$O(N \log N)$ Multilevel Calculation of N Eigenfunctions

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Lecture to be given Thursday, 9:00 AM.

Lecture Sections

1. Goal

2. Problem

3. The Key Principle

4. Algorithm

5. Applications

Goals

1. Compute N eigenfunctions and eigenvalues in $O(N \log N)$

2. Expand in N eigenfunctions in $O(N \log N)$

3. Compute other quantities, e.g.,

$$\rho(x) = \sum_{i=1}^{N} |\Psi_i(x)|^2 \text{ for all x, in } O(N \log N)$$

Main Example: Schrödinger

$$(-\Delta + V(x))\Psi(x) = \lambda\Psi(x), \quad x \in \Omega$$

No localization assumed!

Computational Obstacles

1. Many distinct eigenfunctions **O(N)**

2. Many spatial gridpoints **O(N)**

Oscillatory eigenfunctions

N atoms $\Longrightarrow$ in V(x)

3. Many orthogonalization steps per eigenfunction **O(N)**

Total Complexity: **$O(N^3)$**

Current Eigensolvers

Year	Algorithm	q e.f. on N gridpoints
≤1970	Algebraic Solvers	$\sim O(N^3)$
1983	Multigrid-Ritz	$O(q^2N + q^3)$
1990	Multigrid: CT	$O(qN + q^3)$

Underlying Slowness: (for $q = O(N)$)

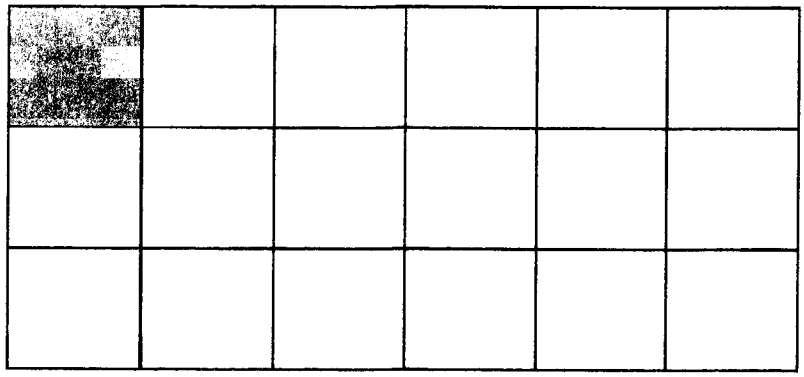
Operations	$\mathbf{O(N^3)}$
Storage	$\mathbf{O(N^2)}$

Objective: **O(N log N)** operations, storage

Localized Systems

N = #atoms in periodicity "super-cell"

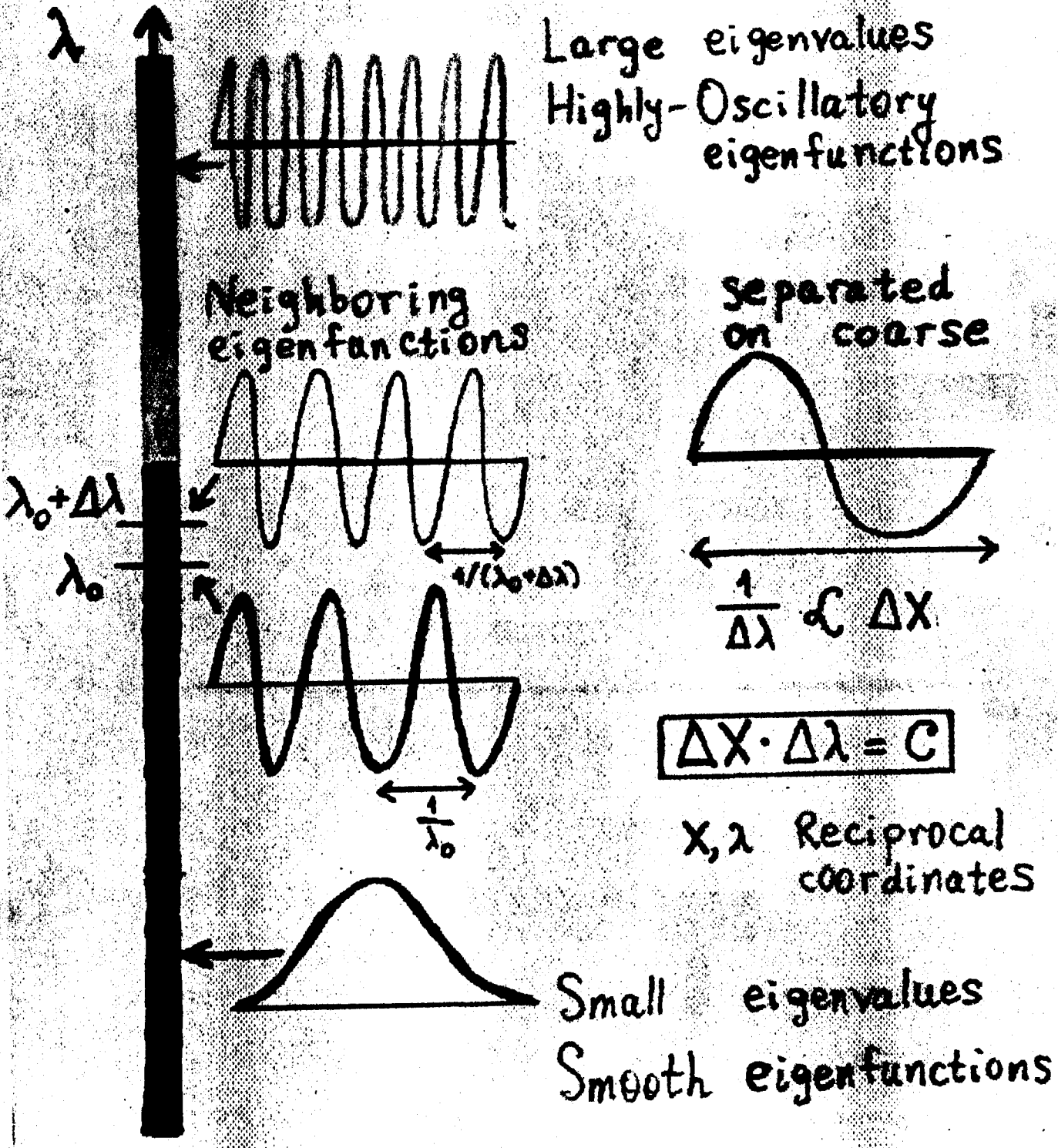
N_{local} = #atoms in local region



	Localized Case	No Localization
Direct Solvers	$O(N N_{local}^2)$	$O(N^3)$
Collective Approach	$O(N \log N_{local})$	$O(N \log N)$

The Key Principle of

Reciprocal Resolution

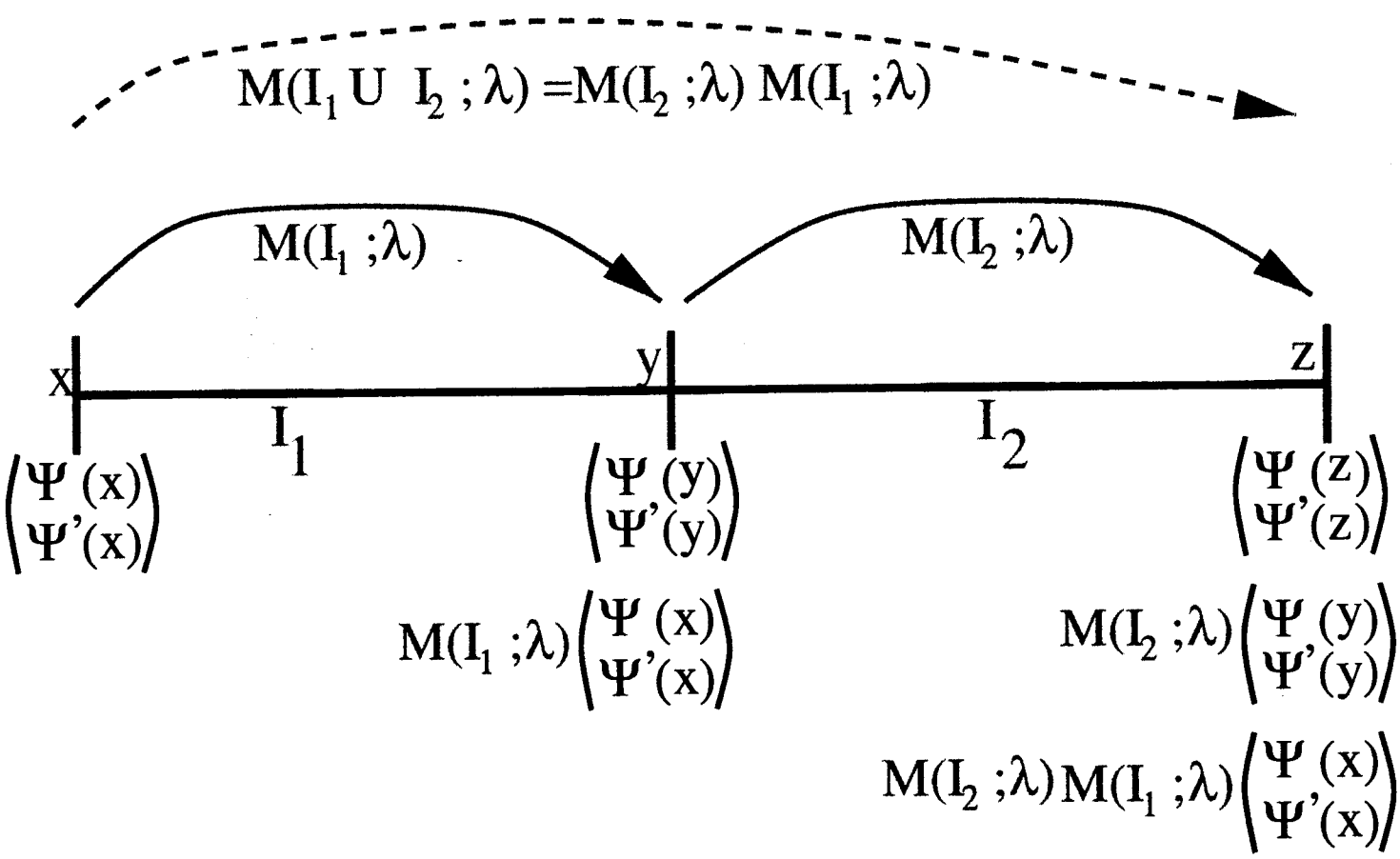


Building Block: Monodromy

$$\Psi''(x) + (\lambda - V(x))\Psi(x) = 0$$

$$\Downarrow$$

2 × 2 Monodromy transformation $M(I_x; \lambda)$



- Local calculation
- B.C. expressible in terms of $\mathcal{M} = M(\Omega; \lambda)$
  $\Longrightarrow$ secular equation for eigenvalues

Examples

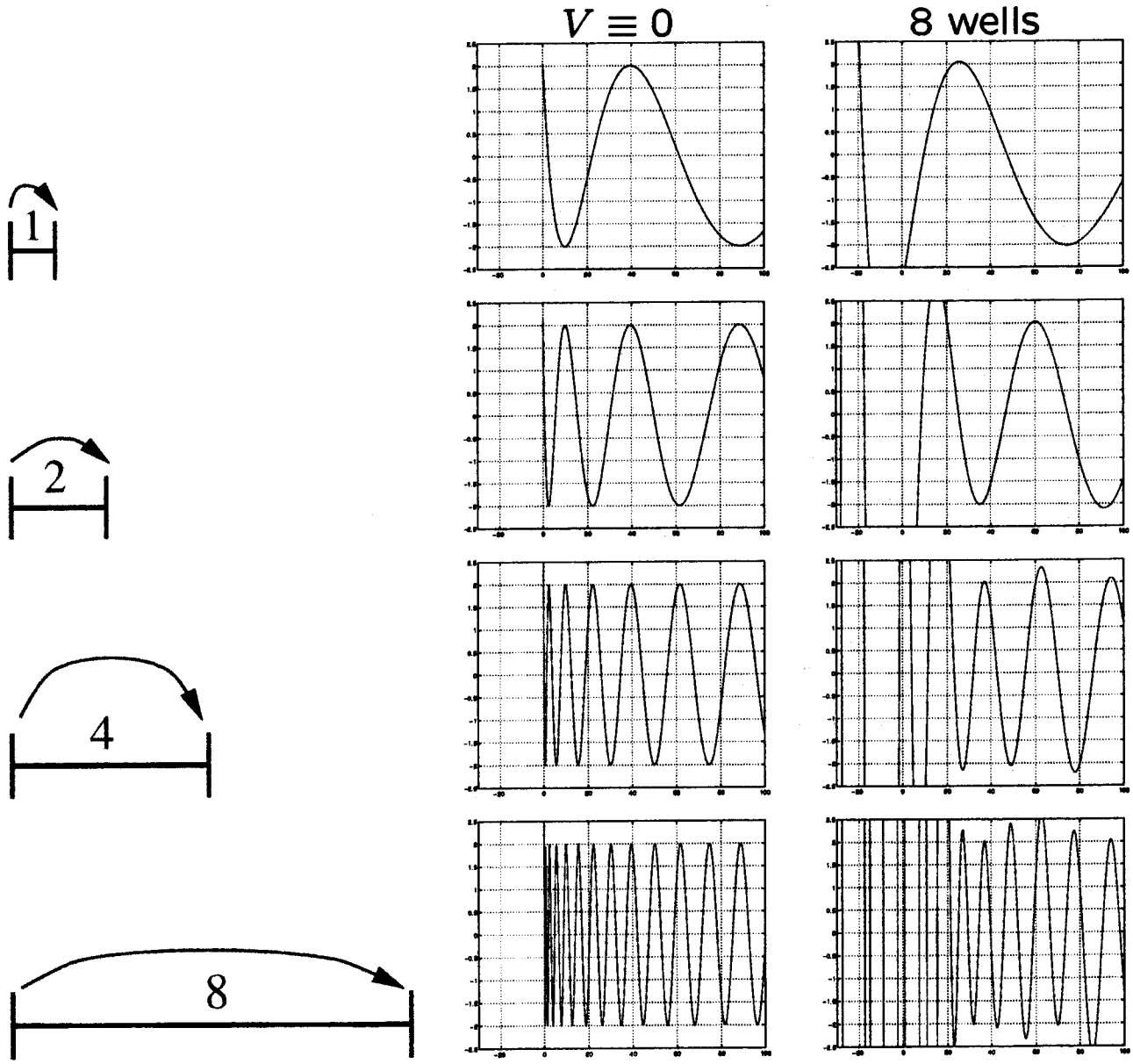
B.C.	Secular Equation
Dirichlet	
$\Psi(0) = \Psi(L) = 0$	$\mathcal{M}_{12}(\lambda) = 0$
Periodic	
$\Psi(x+L) = \Psi(x)$	$\mathcal{M}_{11}(\lambda)+\mathcal{M}_{22}(\lambda) = 2$
Quasi-Periodic	
$\Psi(x + L) = e^{i\beta L}\Psi(x)$	$\lvert\mathcal{M}_{11}(\lambda)+\mathcal{M}_{22}(\lambda)\rvert \leq 2$
	Band spectrum

The Key Principle

Reciprocal Smoothness of $M(I_x; \lambda)$

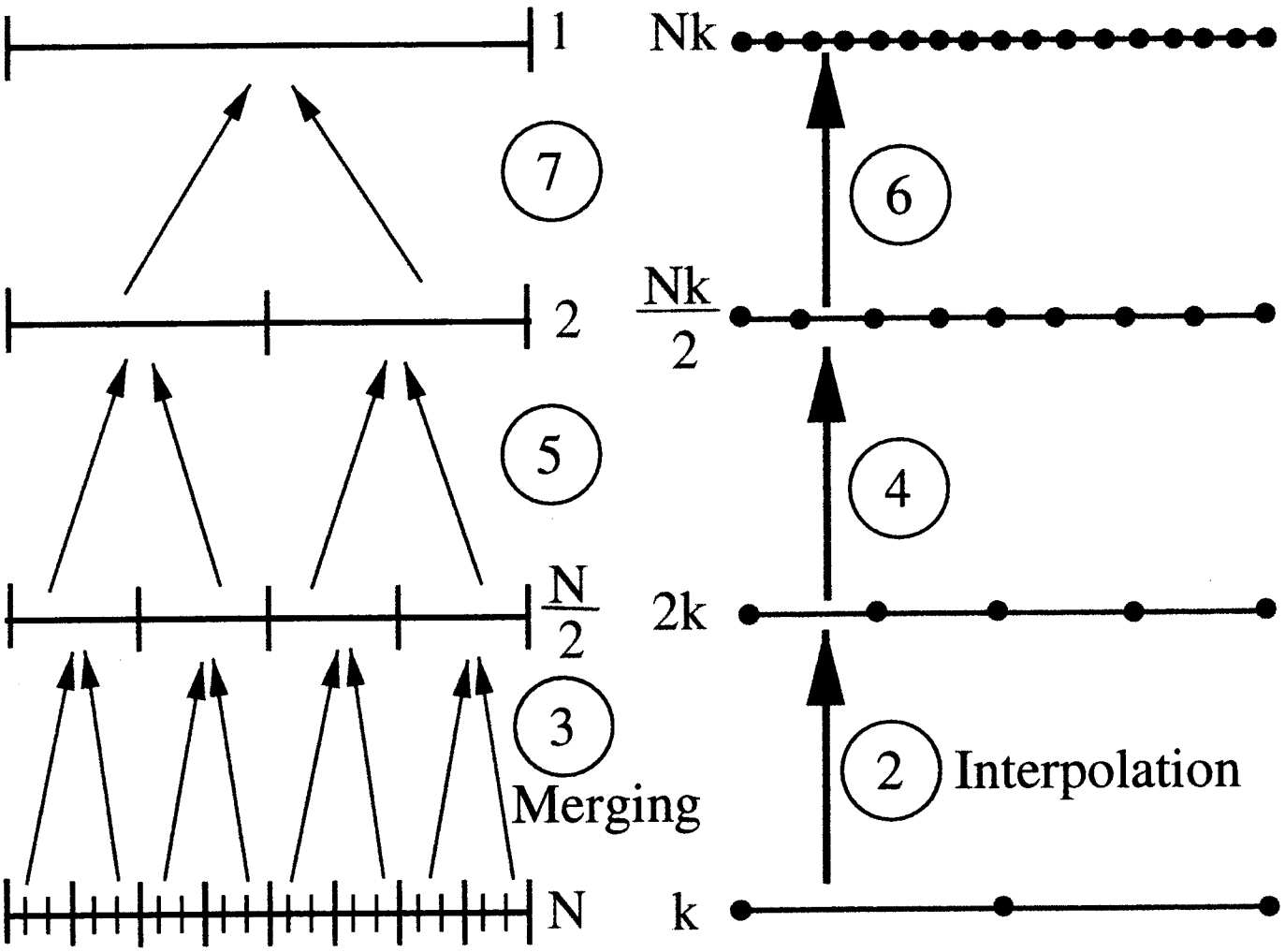
I_x

$M_{11}(I_x; \lambda)$ versus λ



Larger I_x $\Rightarrow$ More oscillatory $M(I_x; \cdot)$

Multiscale Eigenbasis



(1) Evaluation

Total Work = #stages x Work per stage = pkN x log(N)

Optimal $p = O(\log \frac{1}{\varepsilon}) \Longrightarrow$ Work $= O(N \log N \log \frac{1}{\varepsilon})$

Applications

1. Discrete Evaluations
   General B.C.
   $O(\log(1/\varepsilon))$ per eigenvalue
   $O(\log(1/\varepsilon))$ per eigenfunction evaluation

2. Electronic Density Integration

   $$\rho(x) = \sum_i |\psi(x;\lambda_i)|^2, \quad \int |\psi(x;\lambda)|^q d\beta(\lambda)$$

   $O(N \log N \log(1/\varepsilon))$

3. Expansion in the eigenbasis

   - Generalization of FFT
   - Fast Sturm-Liouville Transforms

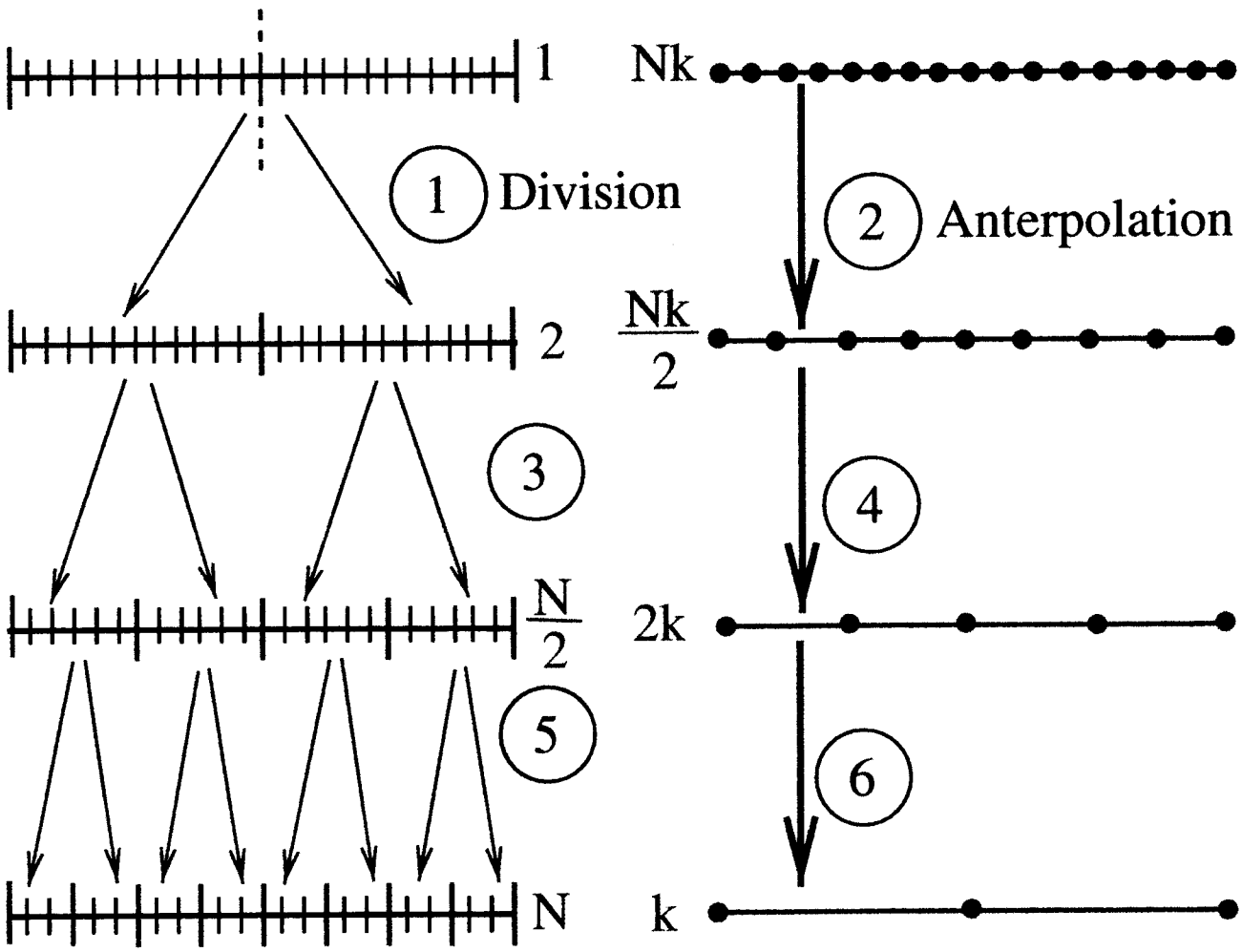
     $$\frac{d}{dx}(p(x)\frac{du}{dx}(x)) + q(x)u(x) = \lambda r(x)u(x)$$

     Legendre, Chebyshev, Hermite, Lagrange

   $O(N \log N \log(1/\varepsilon))$

Fast Summation

$$g(x_j) = \sum_{i=1}^{N} f(\lambda_i)\Psi(x_j;\lambda_i), \qquad j = 1, \ldots, N$$



Total Work = #stages x Work per stage = pkN x log(N)

Optimal p = $O(\log \frac{1}{\varepsilon})$ $\Longrightarrow$ Work = $O(N \log N \log \frac{1}{\varepsilon})$

Summary

MEB = Fundamental structure for general eigenbasis computations

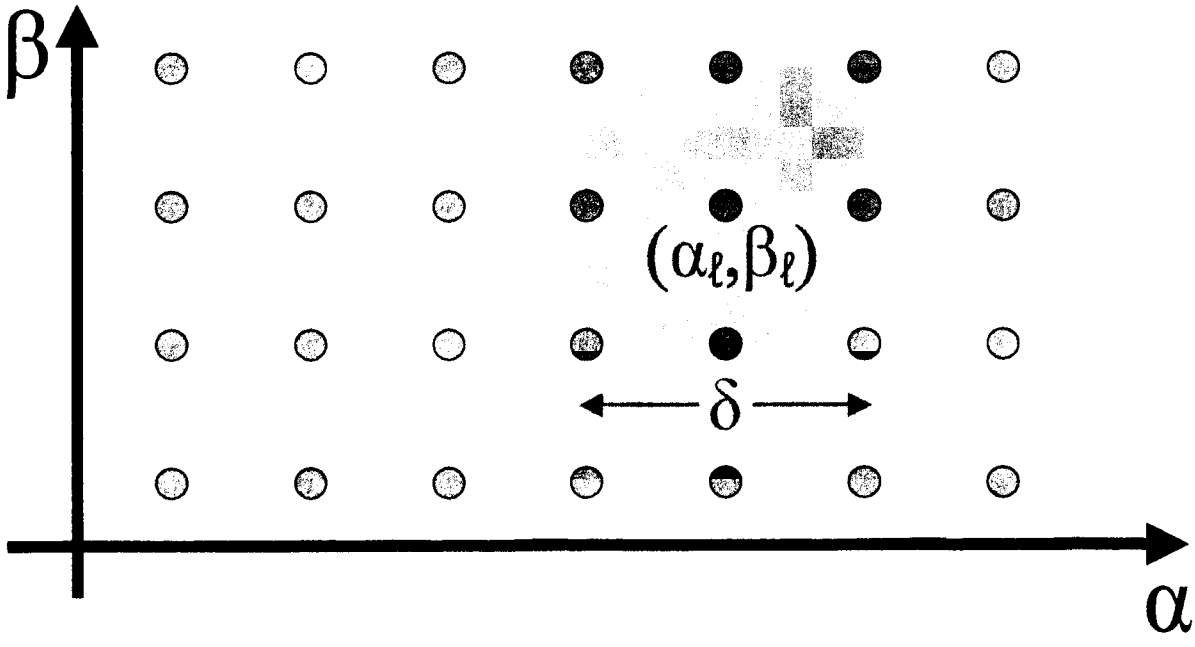
- **Fast** construction & applications **O(N log N)**
- **Generic**
  - General differential operator
  - General boundary conditions
  - Generally spaced gridpoints
  - Parallelization possible

Future Plan

- Multiscale Eigenbasis in 2D, 3D
- Self-consistent (nonlinear) eigenproblems
- Oscillatory integrals $G(x,y) \approx e^{ik|x-y|}$

Eigenfunction Structure

$$-\Delta\, e^{i(\alpha x + \beta y)} = (\alpha^2+\beta^2)\, e^{i(\alpha x + \beta y)}$$



$$e^{i(\alpha x + \beta y)} = A(x,y)\, e^{i(\alpha_\ell x + \beta_\ell y)}$$

- A(x,y) smooth in (x,y) on scales $h \le \frac{\pi}{\delta}$

- Equation for A(x,y) depends <u>smoothly</u> on (α,β) on scales $\delta \le \frac{\pi}{h}$

N Eigenfunctions

e.g., in d-dimensional periodicity cell

Level 0: meshsize h_0

gridpoints $n = O(N)$

Level 1: $h_1 = 2h_0$, $n_1 = n / 2^d$

represented eigenfunctions: 2^d

$\Longrightarrow$ # total data: n

•
•
•

levels: O(log m)

m = # satoms in the local region

➡ Total operations, storage: **O(N log m)**

Eigenfunction Structure

$\mathbf{L}\, U_\alpha(x) = \lambda_\alpha U_\alpha(x)$ e.g. $L = -\Delta + V$

$\alpha = 1,\ldots,N$ U_α **complex**

$$U_\alpha(x) = A_\alpha(x)\, \varphi_{\ell(\alpha)}(x)$$

$$L\, \varphi_\ell(x) \approx \lambda\, \varphi_\ell(x)$$

$A_\alpha(x)$ smooth

$\varphi_\ell(x)$ found by relaxation

$A_\alpha(x)$ represented on a coarser grid

Objective: **O(N log m)** operations, storage

Feasibility studies: 1D Kohn-Sham

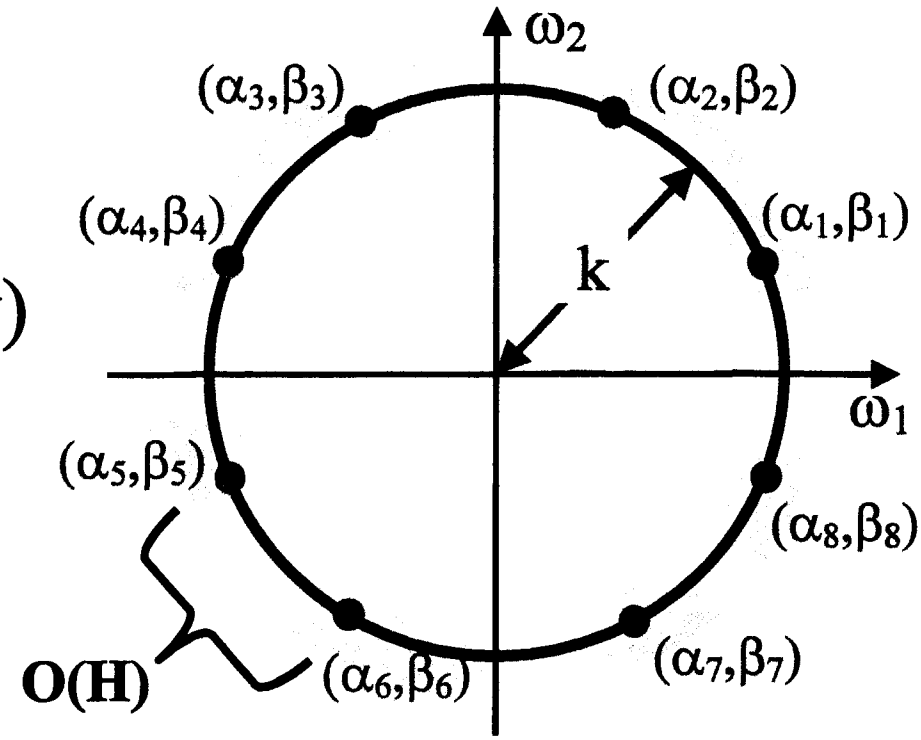
2D Helmholz

2D Wave Equation: $\Delta u + k^2 u = f$

Non-local:

$$e^{i(\omega_1 x + \omega_2 y)}$$

$$\omega_1^2 + \omega_2^2 \approx k^2$$



On coarser grid (meshsize **H**):

$$v(x) = \sum_{r=1}^{c\,H} A_r(x,y)\, e^{i(\alpha_r x + \beta_r y)}$$

- Fully efficient multigrid solver
- Tends to Geometrical Optics
- Radiation Boundary Conditions: directly on coarsest level