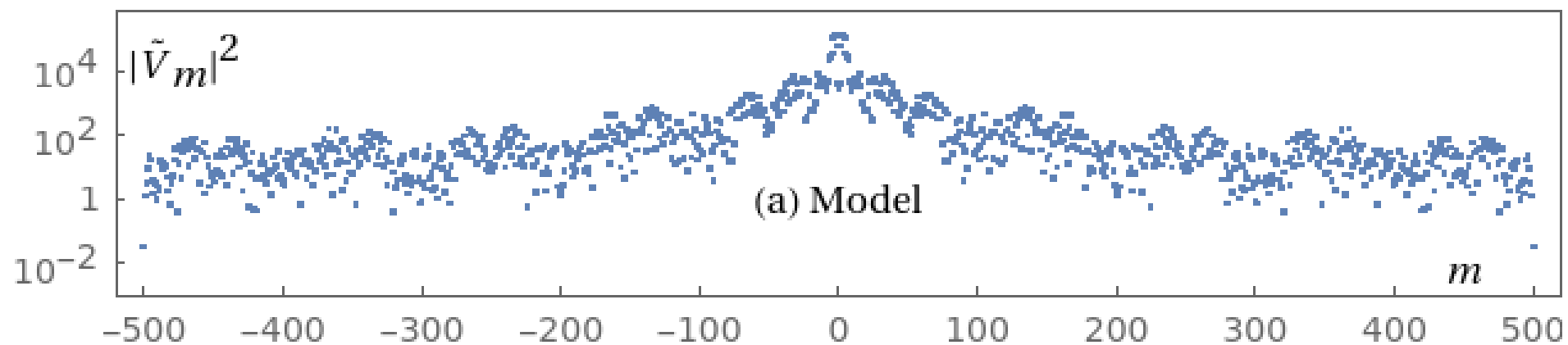
$$L = 25$$

$$M/2L = 10$$

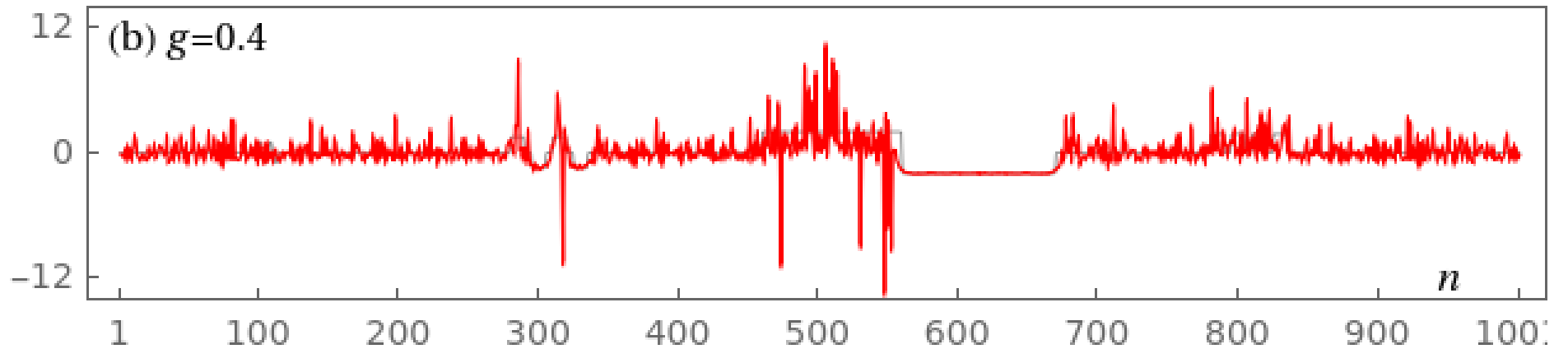
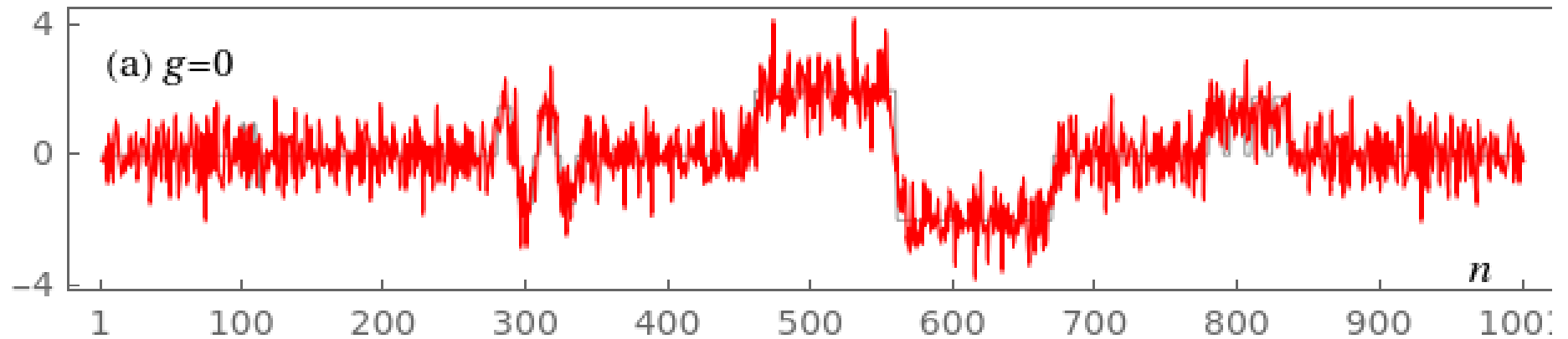
Only about 1/10 of
DFT coefficients
are known
(linear problem
is strongly
band-limited)



Unknown coefficients set to 0
Not the minimum norm of V solution.



Toy Problem 3: This is what happens if we fill the unknown coefficients with random values, which does not make sense but we tried it anyway
 $2L/M=0.1$

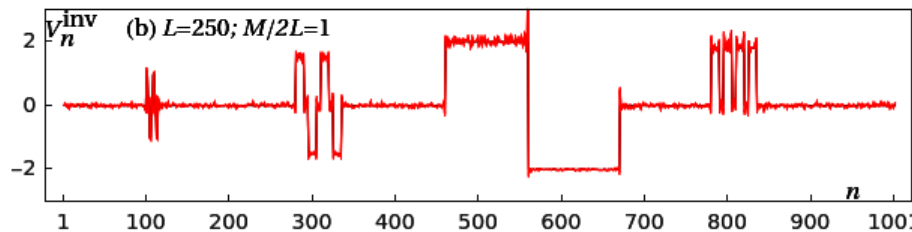
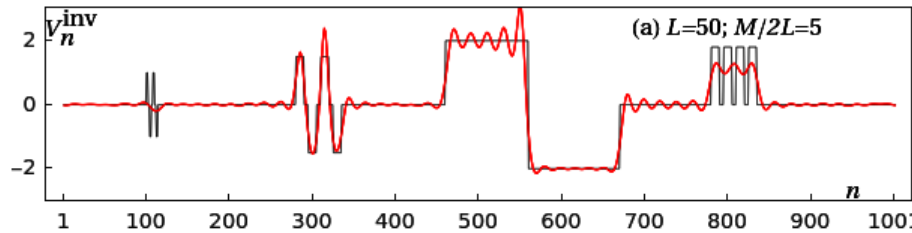


TOY PROBLEM 3: Reconstructions with noise in the known coefficients (unknown are set to 0)

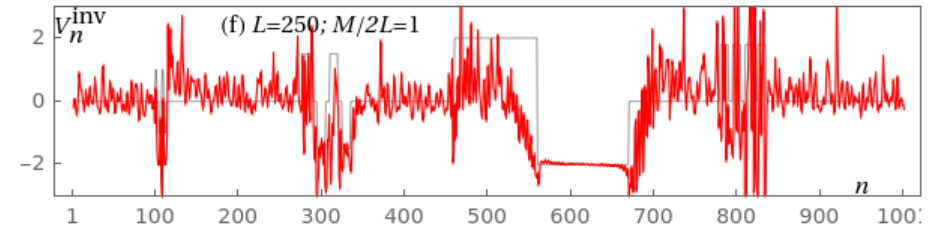
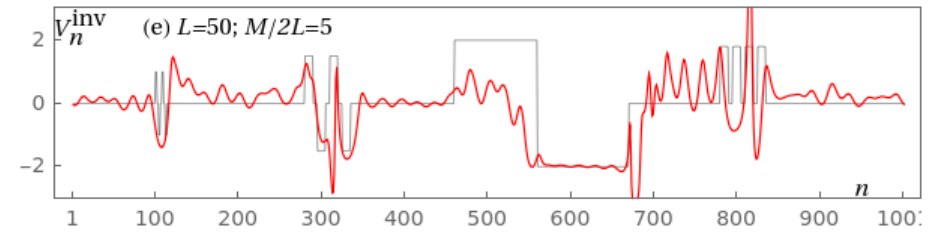
$$\phi_{jl} \longrightarrow \phi_{jl} + RZ \sqrt{\langle |\tilde{\kappa}|^2 \rangle} \quad P[|Z|] = \sqrt{2/\pi} \exp(-|Z|^2/2)$$

Phase of Z is random

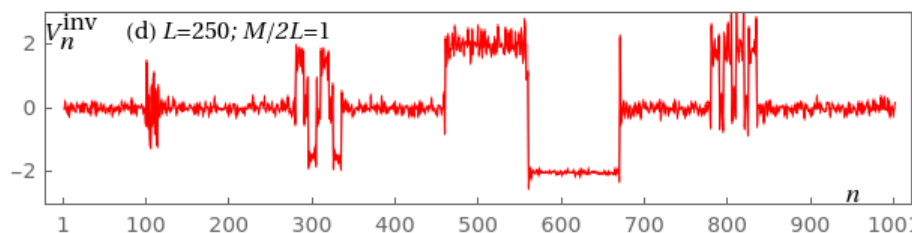
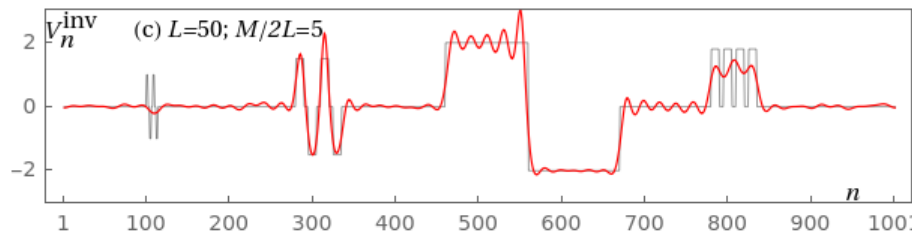
$g=0.2, R=0.1$



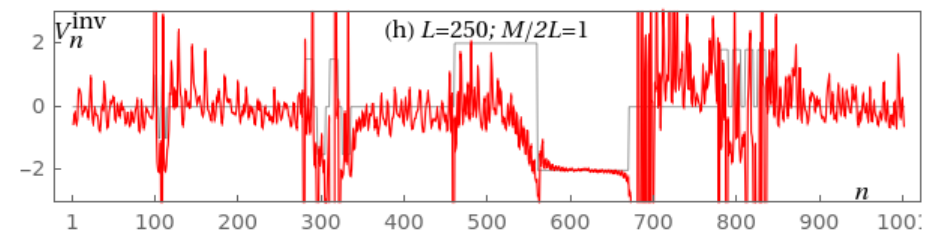
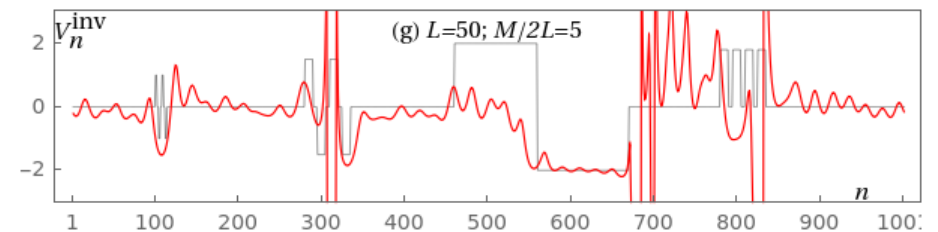
$g=0.4, R=0.1$



$g=0.2, R=0.2$



$g=0.4, R=0.2$



5a. Distorted Born Approximation and Tangent Spaces

$$U = D + V$$

Annotations:
- Blue arrow pointing to U : Total potential
- Red arrow pointing to D : Some initial guess
- Green arrow pointing to V : Small deviation from initial guess

$$T[U] = T[D + V] \approx T[D] + S[D] V S^T[D]$$

where

$$S[X] = (I - XG)^{-1}, \quad S^T[X] = (I - GX)^{-1}$$

$$(AS[D]) V (S^T[D]B) = \Phi - AT[D]B \equiv \Psi[D]$$

Annotations:
- Blue arrow pointing to V : Linear equation for V
- Red arrow pointing to $\Psi[D]$: New data matrix (known)

Linear equation for V

5b. Distorted Born Approximation

$$U = D + V$$

Annotations:
- U : Total potential (blue arrow)
- D : Some initial guess (red arrow)
- V : Small deviation from initial guess (green arrow)

$$T[U] = T[D + V] \approx T[D] + S[D] V S^T[D]$$

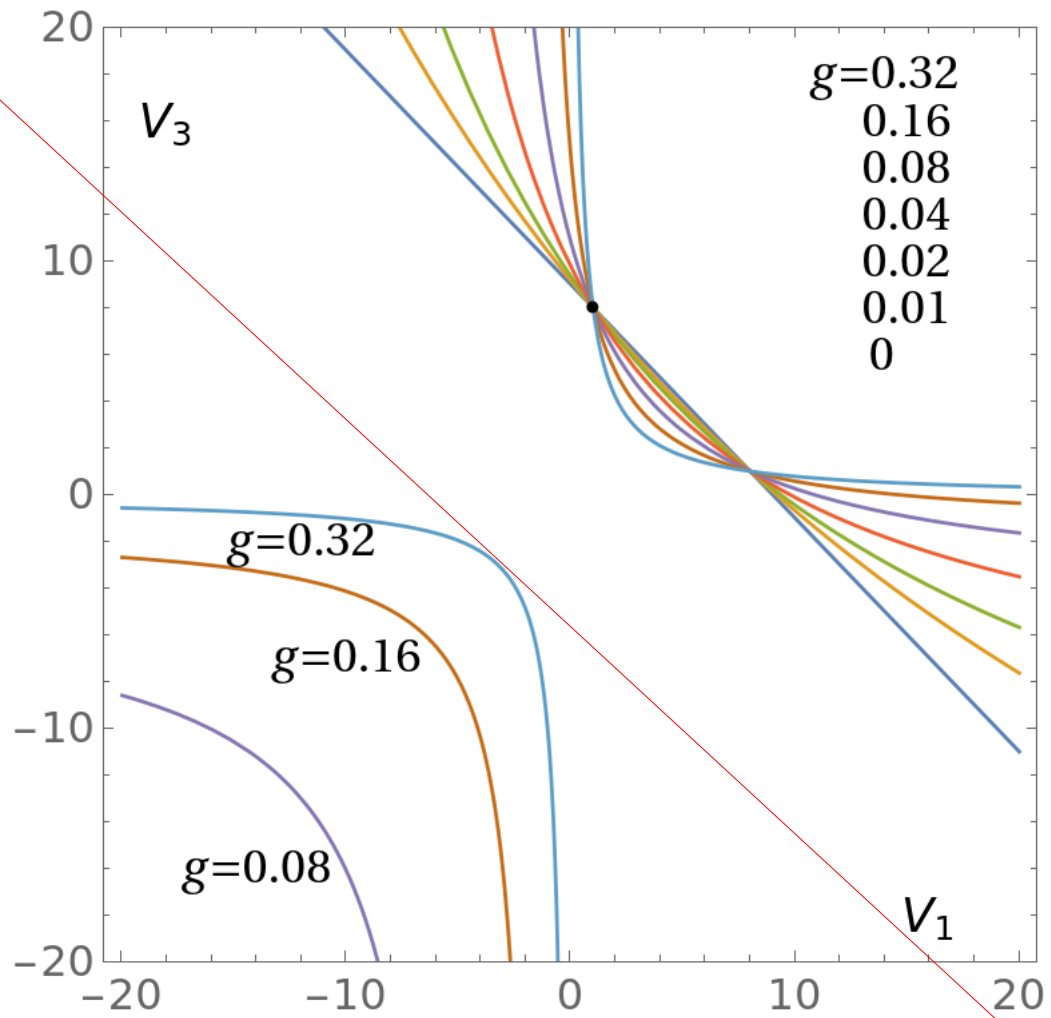
where

$$S[X] = (I - XG)^{-1}, \quad S^T[X] = (I - GX)^{-1}$$

$$(AS[D]) V (S^T[D]B) = \Phi - AT[D]B \equiv \Psi[D]$$

New data matrix (known)

Linear equation for V



6a. Example 4 -- Realistic Interaction

Chain with $N=51 \times 51 = 2601$ voxels/particles

$$G_{nm} = g(1 - \delta_{nm}) \frac{e^{ik|\mathbf{r}_n - \mathbf{r}_m|}}{|\mathbf{r}_n - \mathbf{r}_m|/h}, \quad k = \frac{\omega}{c}$$

Dimensionless parameter characterizing the strength of interaction
(multiple scattering)

$$A_{ln} = e^{-i(l/L)kz_n}, \quad B_{nl} = e^{i(l/L)kz_n}$$

$$-L \leq l \leq L, \quad 1 \leq n \leq N, \quad z_n = nh$$

$(l/L)k$ ← projection of the incident (detected) wave vector onto the chain

$$\sum_n (\mathbf{AS}[\mathbf{D}])_{ln} V_n (\mathbf{S}^T[\mathbf{D}]\mathbf{B})_{nm} = \psi_{lm}$$

(Distorted Born)

6b. Example 4: Pseudo-inverse for V using shifted Born

$$W_{nm}[D] = \left((AS[D])^* (AS[D]) \right)_{nm} \left((S^T[D]B) (S^T[D]B)^* \right)_{mn}$$

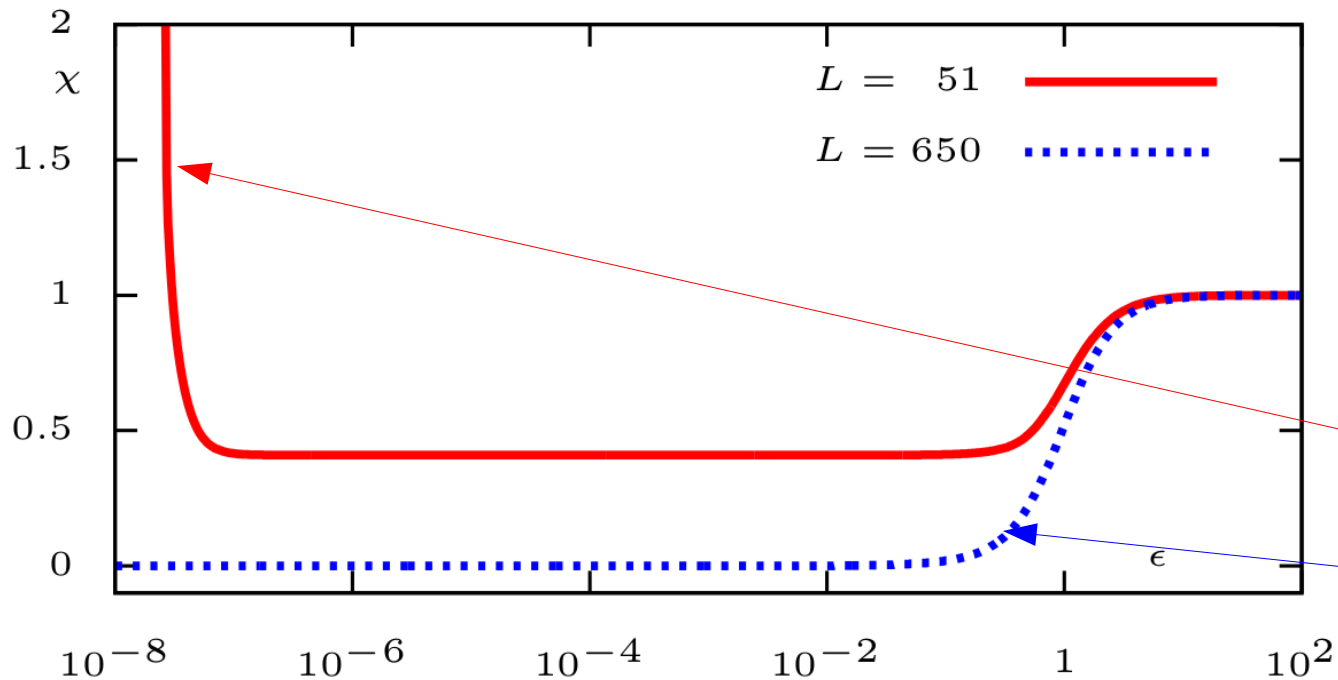
v is vector of diagonal elements of V

$b[D]$ is data matrix $\Psi[D]$ unrolled, i.e., $b_{(lm)} = \psi_{l,m}$

$$[W[D] + \lambda^2 I]v = b[D]$$

Tikhonov regularization
parameter

6c. Example 4: Pseudo-inverse at D=0, inverse crime



Error of the linearized
pseudo-inverse of a model
(shown below)
at D=0
with N=1,601

Inverse crime

Band-limited measurements

Non-band-limited
measurements

Here “chi” is shown where “chi-squared” is

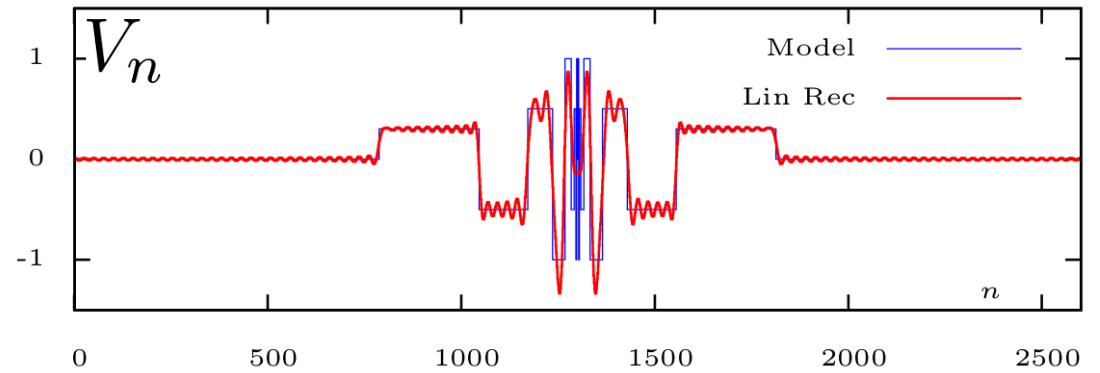
$$\chi^2 = \frac{\sum_n |V_n^{\text{inv}} - V_n^{\text{mod}}|^2}{\sum_n |V_n^{\text{mod}}|^2}$$

6c. Example 4: Pseudo-inverse reconstructions with band-limited measurements

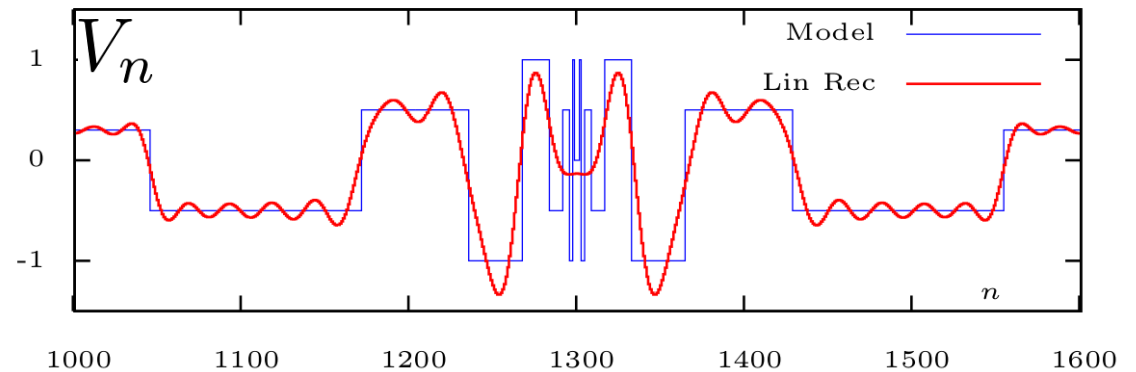
$L=51$

(inverse crime)

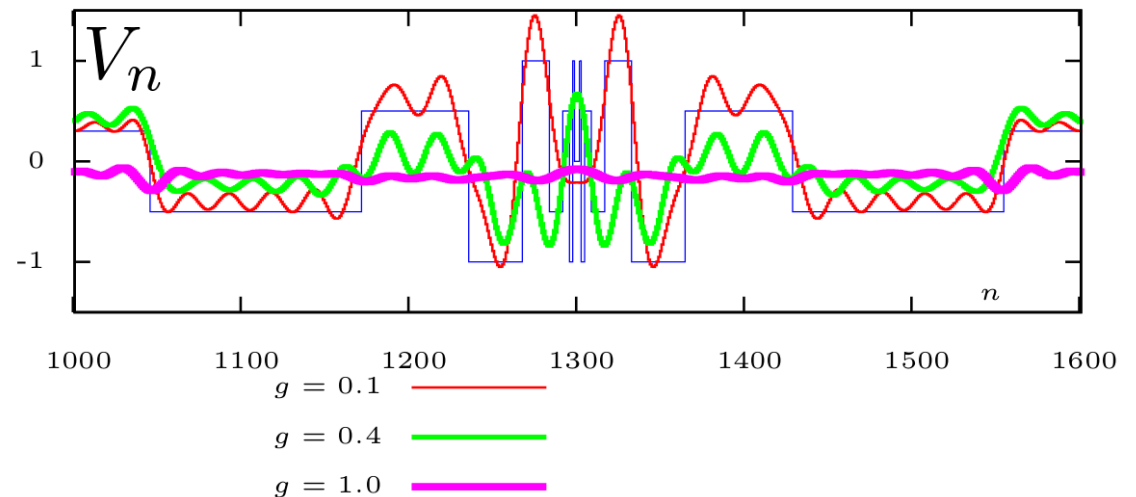
(a) Linearized reconstruction with inverse crime data



(b) Same as in (a) zoom-in



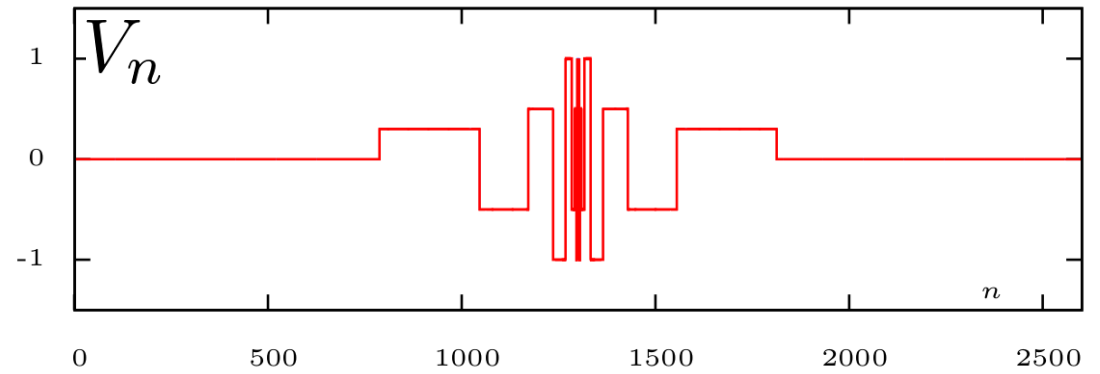
(c) Linearized reconstructions with exact data



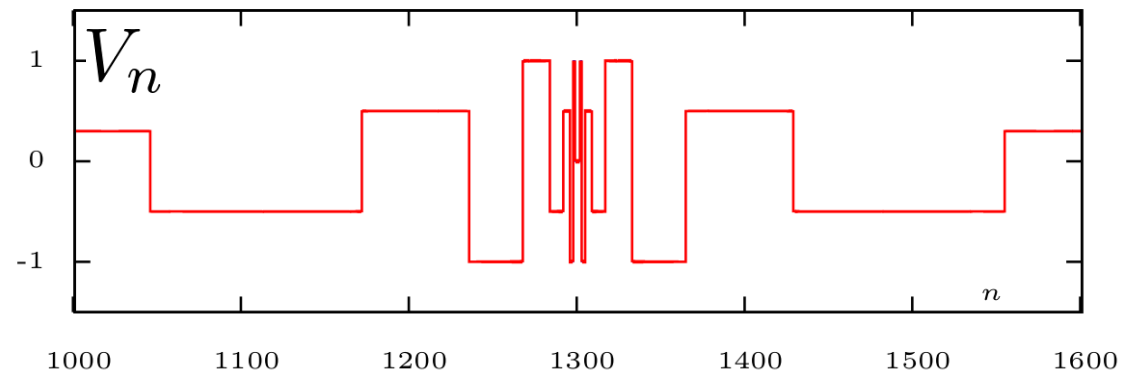
6d. Example 4: Pseudoinverse reconstructions with non-band-limited measurements

$L=650$

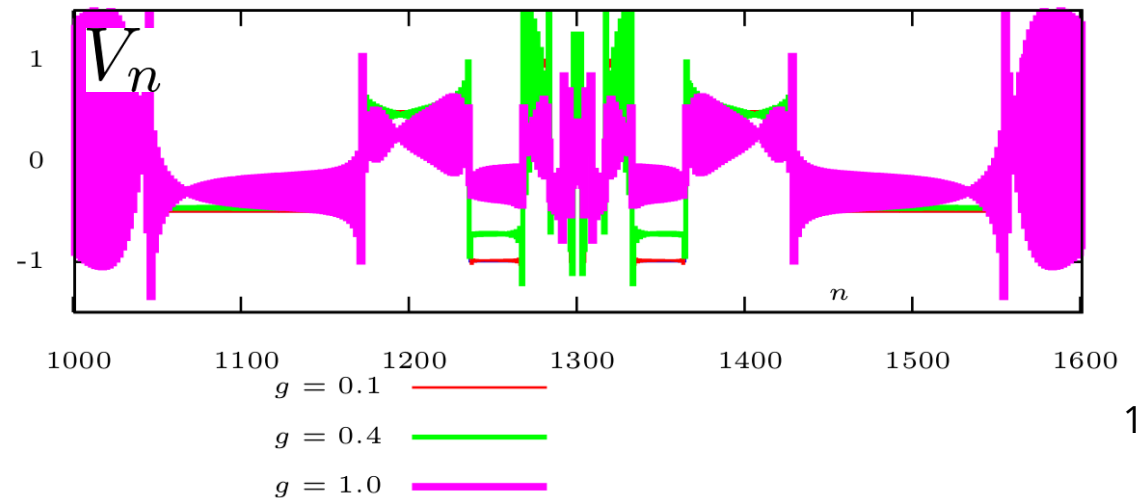
(a) Linearized reconstruction with inverse crime data



(b) Same as in (a) zoom-in



(c) Linearized reconstructions with exact data

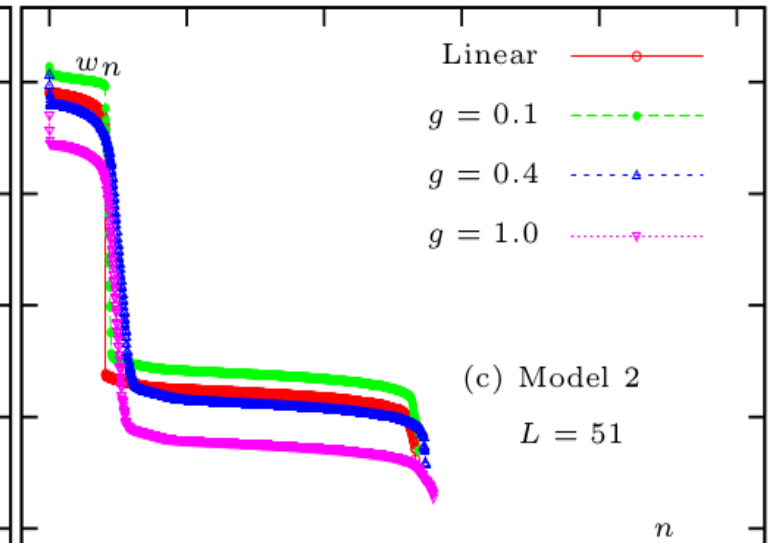
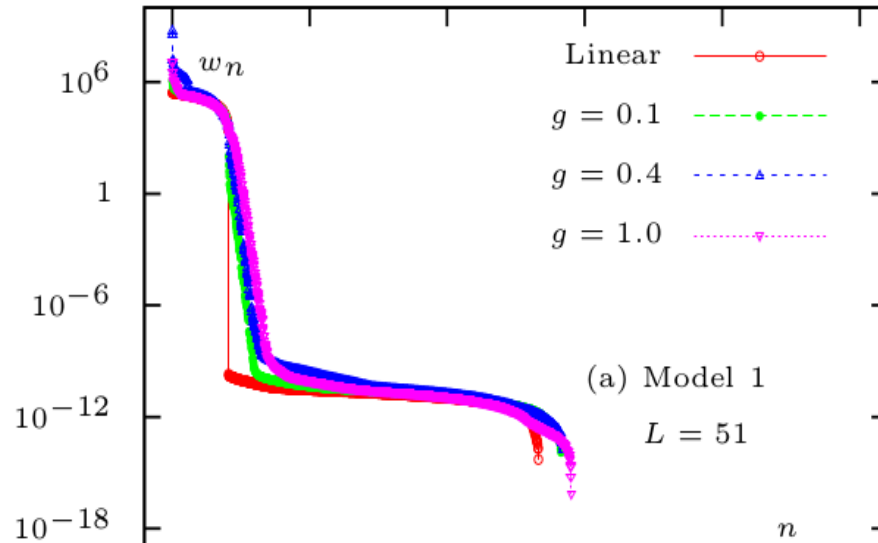


6e. Eigenvalues of $W[D]$, size $N=2,601$

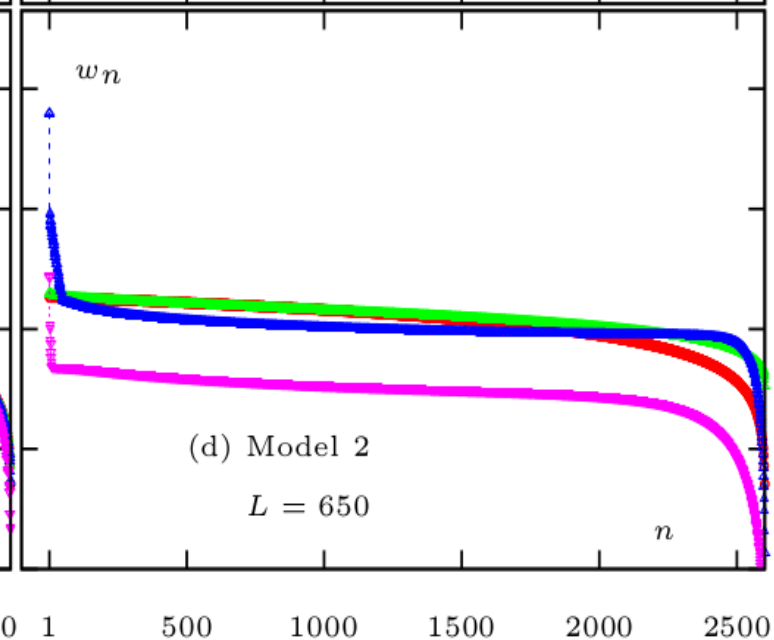
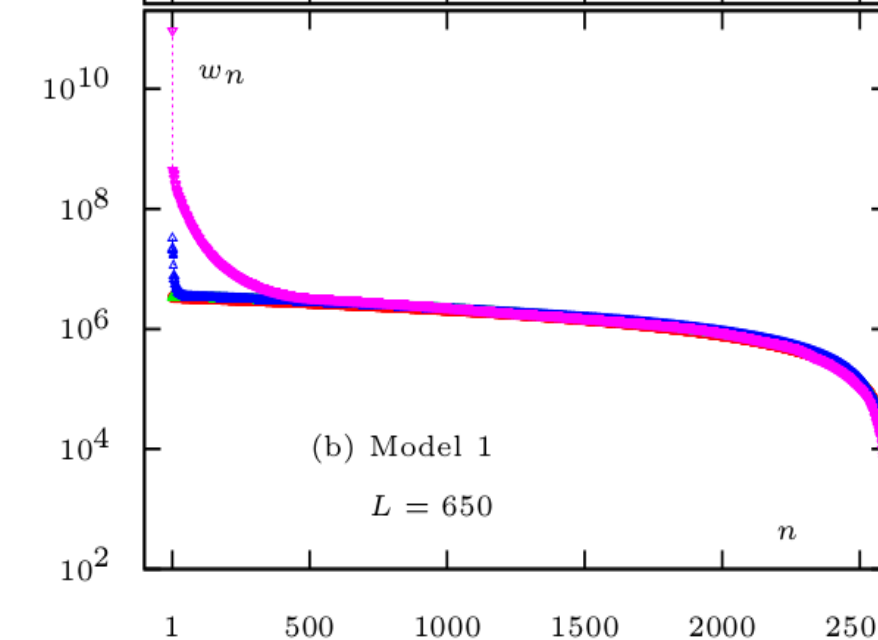
Model 1 for D [pulses]

Model 2 for D [constant]

Band limited



Not band limited

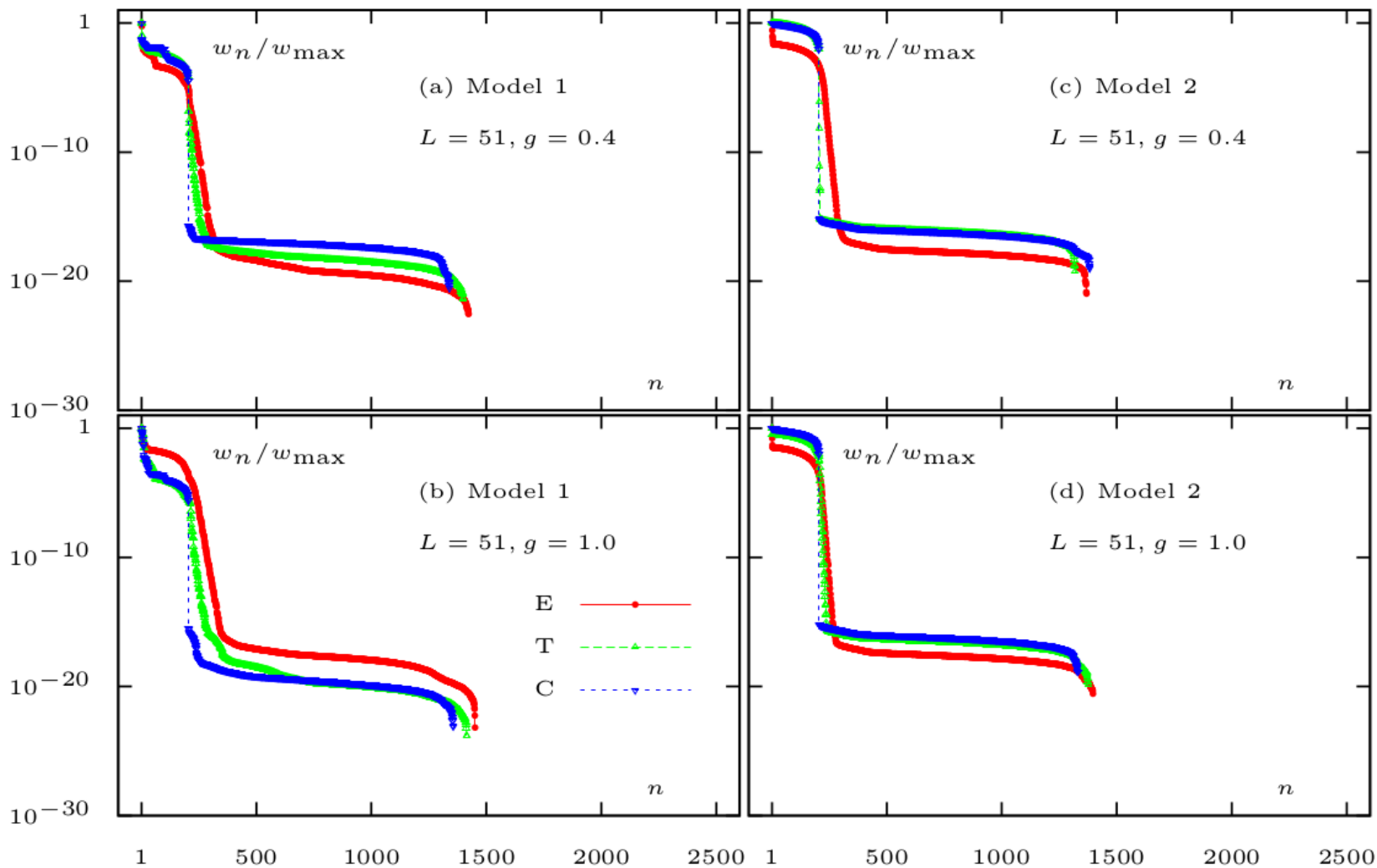


6f. Eigenvalues of $W[D]$, different interactions

Model 1 for D [pulses]

Model 2 for D [constant]

Band limited



Also band limited

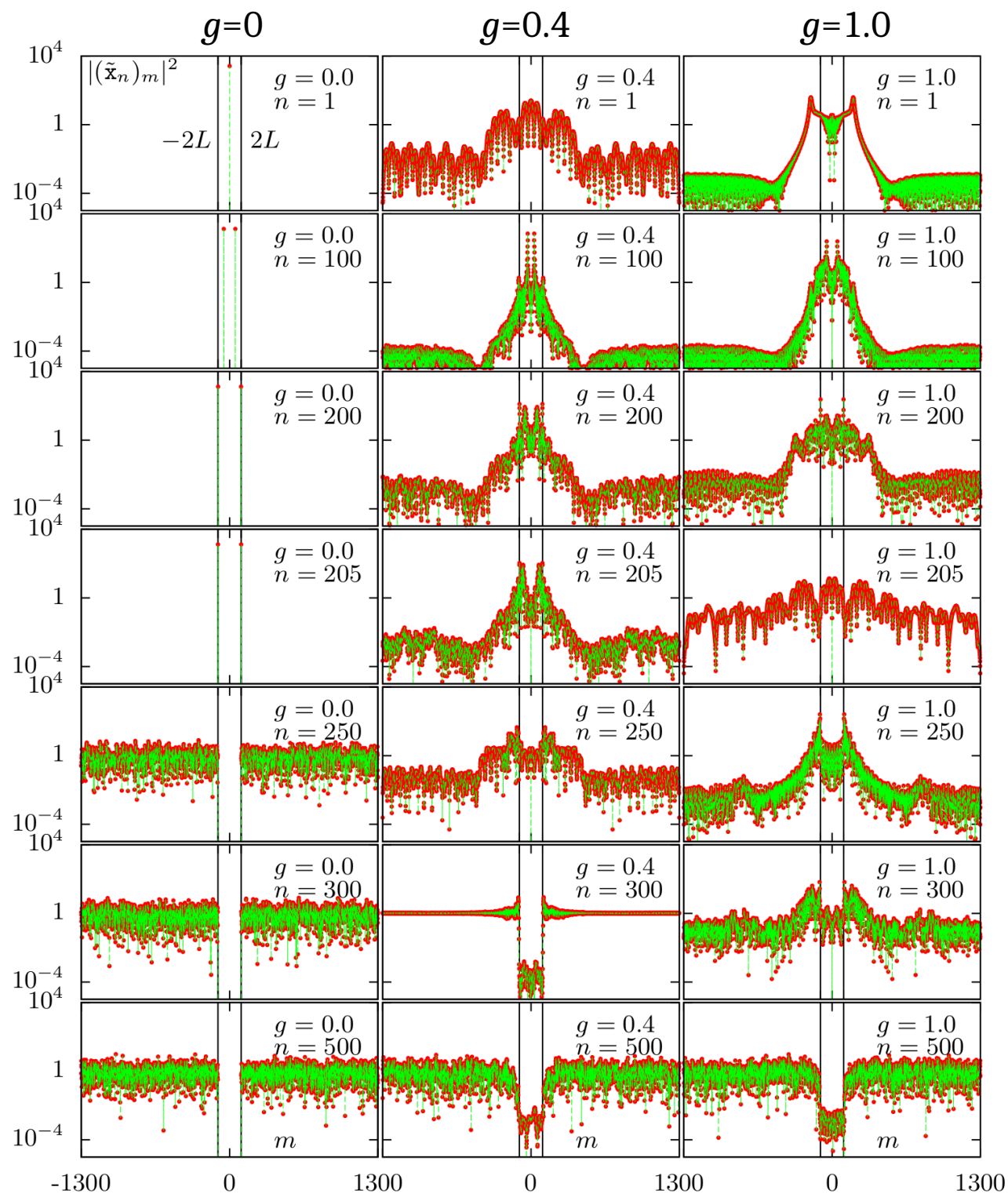
E-Exponential (realistic) T-Tight-binding C-Fully connected

6g. Eigenvalues of $W[D]$

$L=51$
Number of
"significant"
eigenvectors:
 $4L+1=205$

Transition region:
205 to 350

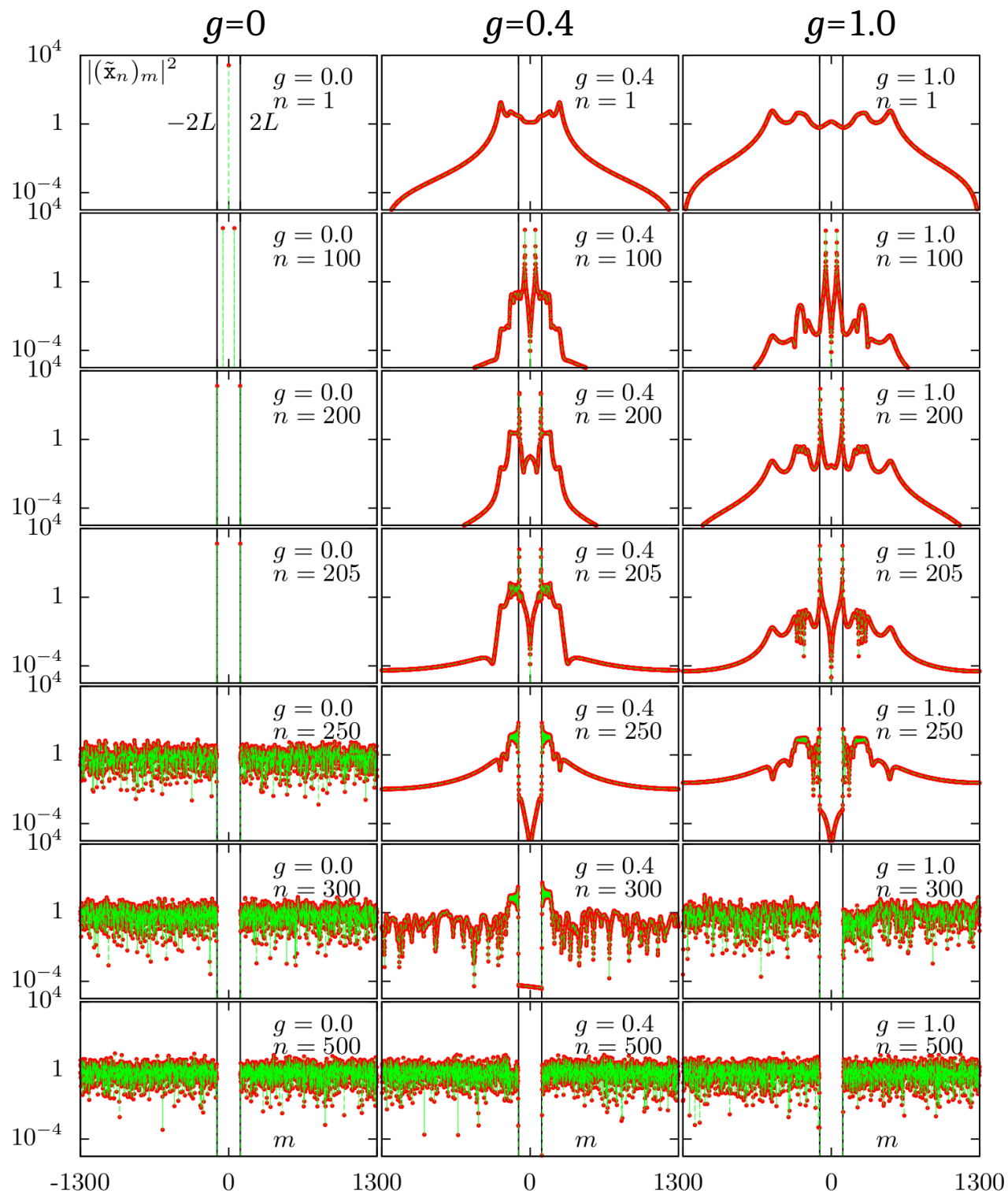
Model 1 for D



6h. Eigenvalues of $W[D]$

$L=51$
Number of "significant" eigenvectors:
 $4L+1=205$

Transition region:
205 to 350





CONCLUSIONS

- Nonlinearity of ISP is unlikely to help significantly with resolution. At least, it is an uphill struggle.
- On the other hand, nonlinearity can easily make the ISP ill-posed even if it is/qs well-posed in the linear regime.
- Perturbation of inverse solutions in the strength of interaction can be singular. This makes analysis difficult.
- Resolution limit exists

Several Lorentzians

$$L(x) = \frac{1}{\pi} \frac{\delta}{(x - a)^2 + \delta^2}$$

FT \rightarrow

$$\tilde{L}(k) = e^{ika - |k|\delta}$$

