The Finite Element Discrete Variable Method for the Solution of the Time Dependent Schroedinger Equation

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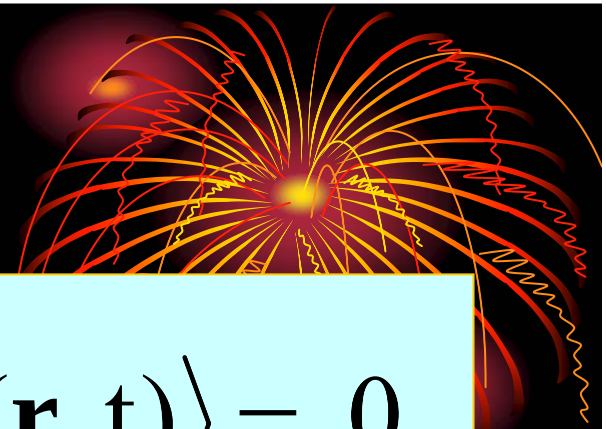
Basic Equation



$$i\hbar \frac{\partial}{\partial t}\left|\Psi(\mathbf{r},t)\right\rangle - H(\mathbf{r},t)\left|\Psi(\mathbf{r},t)\right\rangle = 0$$

Where

Possibly
Non-Local
or
Non-Linear

$$H(\mathbf{r},t) = -\frac{\hbar^2}{2}\sum_i \frac{\nabla_i^2}{m_i} + V(\mathbf{r},t)$$

Objectives

- Flexible Basis (grid) – capability to represent dynamics on small and large scale
- **Good scaling properties – O(n)**
- **Matrix elements easily computed**
- **Time propagation stable and unitary**
- **"Transparent" parallelization**

Enabling Technology

Outline

- Spatial Representations
  - Grids / Finite Differences
  - Spectral Methods - Discrete Variable Representation (DVR)
  - Finite Elements
  - Finite Element – DVR
- Time Propagation
  - General Integrators
  - Lanczos-Arnoldi
  - Real Space Product Formula
- Examples

Discretizations & Representations

- Grids are simple - converge poorly

$$\Psi(\mathbf{r}) = \sum_i \Psi(\mathbf{r_i})\,\delta(\mathbf{r} - \mathbf{r_i})$$

$$\text{Second Derivatives; } \begin{pmatrix} 3 \\ 5 \\ 7 \end{pmatrix} \text{- Order Formulas}$$

$$\frac{d^2}{dx^2}\Psi(x_i, y, z) \approx \frac{1}{h^2} *$$

$$\begin{bmatrix} -2 & 1 & 0 & 0 \\ -30/12 & 16/12 & -1/12 & 0 \\ -1960/720 & 1080/720 & -108/720 & 8/720 \\ & & & \end{bmatrix} \begin{bmatrix} \Psi(x_i, y, z) \\ \Psi(x_{i+1}, y, z) \\ \Psi(x_{i+2}, y, z) \\ \Psi(x_{i+3}, y, z) \end{bmatrix}$$

- Global or Spectral Basis Sets – exponential convergence but can require complex matrix element evaluation

$$\Psi(\mathbf{r}) = \sum_i C_i\,\Phi_i(\mathbf{r})$$

One needs to calculate matrix elements;

$$\langle \Phi_i | \mathbf{H} | \Phi_j \rangle$$

For many expansion basis these can only be done by quadrature.

Can we avoid matrix element quadrature, maintain locality and keep global convergence ?

Properties of Classical Orthogonal Functions

- Orthonormality w.r.t. some positive weight function.

$$\left\langle \chi_n \middle| \chi_m \right\rangle = \int_a^b dx\; w(x)\; \chi_n(x)\; \chi_m(x) = \delta_{n,m}$$

- The functions satisfy a three term recursion relationship of the form;

$$\beta_n \chi_n(x) = (x - \alpha_{n-1}) \chi_{n-1}(x) - \beta_{n-1} \chi_{n-2}(x)$$

  * The recursion coefficients may be computed using the Lanczos procedure

- A set of Gauss quadrature points, x_i and weights, w_i may be found which exactly integrate any polynomial integrand of order (2n - 1) or less with respect to the weight function.
- The points and weights may be found by diagonalizing the tridiagonal matrix made up of the α and β coefficients.
- Completeness

$$\sum_n \chi_n(x)\; \chi_n(x') = \delta(x - x');$$

More Properties

- A discrete orthonormality relationship

  Note that the orthonormality integral can be performed exactly by p-point Gauss quadratures for all φ_q where $q \le p$

$$\langle \chi_n | \chi_m \rangle = \sum_{i=1}^{p} w_i \, \chi_n(x_i) \chi_m(x_i) = \delta_{n,m}$$

This is true because the integrand is a polynomial which can be integrated exactly by the quadrature.

- Corollary

  Given an expansion,

$$\Psi(x) = \sum_{q=1}^{p} c_q \chi_q(x)$$

$$c_q = \int_a^b dx \; w(x) \, \chi_q(x) \, \Psi(x) = \sum_{i=1}^{p} \chi_q(x_i) \, w_i \Psi(x_i)$$

Matrix Elements

Consider, a matrix element of the potential,

$$V_{q,q'} = \langle \varphi_q | V(x) | \varphi_{q'} \rangle$$

Conceptually, this matrix element may be evaluated if we know the matrix representation of the position operator. Then,

$$\mathbf{V} = V(\mathbf{x})$$

as long as the basis set is complete. This remains quite useful even for finite basis sets and suggests that an excellent approximation to the matrix is obtained,

$$V_{q,q'} = \sum_i T_{q,i}\, V(x_i)\, T_{q',i}$$

where **T** is the transformation from the original representation to one which diagonalizes x. Note, that this looks like a quadrature formula.

Properties of Discrete Variable Representation

- Define a new set of "coordinate" functions,

$$u_i(x) = \sqrt{w_i}\sum_{q=1}^{p} \chi_q(x)\, \chi_q(x_i)$$

with the property that,

$$u_i(x_j) = \frac{\delta_{i,j}}{\sqrt{w_i}}$$

and

$$\langle u_i|x|u_j\rangle = x_i \delta_{i,j}$$

- Consider the matrix element

$$F_{i,j} = \langle u_i|F(x)|u_j\rangle$$

In general this will not be equal to

$$F_{i,j} = F(x_i)\, \delta_{i,j}$$

unless the basis/or quadrature is complete.

(Think power series expansion and matrix mutiply)

In the DVR, its is assumed that this is true.

In practice it appears to be an excellent approximation.

The Key Point

More Properties

- A simple representation

$$u_i(x) = \frac{1}{\sqrt{W_i}} \prod_{j \neq i} \frac{(x - x_j)}{(x_i - x_j)}$$

where x_i are the Gauss quadrature points.

Matrix elements of the derivative operators may be evaluated using the quadrature rule, but its **trivial**. For Cartesian coordinates :

$$\left\langle u_i \left| \frac{d^2}{dx^2} \right| u_j \right\rangle = w_i u_i(x_i) \left[\frac{d^2}{dx^2} u_j \right]_{x = x_i}$$

Boundary Conditions, Singular Potentials and Lobatto Quadrature

Be Careful

- Physical conditions require wavefuntion to behave regularly
  - ❖ Function and/or derivative non-singular at left and right boundary
  - ❖ Boundary conditions may be imposed using constrained quadrature rules (Radau/Lobatto) – end points in quadrature rule
- Consequence
  - ❖ All matrix elements, even for singular potentials are well defined
  - ❖ ONE quadrature for all angular momenta
  - ❖ No transformations of Hamiltonian required

The Finite-Element DVR

- The FEDVR takes these ideas one step further by combining the finite-element method with the DVR:
  - For any dimensional coordinate space is divided into many elements: 
  - Within each element a DVR basis of arbitrary order can be used: 
  - The continuity on the DVR basis in adjacent elements is satisfied by defining a “bridge” function (Gauss-Lobatto quadrature rule will be used):

$$u_N^i(x) = \frac{u_N^i(x) + u_1^{i+1}(x)}{\sqrt{w_N^i + w_1^{i+1}}}$$

- Sparse Representation N Scaling
- Close to Spectral Accuracy

The FEDVR matrix form

- The Hamiltonian matrix that results from the FEDVR can be quite sparse. An example having four finite elements with a (4/3/3/2) basis set looks like:

$$
\begin{pmatrix}
H_{11} & H_{12} & H_{13} & H_{14} & 0 & 0 & 0 & 0 & 0 \\
H_{21} & H_{22} & H_{23} & H_{24} & 0 & 0 & 0 & 0 & 0 \\
H_{31} & H_{32} & H_{33} & H_{34} & 0 & 0 & 0 & 0 & 0 \\
H_{41} & H_{42} & H_{43} & H_{44} & H_{45} & H_{46} & 0 & 0 & 0 \\
0 & 0 & 0 & H_{54} & H_{55} & H_{56} & 0 & 0 & 0 \\
0 & 0 & 0 & H_{64} & H_{65} & H_{66} & H_{67} & H_{68} & 0 \\
0 & 0 & 0 & 0 & 0 & H_{76} & H_{77} & H_{78} & 0 \\
0 & 0 & 0 & 0 & 0 & H_{86} & H_{87} & H_{88} & H_{89} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & H_{98} & H_{99}
\end{pmatrix}
$$

Multidimensional Problems

- Tensor Product Basis
  - Consequences

$$
\begin{aligned}
\langle i,j,k|H|l,m,n\rangle = {} & \langle i|T|l\rangle \quad \delta_{j,m}\delta_{k,n} + \\
& \langle j|T|m\rangle \; \delta_{i,l}\delta_{k,n} \; + \\
& \langle k|T|n\rangle \; \delta_{i,l}\delta_{j,m} \; + \\
& \langle i,j,k|V|l,m,n\rangle \, \delta_{i,l}\delta_{j,m}\delta_{k,n}
\end{aligned}
$$

Multidimensional Problems

$$\left|V^{out}_{i,j,k}\right\rangle = \sum_{l,m,n} \left\langle i,j,k\middle|H\middle|l,m,n\right\rangle \left|V^{in}_{l,m,n}\right\rangle =$$

$$\sum_{m,n}\sum_{l}\left\langle i\middle|T\middle|l\right\rangle\left|V^{in}_{l,m,n}\right\rangle$$

$$+\sum_{l,n}\sum_{m}\left\langle j\middle|T\middle|m\right\rangle\left|V^{in}_{l,m,n}\right\rangle$$

$$+\sum_{l,m}\sum_{n}\left\langle k\middle|T\middle|n\right\rangle\left|V^{in}_{l,m,n}\right\rangle$$

$$+\left\langle i,j,k\middle|V\middle|i,j,k\right\rangle\left|V^{in}_{i,j,k}\right\rangle$$

Nested sums.

Time Propagation Methods

- Hamiltonian Explicitly Time-Dependent
  - General Initial Value Solvers
    - Runge-Kutta
    - Adams-Bashforth-Moulton
    - Bulirisch-Stoer
    - TDVR

  Good for general and/or rapidly varying time dependencies.
- Short TimePropagation via Exponential

$$\Psi(r, t+\Delta t) = \exp(-i\frac{H(t)\Delta t}{\hbar})\,\Psi(r,t)$$

Time Propagation Methods

- A Cayley Form - Crank-Nicholson

$$\exp\left(i\frac{\Delta t}{2}H\right)\Psi(r, t+\Delta t) = \exp\left(-i\frac{\Delta t}{2}H\right)\Psi(r, t)$$

Expand exponentials to first order to get

$$\Psi(r, t+\Delta t) = \left[1 + i\frac{\Delta t}{2}H\right]^{-1}\left[1 - i\frac{\Delta t}{2}H\right]\Psi(r, t)$$

Note matrix inversion

Linear System Solve

Time Propagation Methods

- Short Iterative Lanczos
  - Lanczos diagonalization over short time periods to represent time propagator – Limited only by time variation of Hamiltonian

$$\left\langle q \middle| \exp(-iH(t_0)\delta t) \middle| q' \right\rangle =$$

$$\sum_i \langle q | i \rangle \exp(-iE_i(t_0)\delta t) \left\langle i \middle| q' \right\rangle$$

Time Propagation Methods

- Lie-Trotter-Suzuki

$$\begin{matrix} h_{11} & h_{12} & h_{13} & h_{14} & & & \\ h_{21} & h_{22} & h_{23} & h_{24} & & & \\ h_{31} & h_{32} & h_{33} & h_{34} & & & \\ h_{41} & h_{42} & h_{43} & h_{44} & h_{45} & h_{46} & \\ & & & h_{54} & h_{55} & h_{56} & \\ & & & h_{64} & h_{65} & h_{66} & h_{67} \\ & & & & & h_{76} & h_{77} \end{matrix}$$

Let

$U_1(\tau) = \exp(-i\,\tau\, H_1)\exp(-i\,\tau\, H_2)$

$H = H_1 + H_2$, then to second order accuracy,

$$\Psi(r, t+\tau) = U_1(\frac{\tau}{2})U_1(\frac{\tau}{2})\,\Psi(r,t) =$$

$$\exp(-i\,\Delta t\,\frac{H_1}{2\hbar})\exp(-i\,\Delta t\,\frac{H_2}{\hbar})\exp(-i\,\Delta t\,\frac{H_1}{2\hbar})\,\Psi(r,t)$$

Note the breakup of the Hamiltonian is arbitrary but a judicious choice can enormously simplify the calculation

To fourth order(Suzuki, J. Math. Phys.),

$$\Psi(r, t+\tau) = U_2(p\tau)U_2(p\tau)\,U_2((1-4p)\tau)\,U_2(p\tau)U_2(p\tau)\,\Psi(r,t)$$

$$p = \frac{1}{4-4^{1/3}}$$

Time Propagation Methods

- FEDVR Propagation

Decompose the Hamiltonian matrix into,

$$H = H_d + H_a + H_b$$

where H_d is the diagonal and contains all of the time dependence and H_a and H_b are **block** diagonal, overlapping matrices.

$$U_2(\tau) = \exp(-i\frac{H_d\tau}{2\hbar})\exp(-i\frac{(H_a + H_b)\tau}{\hbar})\exp(-i\frac{H_d\tau}{2\hbar})$$

$$=$$

$$\exp(-i\frac{H_d\tau}{2\hbar})\exp(-i\frac{H_a\tau}{2\hbar})\exp(-i\frac{H_b\tau}{\hbar})\exp(-i\frac{H_a\tau}{2\hbar})\exp(-i\frac{H_d\tau}{2\hbar})$$

The RSP formalism

- **The kinetic-energy matrices can be further divided into “odd” and “even” blocks:**

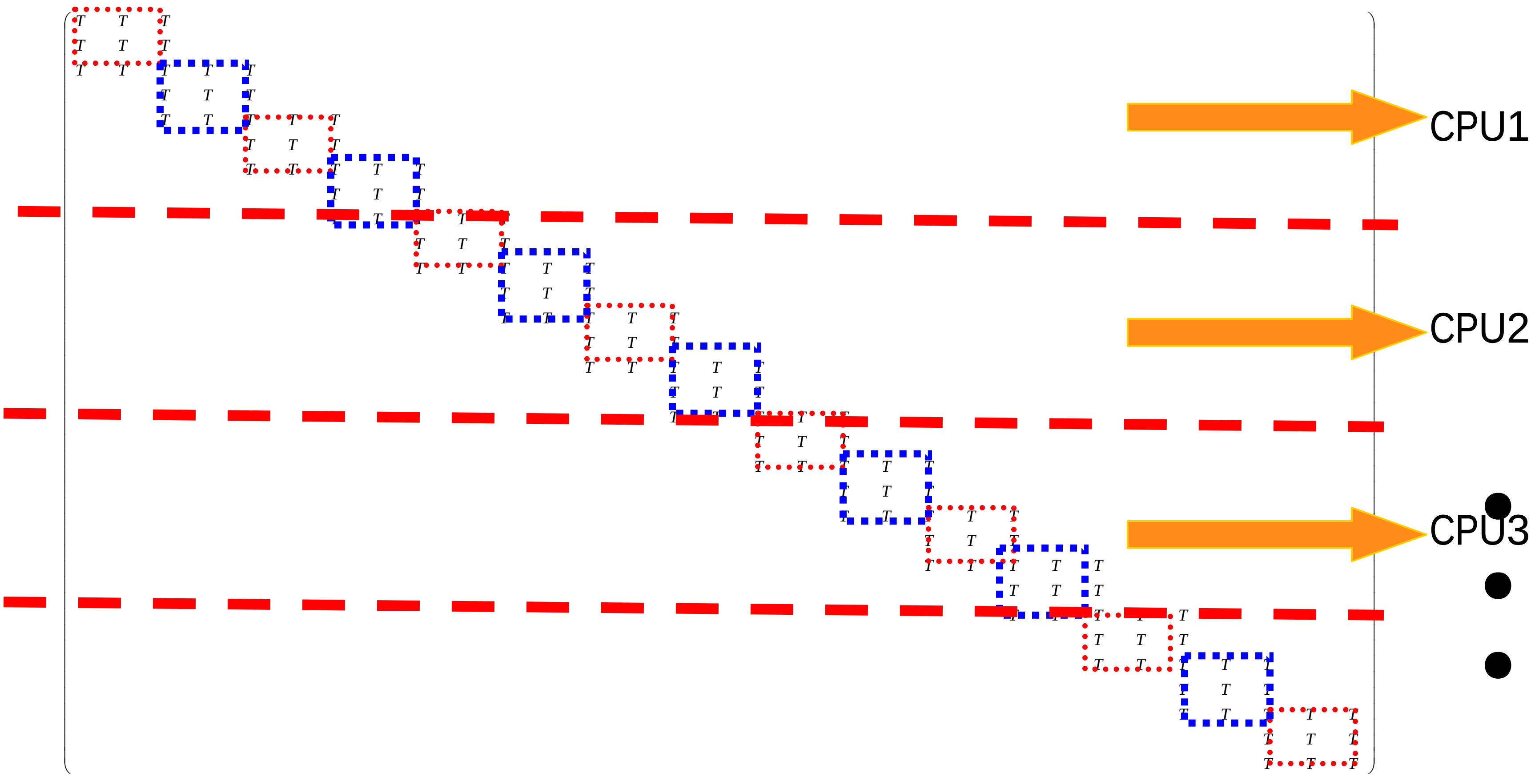
$$
\begin{pmatrix}
T_{11} & T_{12} & T_{13} & T_{14} & 0 & 0 & 0 & 0 & 0 \\
T_{21} & T_{22} & T_{23} & T_{24} & 0 & 0 & 0 & 0 & 0 \\
T_{31} & T_{32} & T_{33} & T_{34} & 0 & 0 & 0 & 0 & 0 \\
T_{41} & T_{42} & T_{43} & T_{44} & T_{45} & T_{46} & 0 & 0 & 0 \\
0 & 0 & 0 & T_{54} & T_{55} & T_{56} & 0 & 0 & 0 \\
0 & 0 & 0 & T_{64} & T_{65} & T_{66} & T_{67} & T_{68} & 0 \\
0 & 0 & 0 & 0 & 0 & T_{76} & T_{77} & T_{78} & 0 \\
0 & 0 & 0 & 0 & 0 & T_{86} & T_{87} & T_{88} & T_{89} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{98} & T_{99}
\end{pmatrix}
=
\begin{pmatrix}
T_{11} & T_{12} & T_{13} & T_{14} & 0 & 0 & 0 & 0 & 0 \\
T_{21} & T_{22} & T_{23} & T_{24} & 0 & 0 & 0 & 0 & 0 \\
T_{31} & T_{32} & T_{33} & T_{34} & 0 & 0 & 0 & 0 & 0 \\
T_{41} & T_{42} & T_{43} & T_{44}/2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & T_{66}/2 & T_{67} & T_{68} & 0 \\
0 & 0 & 0 & 0 & 0 & T_{76} & T_{77} & T_{78} & 0 \\
0 & 0 & 0 & 0 & 0 & T_{86} & T_{87} & T_{88}/2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
+
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & T_{44}/2 & T_{45} & T_{46} & 0 & 0 & 0 \\
0 & 0 & 0 & T_{54} & T_{55} & T_{56} & 0 & 0 & 0 \\
0 & 0 & 0 & T_{64} & T_{65} & T_{66}/2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{88}/2 & T_{89} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & T_{98} & T_{99}
\end{pmatrix}
$$

- **The exponential operator of kinetic-energy matrices can be split as follows:**

$$
\underbrace{\exp[-iT_x\Delta t]}_{U^T(\Delta t)} = \underbrace{\exp(-iT_{odd}\Delta t/2)}_{U^{odd}(\Delta t/2)}\,\underbrace{\exp[-iT_{even}\Delta t]}_{U^{even}(\Delta t)}\,\underbrace{\exp(-iT_{odd}\Delta t/2)}_{U^{odd}(\Delta t/2)}
$$

MPI-Parallelization of RSP-FEDVR

- **The implementation with MPI is done by "domain decomposition". Example is a 1D-decomposition; One can do 2D or even 3D decompositions!**

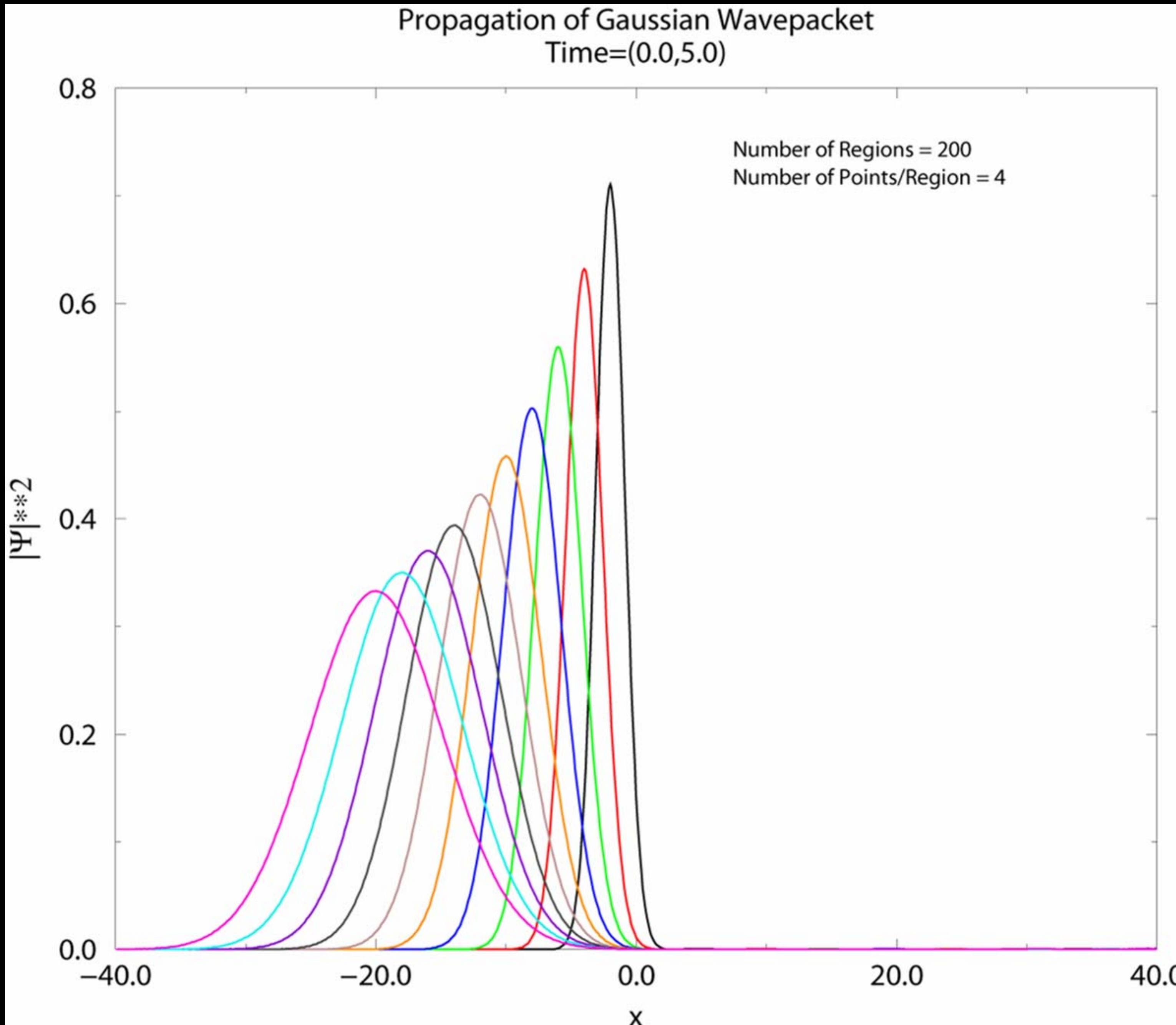


Eigenvalues of Hydrogen Atom (40 Legendre/Lobatto DVR Functions)

State	R=40.0	R=50.0	R=60.0	Exact
1s	-.50000000			-.50000000
2s	-.12500000			-.12500000
2p	-.12500000			-.12500000
3s	-.05555423	-.05555555		-.05555555
3p	-.05555477	-.05555555		-.05555555
4s	-.03055182	-.03120434	-.03124815	-.03125000
4p	-.03070989	-.03121650	-.03124870	-.03125000
5p	-.01221097	-.01817594	-.01966509	-.02000000
6p			-.00991012	-.01388889

Imaginary Time Propagation

Problem	Order	Δt	Matrix Size	Eigenvalue
Well	2	.005	20	5.2696
Well	4	.005	20	4.9377
Well	2	.001	20	4.9356
Well	4	.001	20	4.9348
Fourier	2	.003	80	49.9718
Fourier	4	.003	80	49.9687
Coulomb	2	.005	120	-.499998
Coulomb	4	.005	120	-.499999
Coulomb	4	.01	120	-.499997



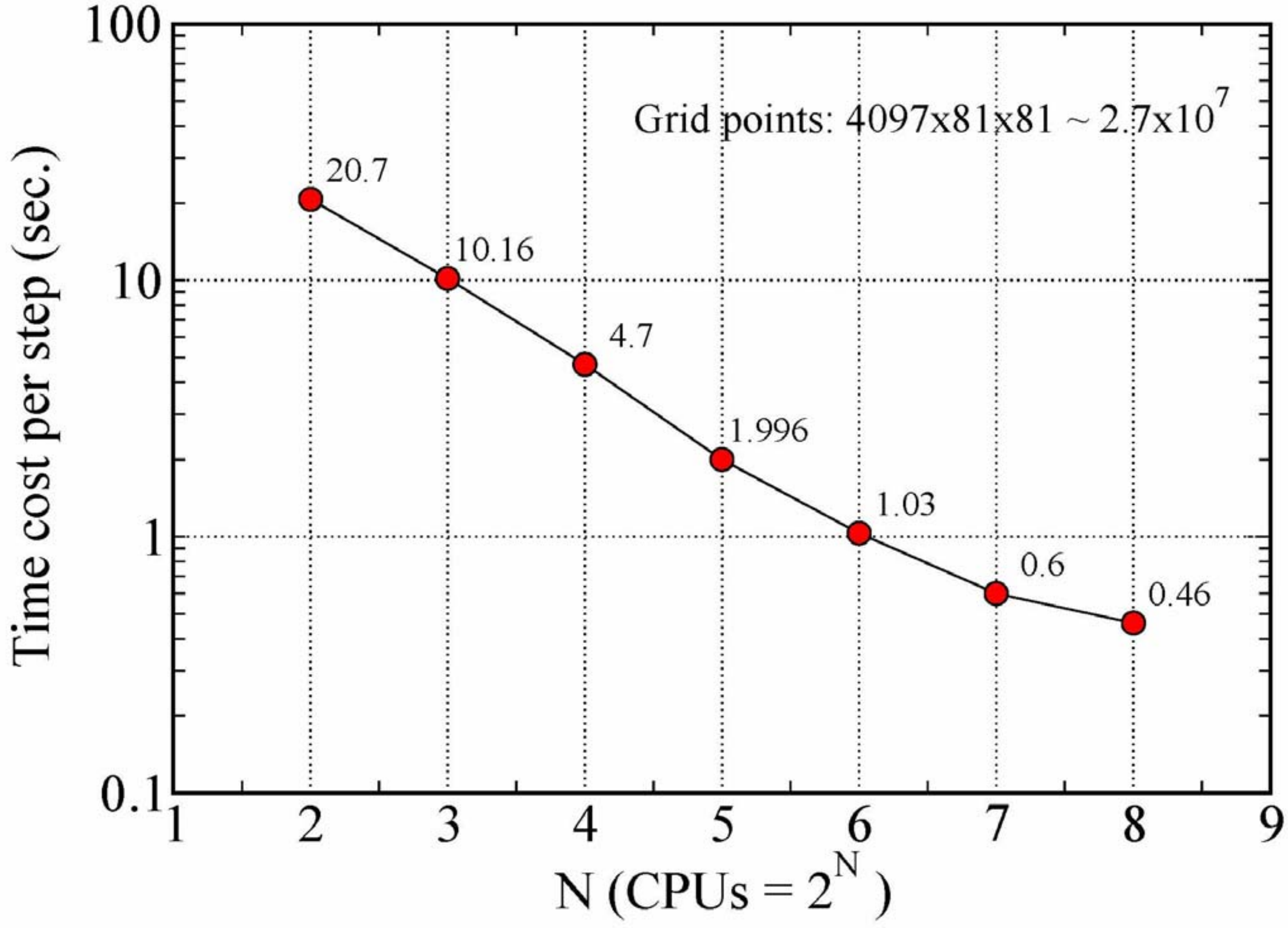
Propagation of Gaussian Wavepacket
Time=(0.0,5.0)
Number of Regions = 200
Number of Points/Region = 4
0.8
0.6
0.4
0.2
0.0
|Ψ|**2
−40.0
−20.0
0.0
20.0
40.0
x

Free Particle Propagation

$$i\hbar \frac{\partial}{\partial t}\psi(r,t) = \left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(r,t)$$

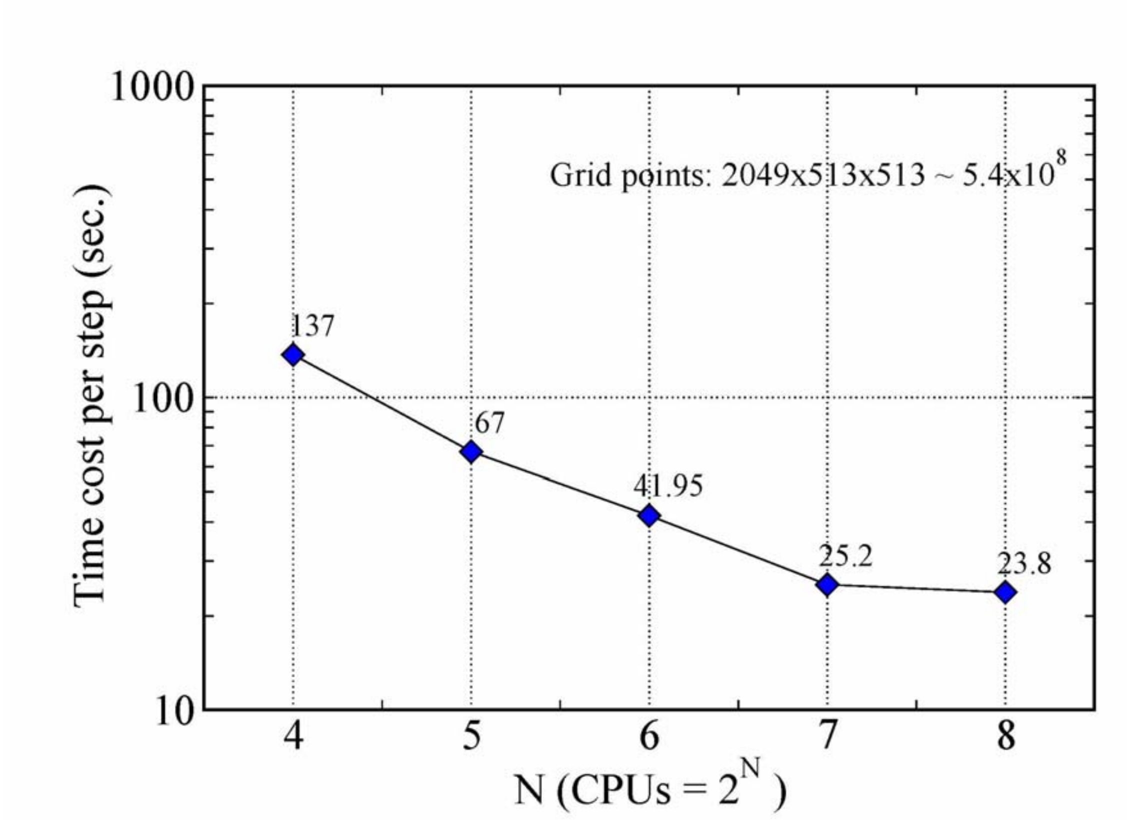
Method	No. Regions	Points/ Region	Time (Alpha/21164)	<x>	$<x^2>$
3pt FD	1	1000	74.5s	1.9629	.7825
DVR	1	700	179.4s	1.9999	.7903
DVR	2	350	126.5s	1.9999	.7905
DVR	4	175	44.7s	1.9999	.7904
DVR	8	100	31.5s	1.9999	.7904
DVR	16	50	13s	1.9999	.7906
DVR	32	25	8s	2.0000	.7906
DVR	32	20	5.6s	1.9999	.7906
DVR	64	7	4s	1.9999	.7906

Propagation of BEC on a 3D Lattice



Superscaling Observed: Due to Elongated Condensate

Propagation of BEC on a 3D Lattice



Almost linear speeding-up up to n=128 CPUs. It breaks down from n=128 to n=256 CPUs for this data set.

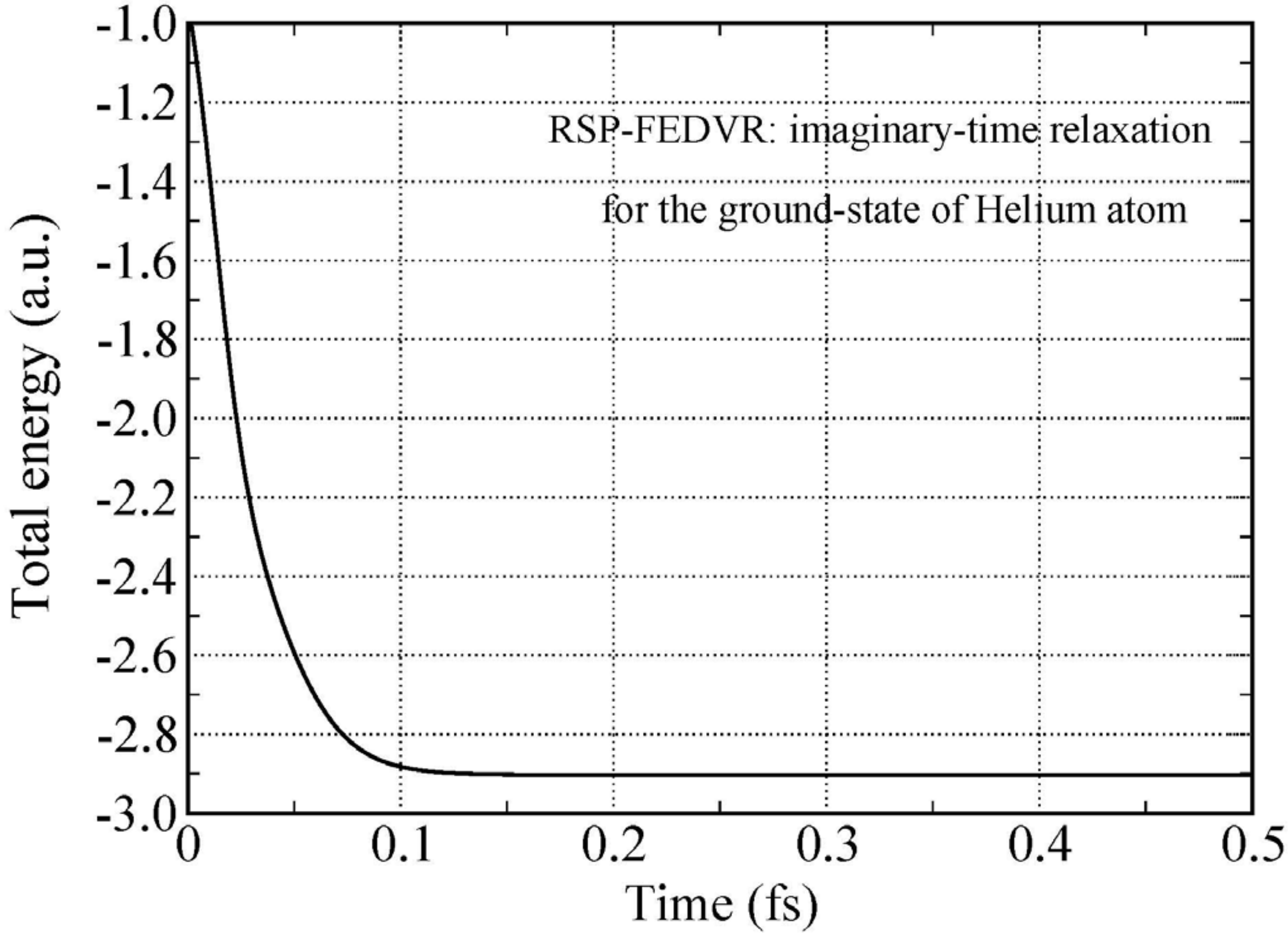
Ground State Energy of BEC in 3D Trap

Method	No. Regions(X Basis)	Points	Energy
RSP-FEDVR	20(x 3)	$(41)^3$	19.85562355
RSP-FEDVR	20 (x 4)	$(61)^3$	19.84855573
RSP-FEDVR	20 (x 6)	$(101)^3$	19.84925147
RSP-FEDVR	20 (x 8)	$(141)^3$	19.84925687
3D Diagonalization			19.847

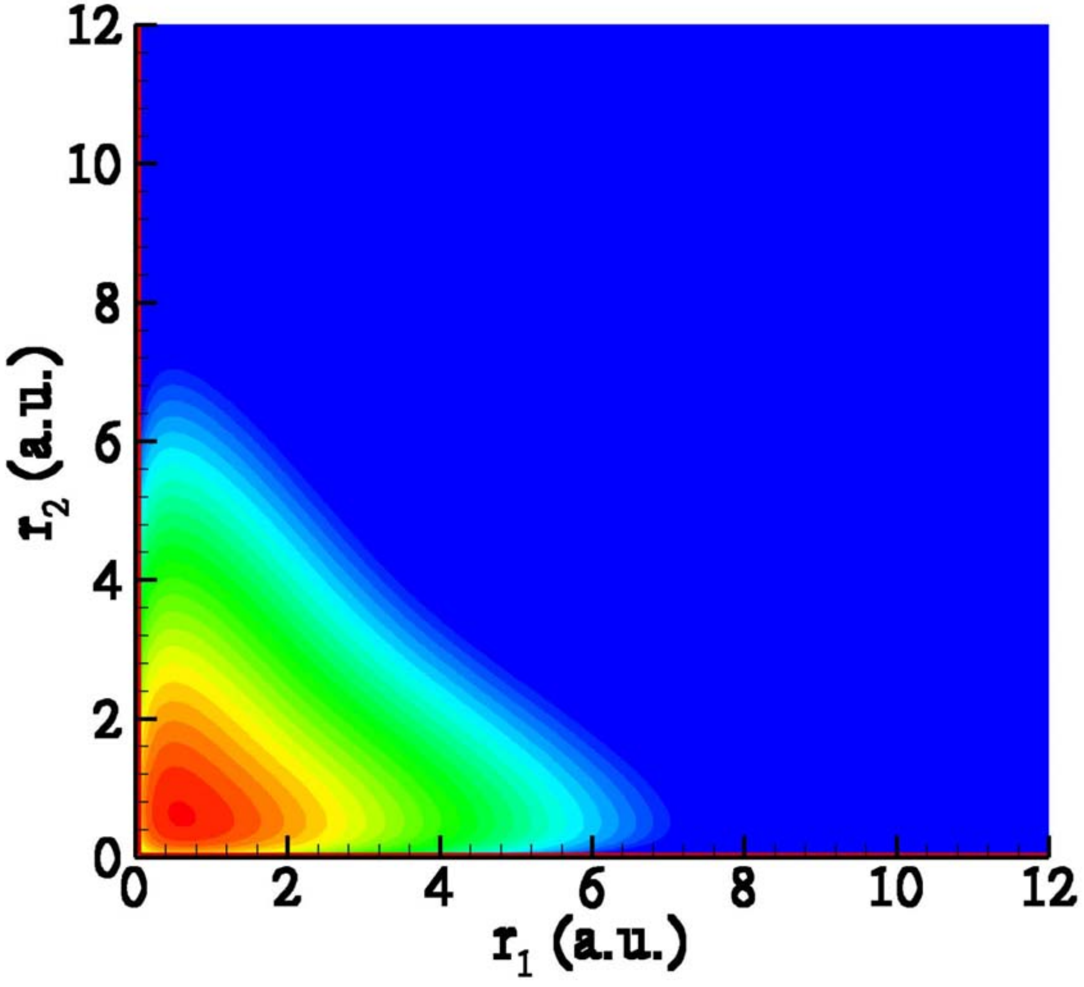
Ground State Energy of 3D Harmonic Oscillator

Method	No. Regions(X Basis)	Points	Energy
RSP-FD	1	$(104)^3$	1.496524844
RSP-FD	1	$(144)^3$	1.498189365
RSP-FD	1	$(200)^3$	1.499061950
RSP-FD	1	$(300)^3$	1.499632781
RSP-FD	1	$(500)^3$	1.499907103
RSP-FEDVR	20(x 3)	$(41)^3$	1.497422285
RSP-FEDVR	20 (x 4)	$(61)^3$	1.499996307
RSP-FEDVR	20 (x 6)	$(101)^3$	1.500000028
RSP-FEDVR	20 (x 8)	$(141)^3$	1.500000001
Exact			1.500000000

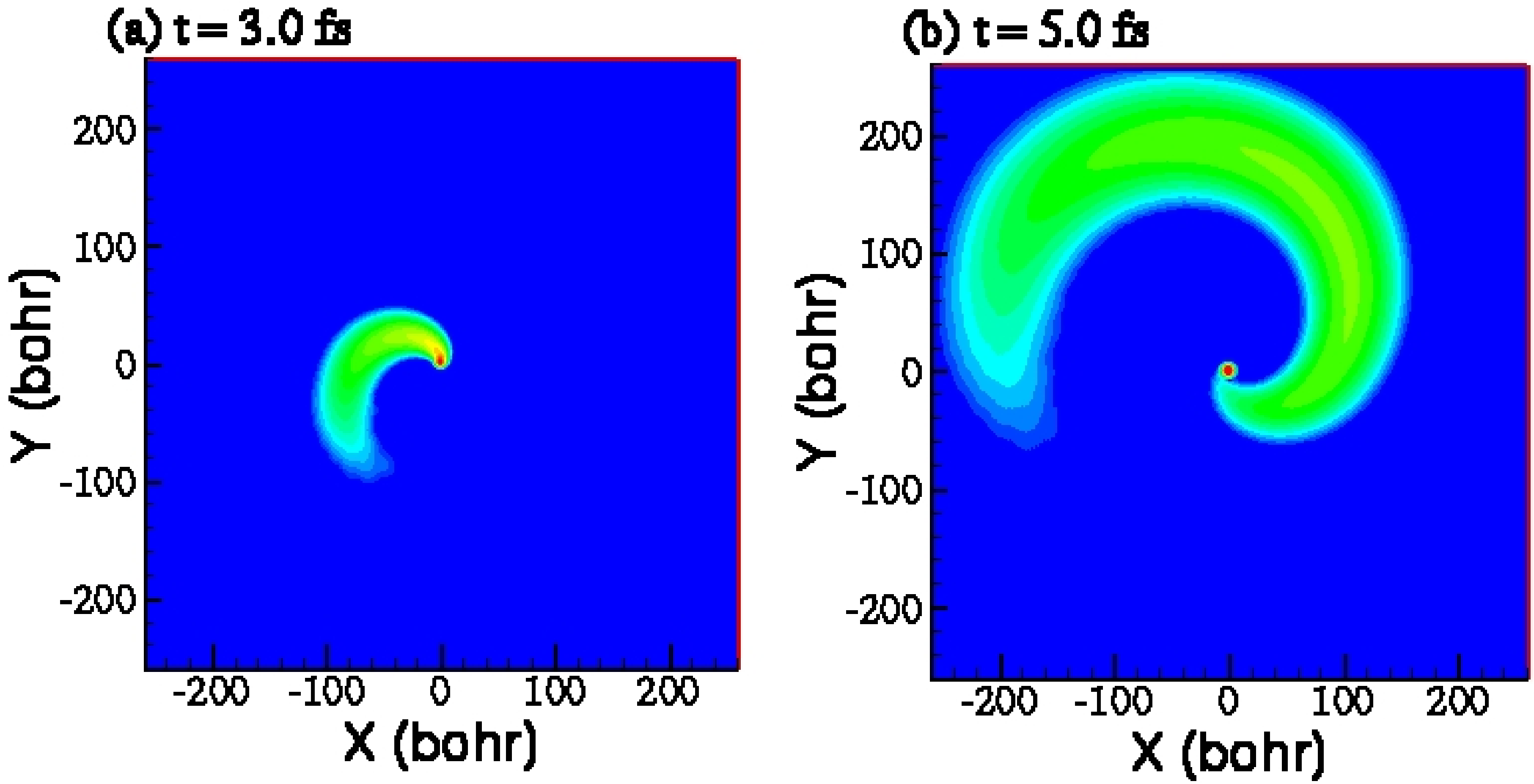
Solution of TD Close Coupling Equations for He Ground State E=-2.903114138 (-2.903724377) 160 elements x 4 Basis



He Probability Distribution



H Atom Exposed to a Circularly Polarized and Intense Few Cycle Pulse



5 fs Pulse, 800nm, I= $2*10^{14}$ W/cm^2

Double Slit Interferometer: BEC

- Potential

$$V(x,y,z,t) = .5\left[\left(\frac{\omega_y^2}{\omega_x^2}\right)y^2 + z^2\right]$$

Harmonic Trap

-

$$\left(\frac{V_0}{\hbar\omega_z}\right)\left[\exp(-\left(\frac{(x - x_0(t))^2}{2\sigma^2}\right) + \exp(-\left(\frac{(x + x_0(t))^2}{2\sigma^2}\right)\right]$$

$$x_0(t) = \alpha\, t + x_0$$

Double Well

Steps

- **Initialize – Load in trap plus double well potential**

- **Separate wells by ramping up the double well**

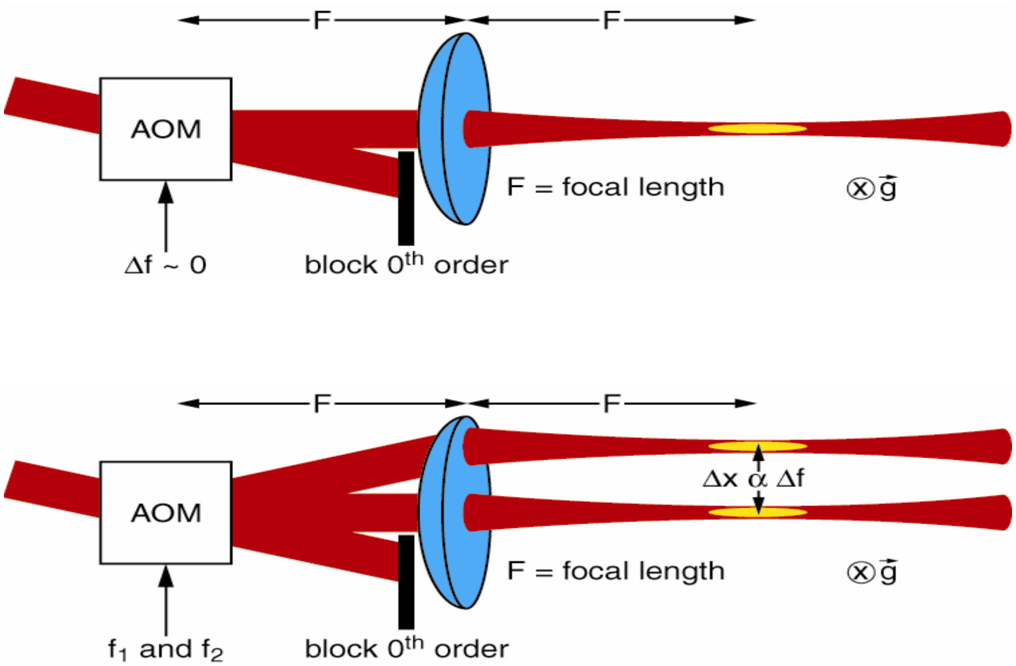
- **Hold**

- **Drop Trap - Ballistically expand**

Questions

- **Role of Collective Excitations created during the splitting**
- **Adiabaticity and time scales in experiment**
- **Validity of GP equation**

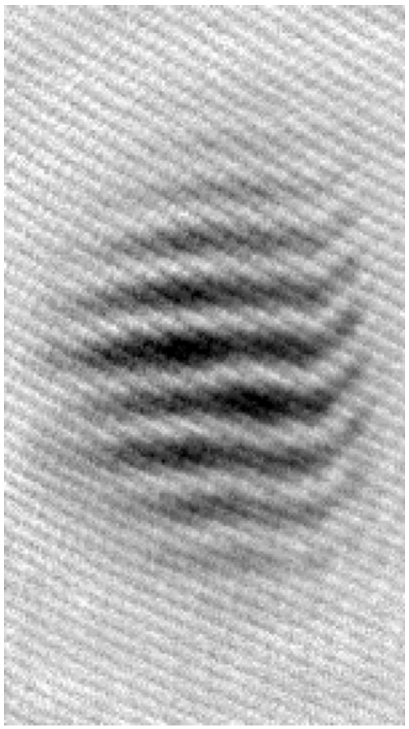
Double Slit Interferometer: Experiment



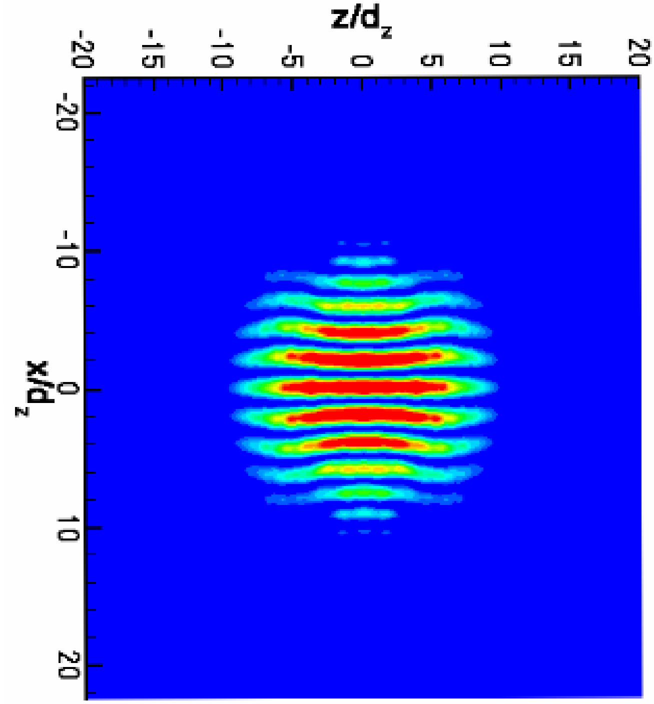
Y. Shin et. al. Phys. Rev. Lett. 92, 050405 (2004)

Interference Patterns

Experiment

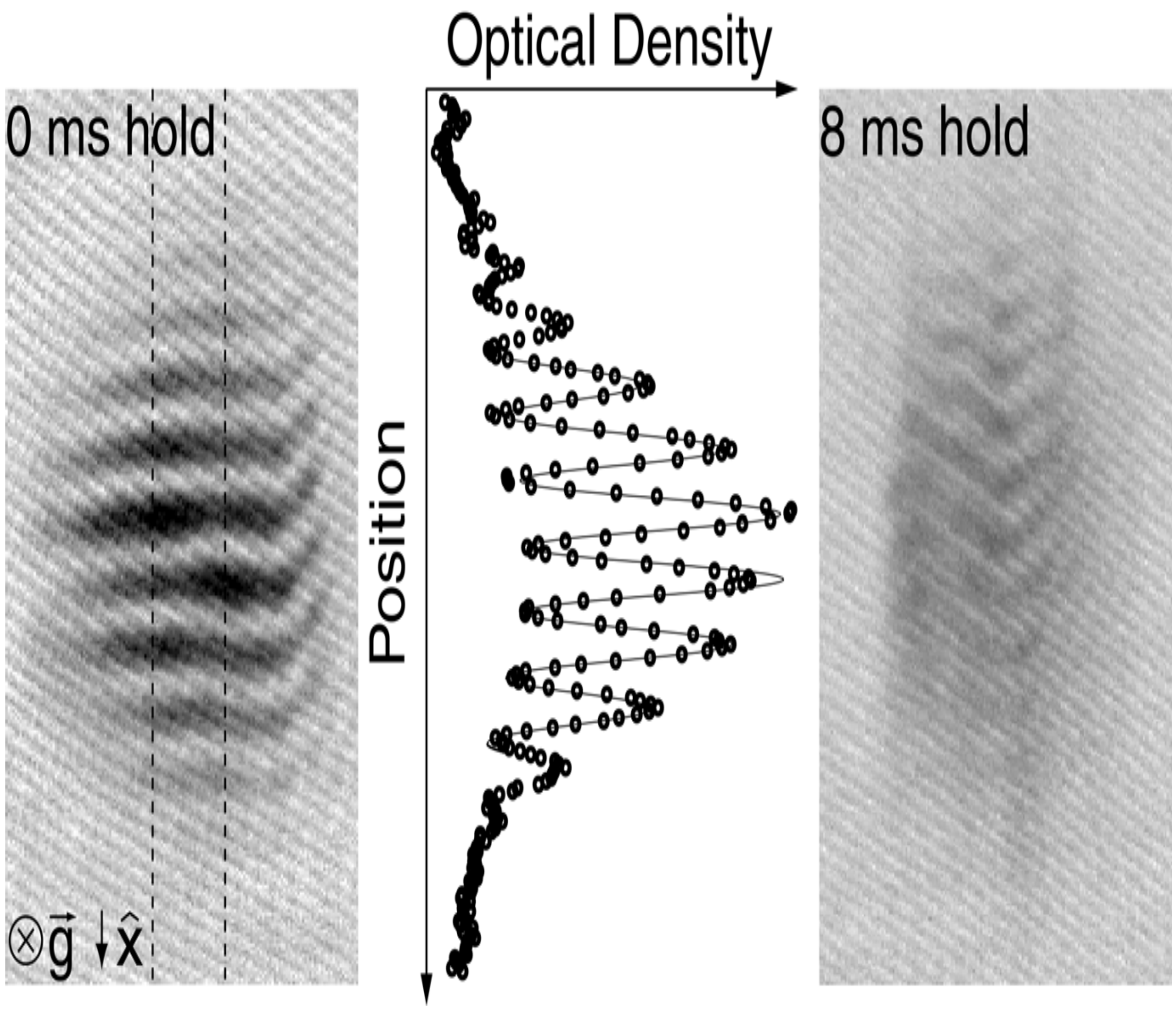


3D Computation



Collins et. al. Phys. Rev. A 71, 033628 (2005)

Interference Patterns



Observations

- Ramp Time
  - Short ramp times distort and dephase – Condensate excitations
  - Radial modes increase with barrier height and maximize when frequency of radial modes equal to Josephson plasma oscillation.
  - Further well separation produces no change
  - Anharmonicity along x axis plays important role in destroying interference pattern
  - Interference pattern stabilizes with longer ramping times –

In Contrast to Exp

Observations

- Hold Time
  - Long hold times degrade interference pattern – Agrees with experiment
  - Degradation saturates – In contrast to experiment
  - Distortion can be reduced with long ramps-In contrast to experiment
  - Shape of interference pattern – kinks and bends - In contrast to experiment

Conclusions

GP Mean Field Dynamics NOT Correct

Adiabaticity fails at long times

Beyond Mean Field

- Quantum Phase Model – Two mode approximation

$$H = \frac{E_c}{4}(a_1^+ a_1^+ a_1 a_1 + a_2^+ a_2^+ a_2 a_2) - \frac{E_j}{N}(a_1^+ a_2 + a_2^+ a_1)$$

where,

$$E_c = \text{on site energy}$$
$$E_j = E_j(0)\exp(-t/\tau) = \text{time-dependent Josephson coupling}$$

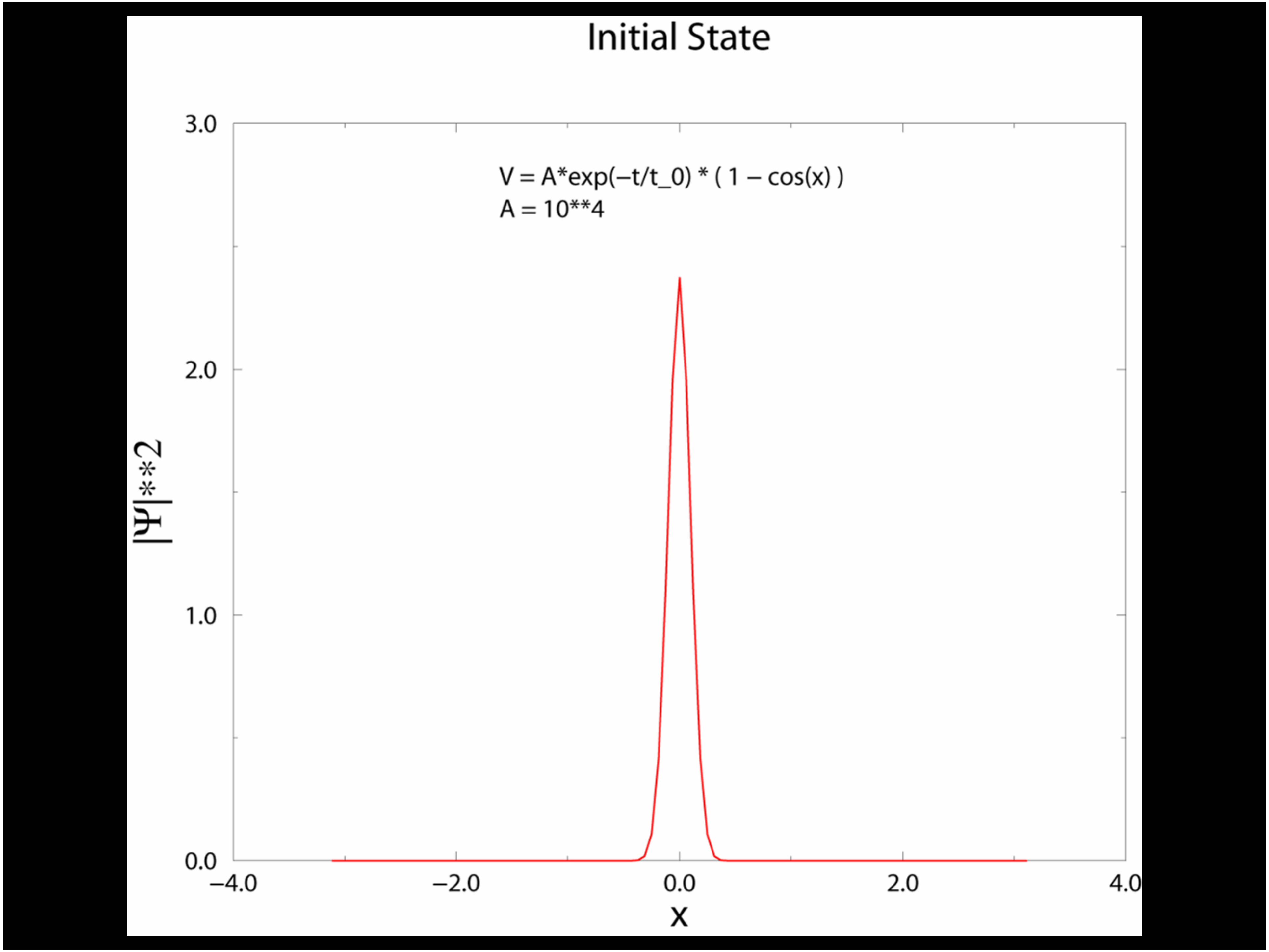
and

$$\tau = \frac{\Delta_R \hbar}{d\sqrt{2m(V_0 - \mu)}}$$

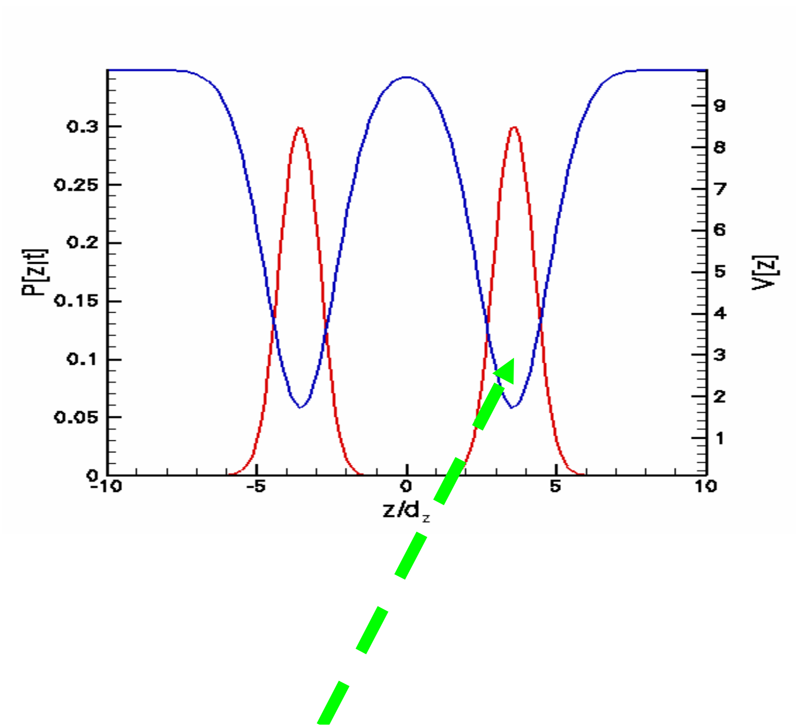
For $E_j << E_c$ where ϕ is the relative phase and

$$i\hbar\frac{\partial}{\partial t}\Psi(\phi,t) = \left[-\frac{E_C}{2}\frac{\partial^2}{\partial\phi^2} - E_j\cos(\phi)\right]\Psi(\phi,t)$$

$$| \Psi >= \int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\Psi(\phi,t) \mid \phi >$$
$$| \phi >= \sum_{-N/2}^{N/2} | n > \frac{\exp(in\phi)\tau}{n!}$$

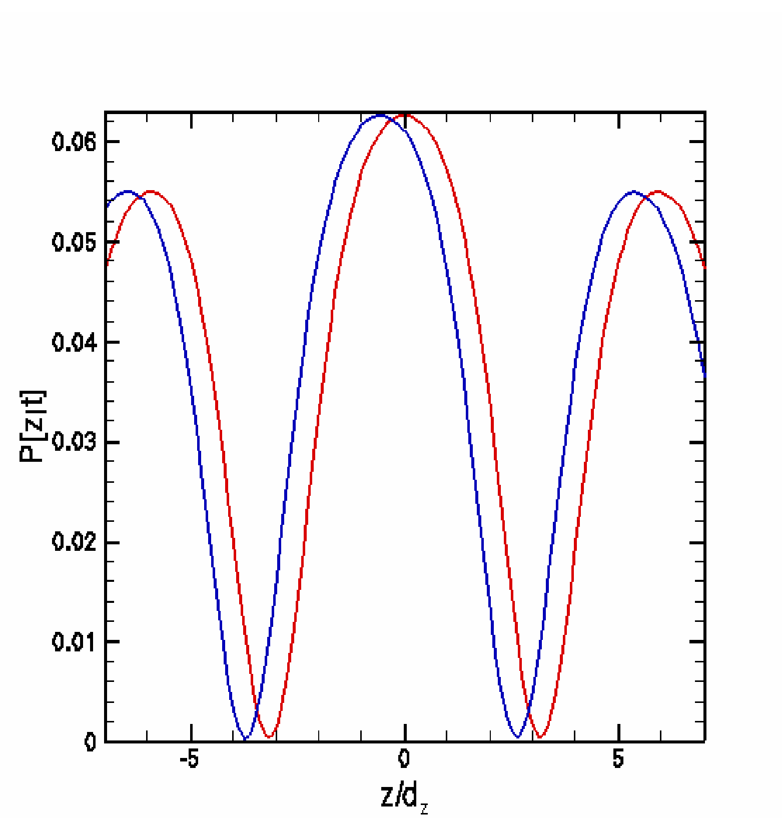

Initial State
V = A*exp(−t/t_0) * (1 − cos(x))
A = 10**4
|Ψ|**2
3.0
2.0
1.0
0.0
−4.0
−2.0
0.0
2.0
4.0
x

Perturbation: One well

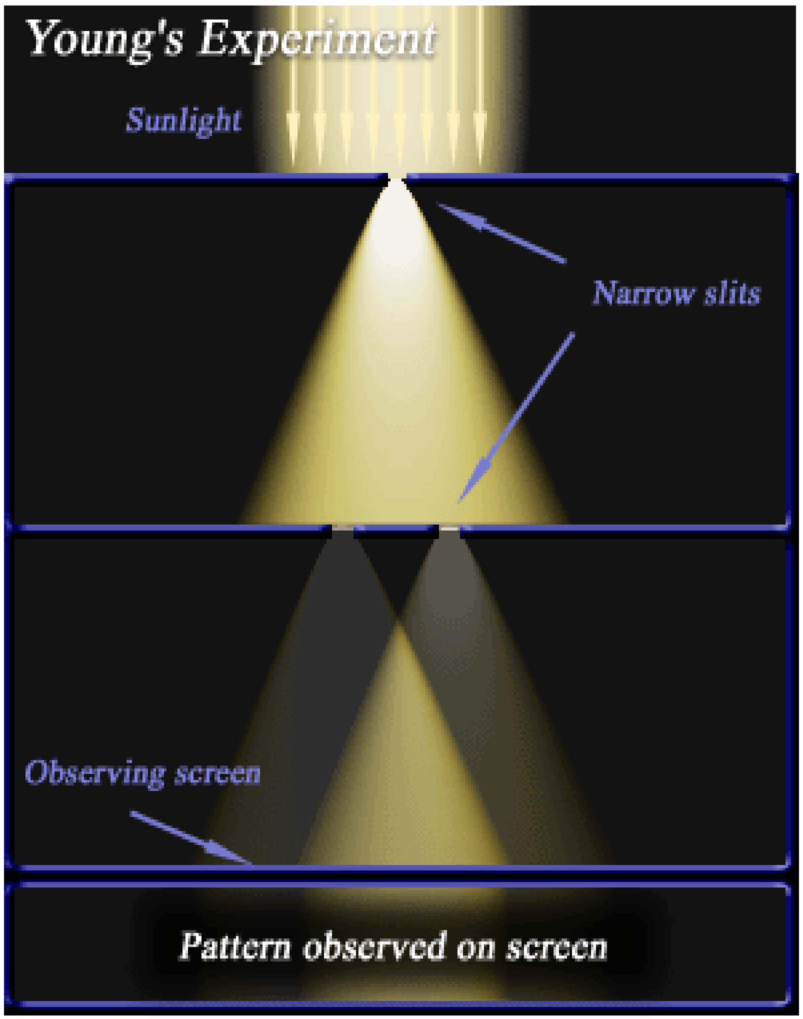


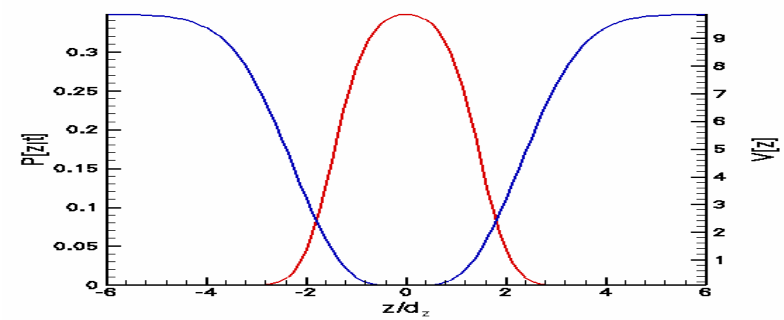
hν: τ_{per}

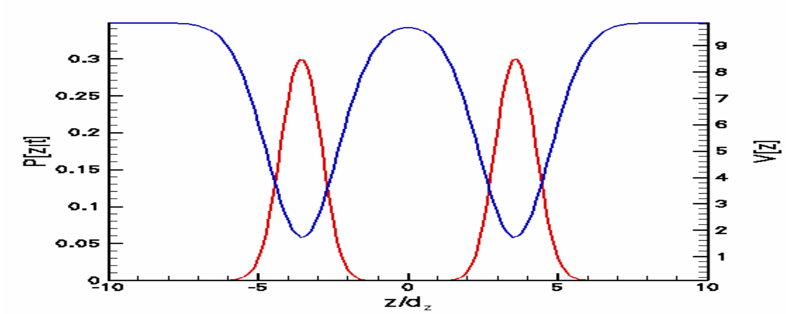
fringe shift: δ

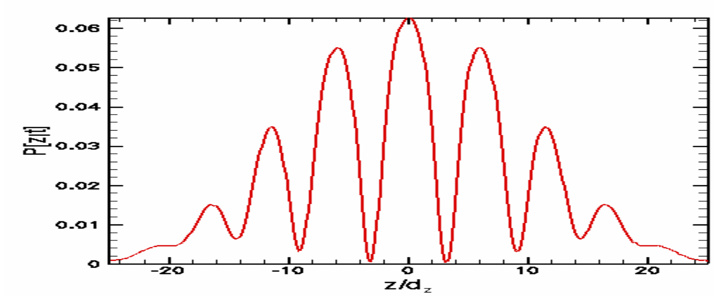


Double Slit Interferometer: BEC

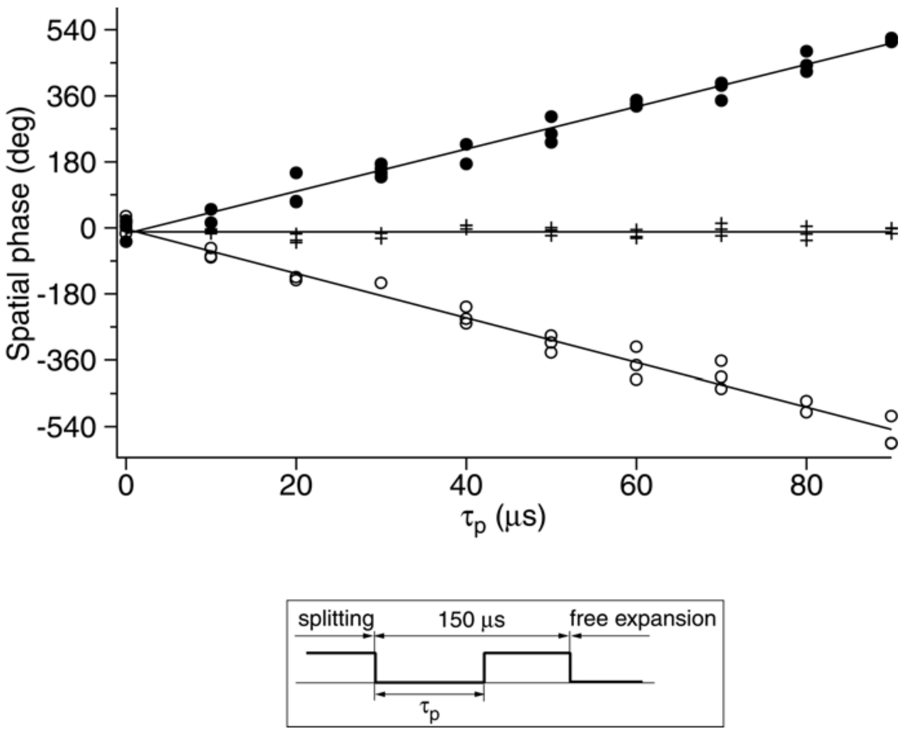


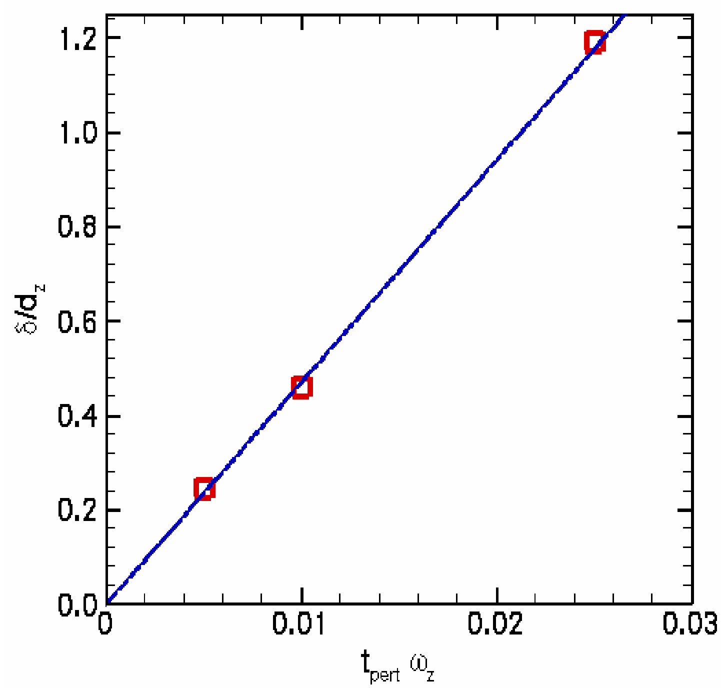


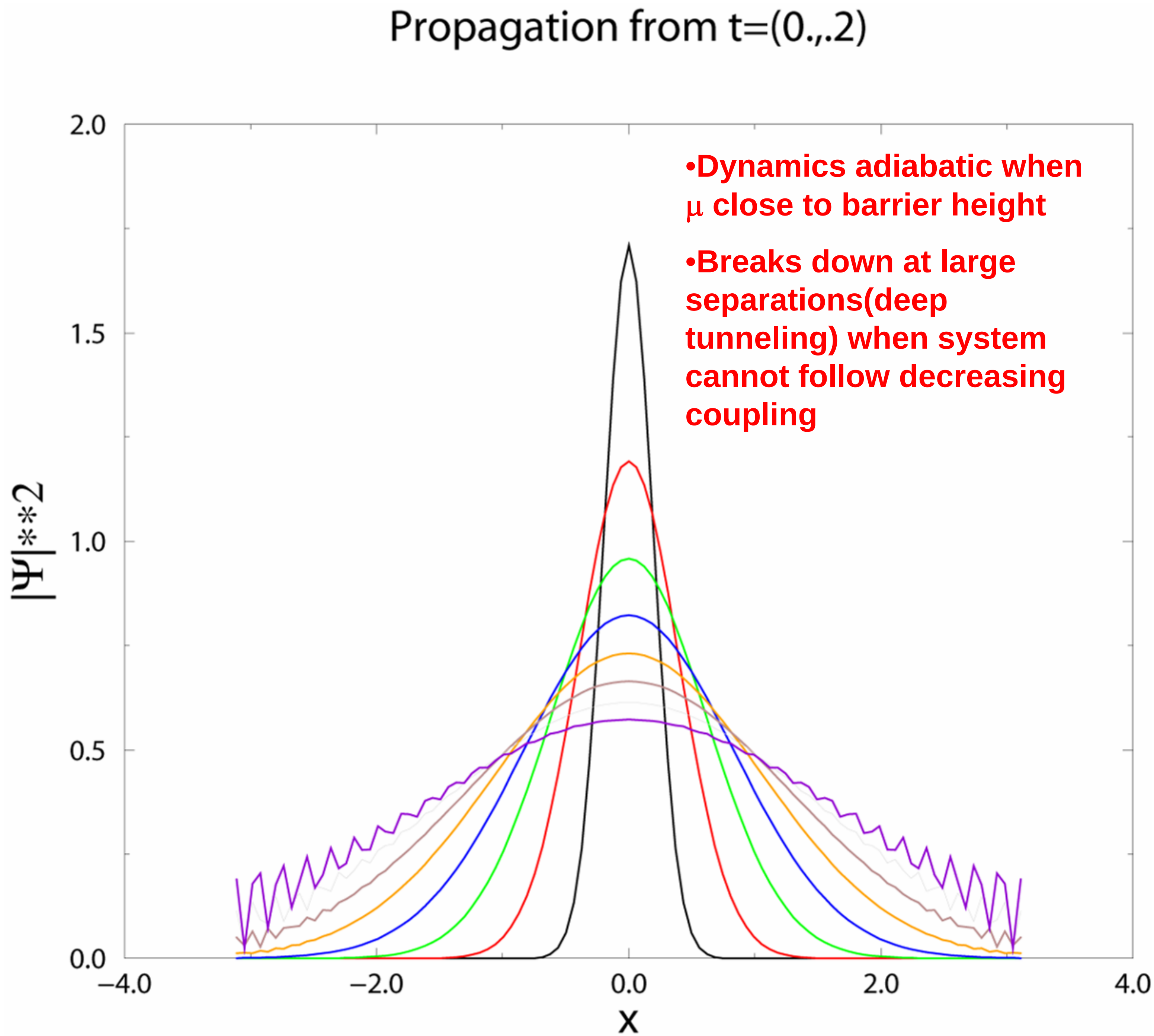




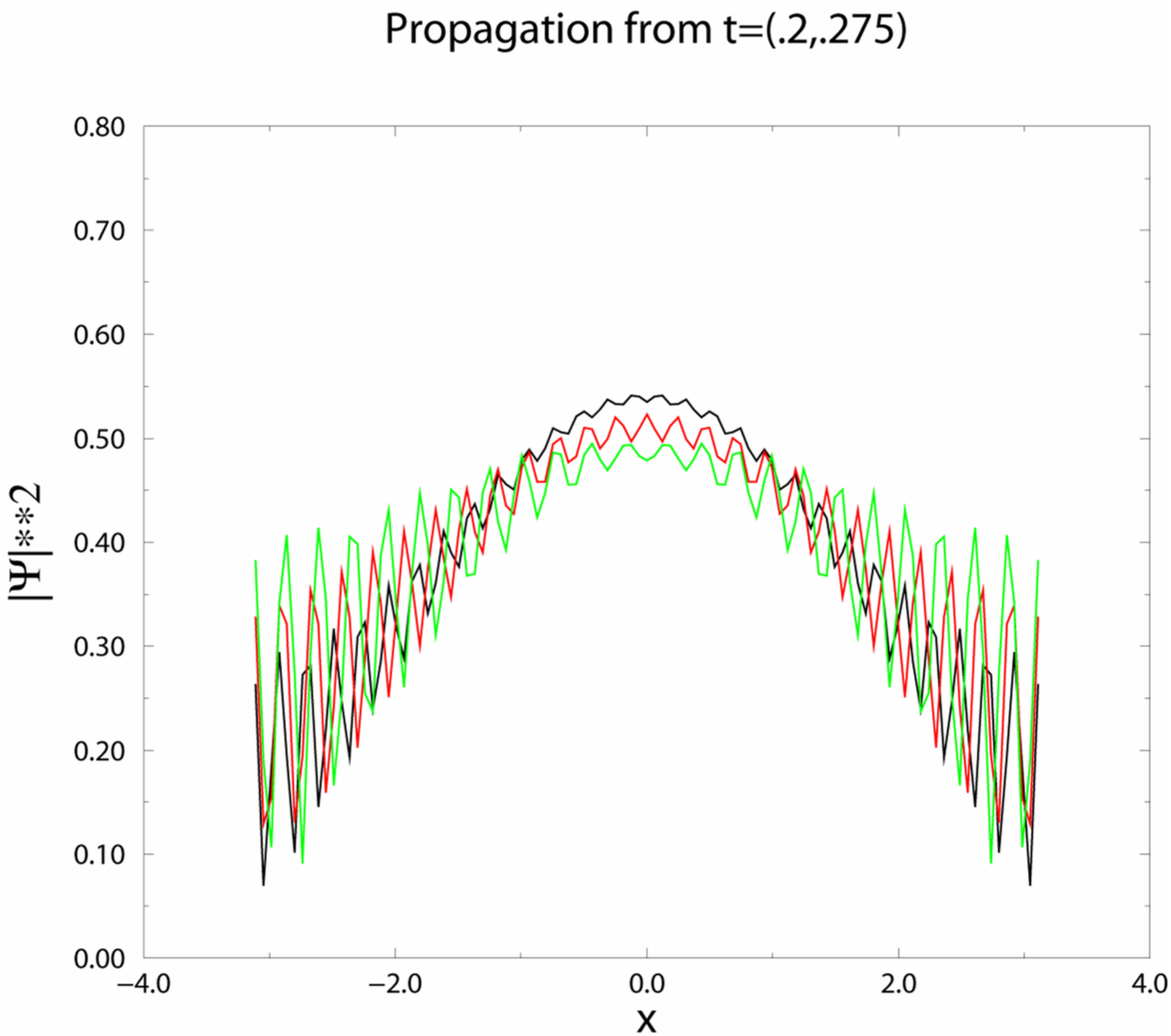
Perturbation: Pattern Shift

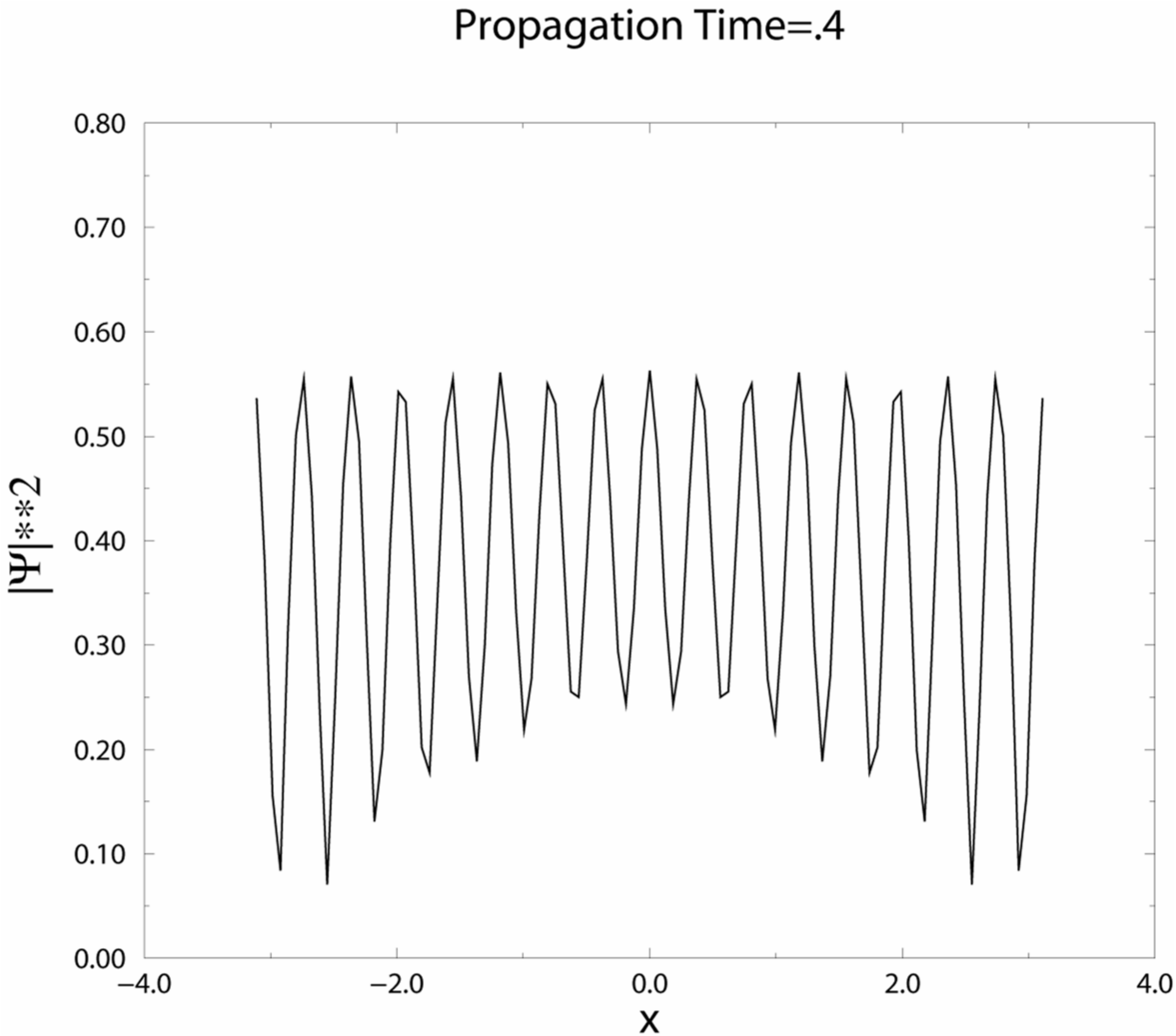


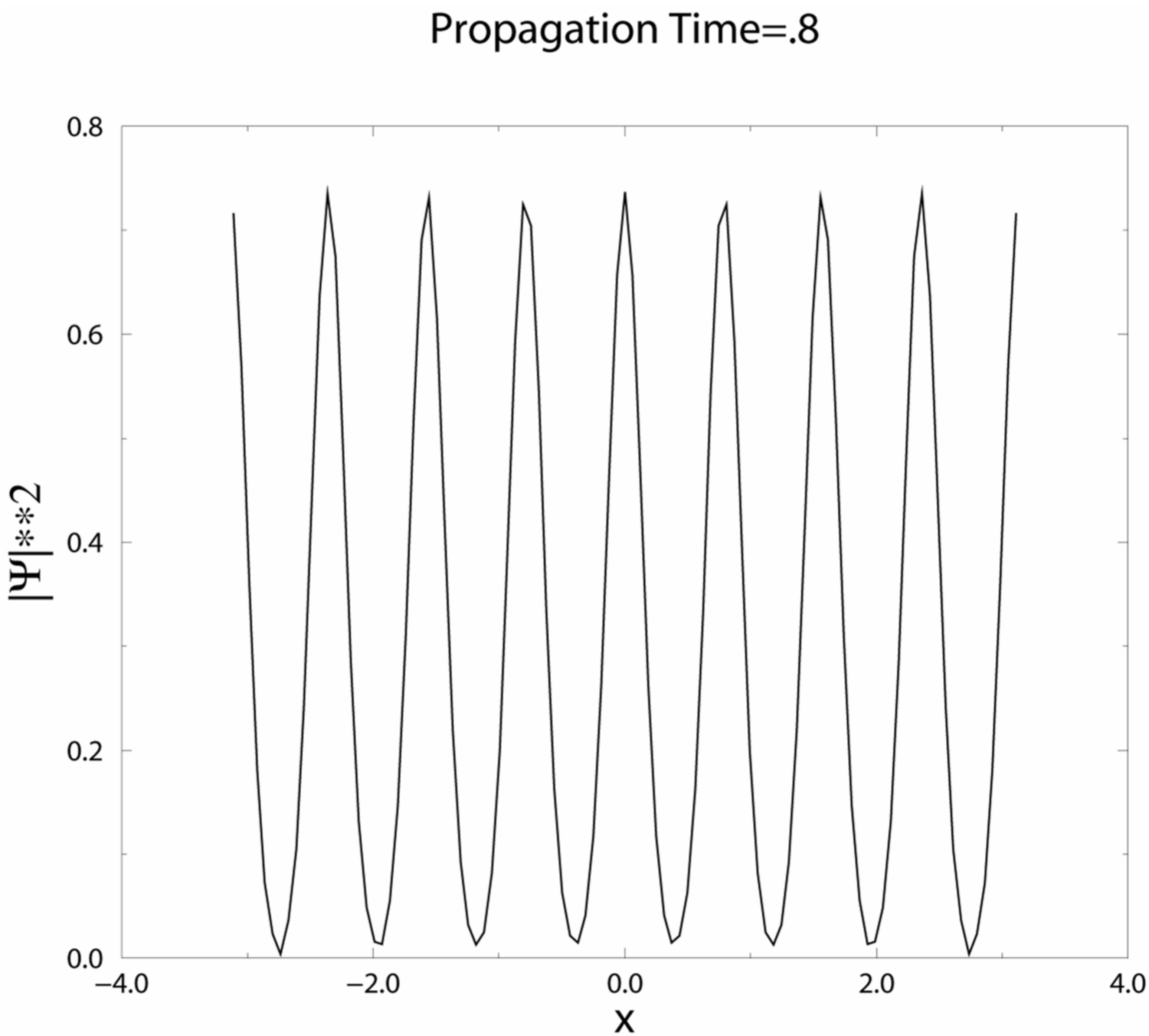


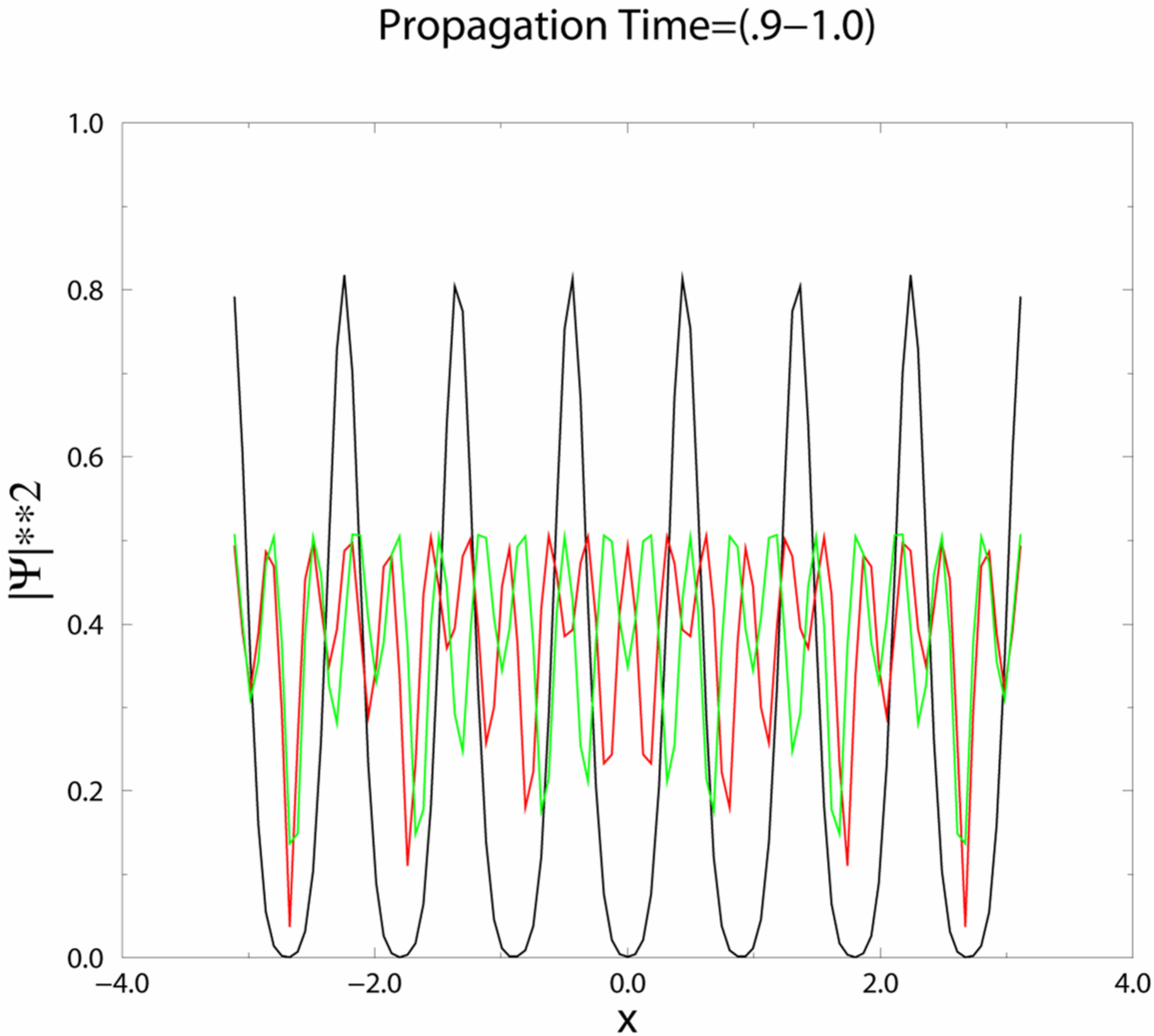


- Dynamics adiabatic when μ close to barrier height
- Breaks down at large separations(deep tunneling) when system cannot follow decreasing coupling


Propagation from t=(.2,.275)
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
|Ψ|**2
−4.0
−2.0
0.0
2.0
4.0
x


Propagation Time=.4
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
|Ψ|**2
−4.0
−2.0
0.0
2.0
4.0
x

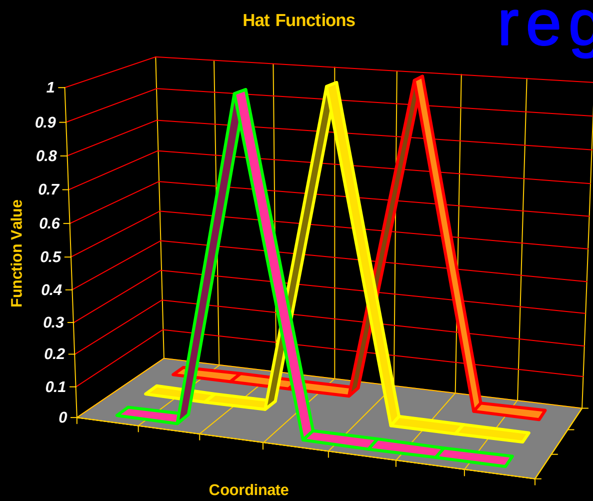

Propagation Time=.8
0.8
0.6
0.4
0.2
0.0
|Ψ|**2
−4.0
−2.0
0.0
2.0
4.0
x

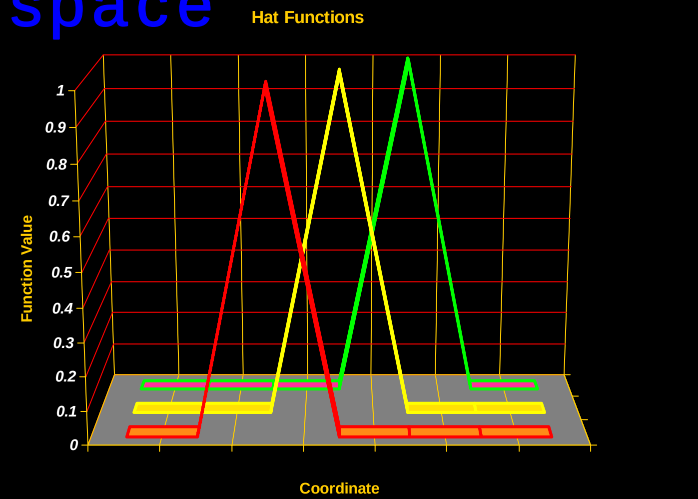


Propagation Time=(.9−1.0)
1.0
0.8
0.6
0.4
0.2
0.0
|Ψ|**2
−4.0
−2.0
0.0
2.0
4.0
x

Discretizations & Representations

- **Finite Element Methods - Basis functions have compact support –** they live only in a restricted region of space





  - **Often** only **functions or low order derivatives** continuous
  - **Ability to treat complicated geometry**
  - **Matrix representations are** sparse **–** discontinuities of derivatives at element boundaries must be carefully handled
    - Matrix elements require quadrature

Finite Element Discrete Variable Representation

- Properties
  - Space Divided into Elements – Arbitrary size
  - "Low-Order" Lobatto DVR used in each element: first and last DVR point shared by adjoining elements

$$F_n^i(x) = \frac{(\, f_n^i(x) + f_1^{i+1}(x)\,)}{\sqrt{w_n^i} + \sqrt{w_1^{i+1}}}$$

- Sparse Representations – N Scaling
- Close to Spectral Accuracy

Elements joined at boundary – Functions continuous but not derivatives

- Matrix elements requires NO Quadrature – Constructed from renormalized, single element, matrix elements

Finite Element DVR

- Structure of Matrix

h_{11}	h_{12}	h_{13}	h_{14}			
h_{21}	h_{22}	h_{23}	h_{24}			
h_{31}	h_{32}	h_{33}	h_{34}			
h_{41}	h_{42}	h_{43}	h_{44}	h_{45}	h_{46}	
			h_{54}	h_{55}	h_{56}	
			h_{64}	h_{65}	h_{66}	h_{67}
					h_{76}	h_{77}