Numerical Steepest Descent for Overlap Integrals of Hagedorn Wavepackets

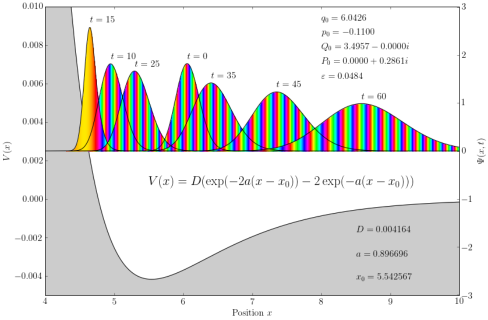
Raoul Bourquin

Disentis 2014

Outline

Motivation

- Simulation of Photoionization of Hg_2
  - Initial value $|\Psi_0\rangle$
  - Time-propagated value $|\Psi_t\rangle$



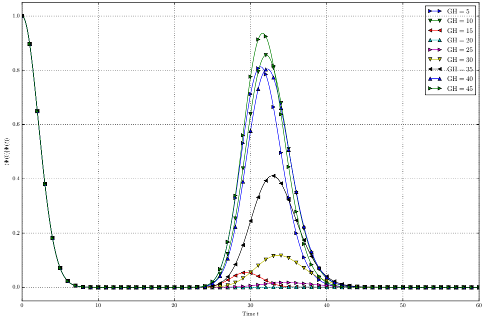
B. Stefanov, O. Iordanov, and L. Zarkova.
Interaction potential in ${}^1\Sigma_g{}^+ Hg_2$: fit to the experimental data.
Journal of Physics B: Atomic and Molecular Physics, 15(2):239, 1982.

Motivation

- Compute autocorrelation $|A(t)|$

$$A(t) := \langle \Psi_0 \,|\, \Psi_t \rangle = \int \cdots \int_{\mathbb{R}^D} \overline{\Psi_0(\underline{x})} \Psi_t(\underline{x}) \mathrm{d}\underline{x}$$

- Common techniques give *wrong* results

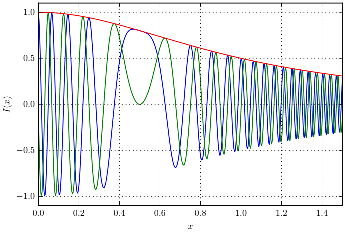


Highly Oscillatory Integrals

Typical Example

$$I = \int_\Omega f(\underline{x}) e^{\imath \omega g(\underline{x})} \mathrm{d}\underline{x}$$

- Oscillator $g(\underline{x})$ (non-oscillatory)
- Envelope $f(\underline{x})$ (non-oscillatory)
- Frequency $\omega \in \mathbb{R}^+$
- Domain $\Omega \subseteq \mathbb{R}^D$



$$f(x) = \frac{1}{1+x^2}$$

$$g(x) = \left(x - \frac{1}{2}\right)^2$$

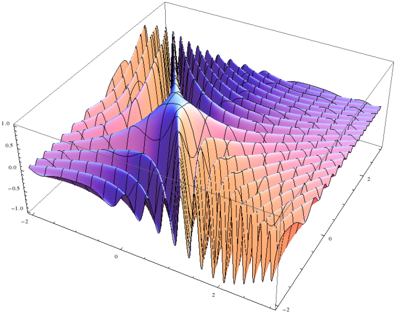
$$\omega = 100$$

Highly Oscillatory Integrals

Typical Example

Compute:

$$\int_{-2}^{3}\int_{-2}^{3} \frac{e^{5\imath\left(x^2-xy-y^2\right)}}{1+(x+y)^2}\mathrm{d}x\mathrm{d}y$$



where:

$$f(x) = \frac{1}{1+(x+y)^2}$$
$$g(x) = x^2 - xy - y^2$$

and $\omega = 5$

Numerical Steepest Descent

Central Observations

Oscillatory part $e^{\imath\omega g(x)}$ of:

$$I = \int_a^b f(x) e^{\imath\omega g(x)} \mathrm{d}x$$

does:

- decay exponentially fast for increasing $\Im g(z)$
- not oscillate for constant $\Re g(z)$

because:

$$e^{\imath\omega g(z)} = e^{\imath\omega(\Re g(z) + \imath\Im g(z))} = e^{\imath\omega\Re g(z)} e^{-\omega\Im g(z)}$$

Numerical Steepest Descent

Main Idea and Overview

- Transform the integrand such that it is no longer oscillatory but rather exponentially decaying.

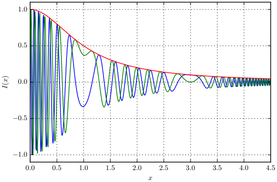
- Find a coordinate transformation $z = h(\tau)$ such that the *real* part of $g(z)$ is constant.
- Apply Cauchy's Theorem for contour integrals along $h(\tau)$.

Numerical Steepest Descent

Contributions to the Integral

Which parts do contribute?

- Endpoints of the interval: $[a, b]$
- *stationary points*: $\nabla g(\underline{x}) = \underline{0}$
- *resonance points*: $\nabla g(\underline{x}) \perp \partial\Omega$



Intuitive explanation:

- Oscillations in integrand generally cancel
- Places with locally no oscillations contribute

Numerical Steepest Descent

The Path Equation

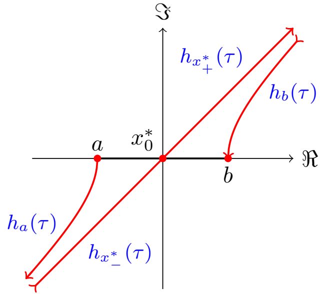
- Set of contributing points:

$$\Theta := \{a, b\} \cup \{x_j^*\}_j$$

- Path equations:
  - $\forall \xi \in \Theta$:

$$g(h_\xi(\tau)) = g(\xi) + \imath\tau$$

  - yields path $h_\xi(\tau)$ with $\tau \in \mathbb{R}_0^+$



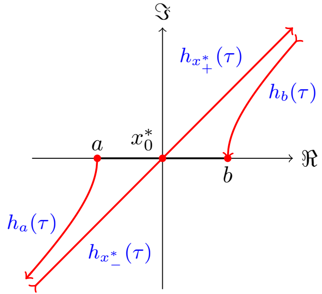
Numerical Steepest Descent

Solving the Path Equation

- Inverse of g possibly multivalued
- Endpoints:
  - compute h_a and h_b
  - choose by conditions:

$$h_a(0) = a, \quad h_b(0) = b$$

- Stationary points:
  - choose two $h_{x_j^*,+}$ and $h_{x_j^*,-}$
  - paths lead to the same *valley*



Numerical Steepest Descent

Assemble the Parts

- Perform transformations $x \mapsto h_\xi(\tau)$

$$J[\xi] := e^{\imath\omega g(\xi)} \int_0^\infty f(h_\xi(\tau))\, h'_\xi(\tau)\, e^{-\omega\tau}\, \mathrm{d}\tau$$

- Apply Cauchy's Theorem

$$I = e^{\imath\omega g(a)} J[a] + \sum_j \left(J[x^*_{j,+}] - J[x^*_{j,-}] \right) - e^{\imath\omega g(b)} J[b]$$

- Restrictions: poles and branch cuts
- Just transformation of the problem

Numerical Steepest Descent

Quadrature

- New problem to compute:

$$J[\xi] := e^{\imath\omega g(\xi)} \int_0^\infty f\left(h_\xi(\tau)\right) h'_\xi(\tau)\, e^{-\omega\tau}\, \mathrm{d}\tau$$

- (Generalized) Gauss-Laguerre quadrature $\{\gamma_k, w_k\}_{k=1}^K$

$$J[\xi] \approx \frac{e^{\imath\omega g(\xi)}}{\omega} \sum_{k=1}^K f\left(h_\xi\left(\frac{\gamma_k}{\omega}\right)\right) h'_\xi\left(\frac{\gamma_k}{\omega}\right) w_k$$

- Integrals (weakly) singular
- There can be many paths

Numerical Steepest Descent

Main Decomposition Theorem

Theorem (Huybrechs and Vandewalle, 2006)

Assume that the functions f and g are analytic in a simply connected and sufficiently (infinitely) large complex region D containing the interval $[a, b]$. Assume further that the equation $g(x) = 0$ has only one solution x^* in D and $x^* \in (a, b)$. Define $g_1 := g|_{[a,x^*]}$ and $g_2 := g|_{[x^*,b]}$. If the following conditions hold:

$$\exists m \in \mathbb{N} : |f(z)| = \mathcal{O}(|z|^m),$$

$$\exists \omega_0 \in \mathbb{R} : |g_1^{-1}(z)| = \mathcal{O}(e^{\omega_0 |z|})$$

$$|g_2^{-1}(z)| = \mathcal{O}(e^{\omega_0 |z|})$$

as $|z| \to \infty$ then

Numerical Steepest Descent

Main Decomposition Theorem, continued

Theorem (Huybrechs and Vandewalle, 2006)

there exist functions $F_j(\xi), j = 1, 2$ of the form:

$$F_j(\xi) := \int_{\Gamma_{\xi,j}} f(z) e^{\imath \omega g(z)} \mathrm{d}z$$

with $\Gamma_{\xi,j}$ a path that starts at ξ, such that:

$$\int_s^t f(z) e^{\imath \omega g(z)} \mathrm{d}z = F_1(s) - F_1(x^*) + F_2(x^*) - F_2(t), \quad \forall \omega > (m+1)\omega_0,$$

for $s \in [a, x^*]$ and $t \in [x^*, b]$. A parameterization $h_{\xi,j}(\tau)$, $\tau \in [0, \infty)$, for $\Gamma_{\xi,j}$ exists such that the integrand of F_j is $\mathcal{O}(e^{-\omega\tau})$.

Numerical Steepest Descent

Extensions and Outlook

This was for closed intervals. What about:

- semi-infinite intervals $[a, \infty)$?
  - works the same (no correct proof yet)
- infinite intervals $(-\infty, \infty)$?
  - decompose into two semi-infinite intervals
- multiple stationary points?
  - apply procedure at each x_i^*
- complex stationary points $x^* \in \mathbb{C} \setminus \mathbb{R}$?
  - put path through the point
- higher dimensions?
  - much more involved and complicated theory

Numerical Steepest Descent

Example $g(x) := x^2$

$$I = \int_{-1}^{1} 1\, e^{\imath\omega x^2} \mathrm{d}x \quad \text{with} \quad g(x) := x^2$$

$$g'(x) = 0 \quad \Rightarrow \quad x^* = 0$$

$$g(h_{-1}) = g(-1) + \imath\tau \Rightarrow h_{-1}(\tau) = -\sqrt{1+\imath\tau}, \quad h'_{-1}(\tau) = -\frac{\imath}{2\sqrt{1+\imath\tau}}$$

$$g(h_1) = g(1) + \imath\tau \Rightarrow h_1(\tau) = \sqrt{1+\imath\tau}, \quad h'_1(\tau) = \frac{\imath}{2\sqrt{1+\imath\tau}}$$

$$g(h_0) = g(0) + \imath\tau \Rightarrow h_{0,\pm}(\tau) = \pm\sqrt{\imath\tau}, \quad h'_{0,\pm}(\tau) = \pm\frac{\imath}{2\sqrt{\tau}}$$

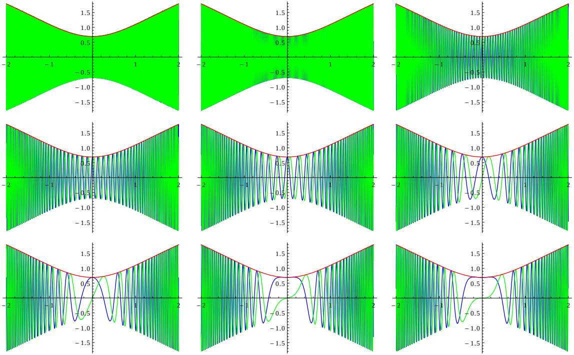
$$I = e^{\imath\omega} \int_0^\infty -\frac{\imath e^{-\omega\tau}}{2\sqrt{1+\imath\tau}} \mathrm{d}\tau - \int_0^\infty -\frac{\imath e^{-\omega\tau}}{2\sqrt{\tau}} \mathrm{d}\tau + \int_0^\infty \frac{\imath e^{-\omega\tau}}{2\sqrt{\tau}} \mathrm{d}\tau - e^{\imath\omega} \int_0^\infty \frac{\imath e^{-\omega\tau}}{2\sqrt{1+\imath\tau}} \mathrm{d}\tau$$

Numerical Steepest Descent

Complex Stationary Points

$$\int_{-2}^{2} \log\left(2+x^2\right) e^{50\imath\left(\delta x + \frac{x^3}{3}\right)} \mathrm{d}x$$

with $\delta \in \{10, 5, 2, 1, \frac{1}{2}, \frac{1}{5}, \frac{1}{10}, \frac{1}{100}, 0\}$ and $x^* = \imath\sqrt{\delta}$

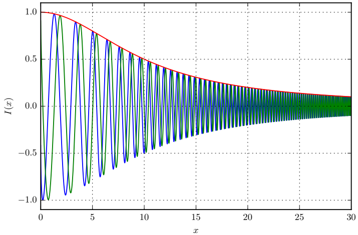


Numerical Steepest Descent

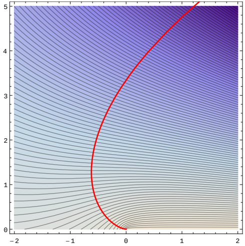
Semi-open Intervals

$$I = \int_0^\infty \frac{100}{100 + x^2} \exp\left(\imath \omega e^{\sqrt{x}}\right) \mathrm{d}x$$

with $\omega = 2$



$$h_a(\tau) = \log(1 + \imath\tau)^2$$



$$I = 200 e^{\imath\omega} \int_0^\infty \frac{\imath \log(1+\imath\tau) e^{-\omega\tau}}{(1+\imath\tau)\left(100 + \log^4(1+\imath\tau)\right)} \mathrm{d}\tau$$

Hagedorn Wavepackets

- Time-dependent Schrödinger Equation (TDSE)

$$\imath\varepsilon^2 \frac{\partial \Psi}{\partial t} = \left(-\frac{\varepsilon^4}{2} \Delta_x + V(\underline{x}) \right) \Psi$$

- semiclassical scaling: ε^2 instead of $\hbar$
  - $0.001 < \varepsilon < 0.1$

Hagedorn Wavepackets

Definition

- Diagonalize quadratic Hamiltonian

$$\mathcal{H} = \frac{1}{2}\left(\alpha p^2 + \beta(xp + px) + \gamma x^2\right)$$

- Position x and momentum p
- Eigenvalues: $k + \frac{1}{2}$
- Eigenfunctions: $\phi_k, \quad k = 0, 1, 2, \ldots$
- Yields wavepackets $\phi_k(x)$

Hagedorn Wavepackets

Explicit Representation in 1D

- Explicit expression

$$\phi_0(x) = (\pi\varepsilon^2)^{-\frac{1}{4}} Q^{-\frac{1}{2}} \exp\left(\frac{\imath}{2\varepsilon^2} PQ^{-1}(x-q)^2 + \frac{\imath}{\varepsilon^2} p(x-q)\right)$$

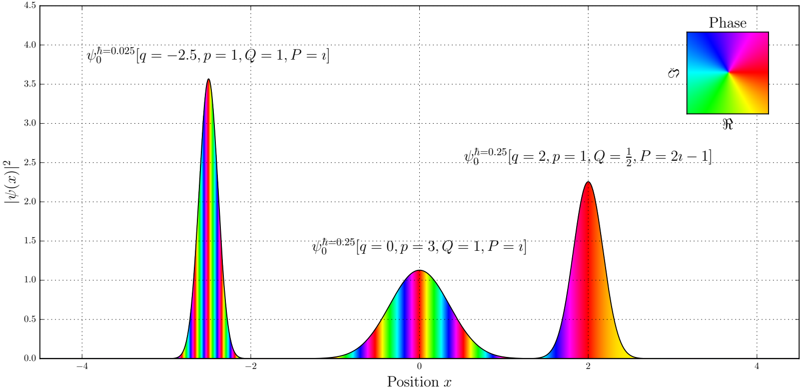
- Parametrized by $q(t), p(t) \in \mathbb{R}$ and $Q(t), P(t) \in \mathbb{C}$
- Raising and Lowering Operators

$$\phi_{k+1} = \frac{1}{\sqrt{k+1}} \mathcal{R}\phi_k \qquad \phi_{k-1} = \frac{1}{\sqrt{k}} \mathcal{L}\phi_k$$

- $\mathcal{L}\phi_0 \equiv 0$
- Orthonormal Basis of $L^2(\mathbb{R})$

Hagedorn Wavepackets

Examples in 1D



Hagedorn Wavepackets

Explicit Representation in Higher Dimensions

- Groundstate

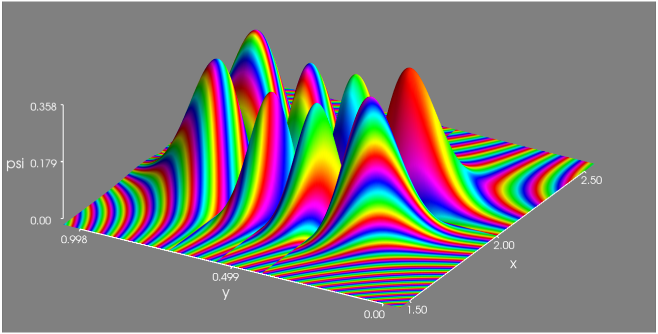
$$\phi_{\underline{0}}(\underline{x}) = (\pi\varepsilon^2)^{-\frac{D}{4}} (\det \mathbf{Q})^{-\frac{1}{2}} \exp\left(\frac{\imath}{2\varepsilon^2}\left\langle(\underline{x}-\underline{q}), \mathbf{P}\mathbf{Q}^{-1}(\underline{x}-\underline{q})\right\rangle + \frac{\imath}{\varepsilon^2}\left\langle \underline{p}, (\underline{x}-\underline{q})\right\rangle\right)$$

- Parameters $\underline{q}(t), \underline{p}(t) \in \mathbb{R}^D$ and $\mathbf{Q}(t), \mathbf{P}(t) \in \mathbb{C}^{D\times D}$
  - Parameter set $\Pi := \{\underline{q}, \underline{p}, \mathbf{Q}, \mathbf{P}\}$
- Multi-index $\underline{k} \in \mathbb{N}_0^D$
- Higher states by raising and lowering operators $\mathcal{R}$, $\mathcal{L}$
- Orthonormal Basis of $L^2(\mathbb{R}^D)$

Hagedorn Wavepackets

Example in 2D

$$\phi_{\underline{k}}[\Pi](\underline{x}) \qquad \underline{k} = (1,3) \quad \varepsilon = \frac{1}{10}$$



$$\underline{q} = \begin{pmatrix} 2 \\ \sqrt{3\varepsilon} \end{pmatrix} \quad \underline{p} = \begin{pmatrix} -\frac{2}{5} \\ \sqrt{\frac{4\varepsilon}{12}} \end{pmatrix} \quad \mathbf{Q} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\sqrt{\frac{4}{5}}} \end{pmatrix} \quad \mathbf{P} = \begin{pmatrix} -2+\imath & -3 \\ -3\sqrt{\frac{4}{5}} & \imath\sqrt{\frac{4}{5}} \end{pmatrix}$$

Hagedorn Wavepackets

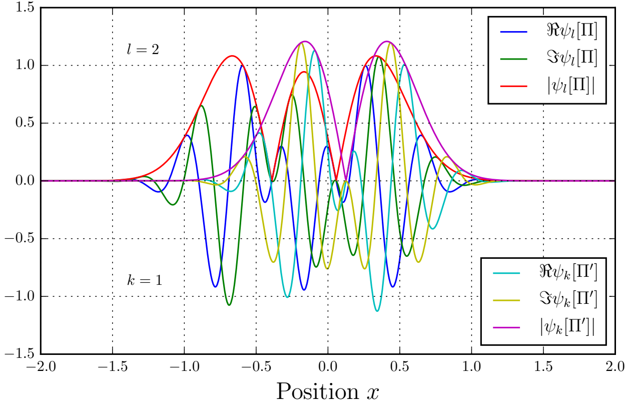
- Overlap integrals

$$I = \left\langle \phi_{\underline{k}}[\Pi] \,\middle|\, \phi_{\underline{l}}[\Pi'] \right\rangle := \int \cdots \int_{\mathbb{R}^D} \overline{\phi_{\underline{k}}[\Pi](\underline{x})}\, \phi_{\underline{l}}[\Pi'](\underline{x}) \mathrm{d}\underline{x}$$

- Parameter sets: Π and Π'
- Highly oscillatory
  - similar position: $\underline{q} \approx \underline{q}'$
  - opposite momentum: $\underline{p} \approx -\underline{p}'$
  - small ε

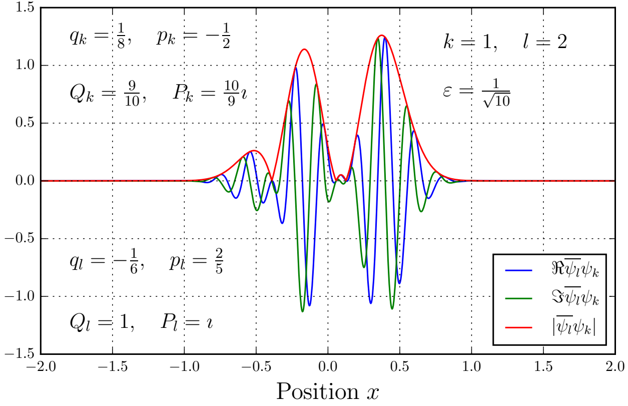
Hagedorn Wavepackets

Two Wavepackets



Hagedorn Wavepackets

The Integrand



Steepest Descent for Wavepackets

Wavepackets

- Wavepackets of the form:

$$\phi(\underline{x}) \sim p\left(\underline{x}\right) \exp\left(\frac{\imath}{\varepsilon^2} g\left(\underline{x}\right)\right)$$

- Oscillator term:

$$g\left(\underline{x}\right) := \frac{1}{2}\left\langle \underline{x} - \underline{q}, \mathbf{PQ}^{-1}\left(\underline{x} - \underline{q}\right)\right\rangle + \left\langle \underline{p}, \underline{x} - \underline{q}\right\rangle$$

- Frequency $\omega = \frac{1}{\varepsilon^2}$

Steepest Descent for Wavepackets

Overlap Integrals

- Integrals look like

$$\langle \phi_k, \phi_l \rangle = \int_{-\infty}^{\infty} \overline{p_k(\underline{x})} p_l(\underline{x}) \exp\left(\frac{\imath}{\varepsilon^2}\left(-\overline{g_k(\underline{x})} + g_l(\underline{x})\right)\right) \mathrm{d}\underline{x}$$

- Combine oscillators $-\overline{g_k(\underline{x})} + g_l(\underline{x})$ into $g(\underline{x})$

Steepest Descent for Wavepackets

Combined Oscillator

- We can find

$$g(\underline{x}) = \underline{x}^{\mathsf{H}} \mathbf{A} \underline{x} + \underline{b}^{\mathsf{T}} \underline{x} + c$$

- where

$$\mathbf{A} = \frac{1}{2} \left(\mathbf{P_l} \mathbf{Q_l}^{-1} - (\mathbf{P_k} \mathbf{Q_k}^{-1})^{\mathsf{H}} \right)$$

- General quadratic form
- Properties of A
  - **A** *not* Hermitian
  - $\Re \mathbf{A}$ and $\Im \mathbf{A}$ symmetric

  $\Rightarrow$ Need new, special techniques

Steepest Descent for Wavepackets

Transformation of the Oscillator

- Goal: Decoupling the paths
- Remove linear Term $\underline{b}^{\mathsf{T}}\underline{x}$
  - Multivariate completion of the square
  - $g(x') = x'^{\mathsf{H}}\mathbf{A}x' + c$
- Diagonalization of $\mathbf{A}$
  - Optimal, *not* possible via unitary matrices ($\mathbf{A}$ not Hermitian)
- Upper-triangular form
  - Schur Decomposition: $\mathbf{A} = \mathbf{U}^{\mathsf{H}}\mathbf{T}\mathbf{U}$
  - $g(x'') = x''^{\mathsf{H}}\mathbf{T}x'' + c'$

Steepest Descent for Wavepackets

Oscillator Decomposition

- Decompose $g(\underline{x}) = \underline{x}^{\mathrm{H}} \mathbf{T} \underline{x}$

$$g\left(x_1, \ldots, x_N\right) = \sum_{i=1}^{N} g_i(x_i, \ldots, x_N)$$

- where

$$g_i\left(x_i, x_{i+1}, \ldots, x_N\right) := t_{i,i} x_i^2 + \sum_{j=i+1}^{N} t_{i,j} x_i x_j$$

- Quadratic in x_i
- Rows of $\mathbf{T}$

Steepest Descent for Wavepackets

Stationary Points

- Compute stationary points

$$\dot{g}_i := \frac{\partial g_i}{\partial x_i} \stackrel{!}{=} 0$$

- Find

$$x_i^* \left(x_{i+1}, \ldots, x_N\right) = -\frac{\sum_{j=i+1}^{N} t_{i,j} x_j}{2 t_{i,i}}$$

- Depends on $x_{i+1}, \ldots, x_N$

Steepest Descent for Wavepackets

Path Equations

- For each oscillator g_i

$$g_i\left(h_i\left(p_i,\ldots\right),\ldots\right) = g_i\left(x_i^*(\ldots),\ldots\right) + \imath p_i$$

- Each $\ldots$ is $x_{i+1},\ldots,x_N$
- Simple quadratic equations
- Paths:

$$h_i^{\pm}(p_i) = \pm\sqrt{\frac{\imath p_i}{t_{i,i}}} - \frac{1}{2t_{i,i}}\sum_{j=i+1}^{N} t_{i,j}x_j$$

- Path derivatives:

$$\dot{h}_i^{\pm}(p_i) = \frac{\partial h_i\left(p_i\right)}{\partial p_i} = \pm\frac{\sqrt{\imath}}{2\sqrt{t_{i,i}}\sqrt{p_i}}$$

Steepest Descent for Wavepackets

Nested Structure of Oscillatory Integrals

- Start with inner-most integrand

$$i_1(x_1, \ldots, x_N) := f(\underline{x}) \exp(i\omega g_1(x_1, \ldots, x_N))$$

- Compute integral

$$I_1(x_2, \ldots, x_N) = \int_{-\infty}^{\infty} i_1(x_1, \ldots, x_N) \, \mathrm{d}x_1$$

- Iterate until ...

$$i_N(x_N) := I_{N-1}(x_N) \exp(i\omega g_N(x_N))$$

- outer-most integral

$$I = I_N() = \int_{-\infty}^{\infty} i_N(x_N) \, \mathrm{d}x_N$$

Steepest Descent for Wavepackets

Transformation of the Integrals

- For each oscillatory part

$$\exp\left(i\omega g_i\left(x_i, \ldots, x_N\right)\right) = C \exp\left(-\omega p_i\right)$$

- Variable transformation by paths

$$I_i^{\pm}[h_i^{\pm}] = C \int_0^{\infty} i_i\left(h_i^{\pm}\left(p_i\right)\right) \dot{h}_i^{\pm}\left(p_i\right) \exp\left(-\omega p_i\right) \mathrm{d}p_i$$

- Singular for $p_i \to 0$
- Substitute $q_i := \sqrt{p_i}$

$$I_i^{\pm}[h_i^{\pm}] = C \int_0^{\infty} i_i\left(h_i^{\pm}\right) \ldots \exp\left(-\omega q_i^2\right) \mathrm{d}q_i$$

Steepest Descent for Wavepackets

Gluing Paths

- Two times half of a Gaussian integral
- Glue paths:
$$I_i[h_i] = I_i^+[h_i^+] - I_i^-[h_i^-]$$
- Transform h_i^- into h_i^+ by $\tau_i := -q_i$
- Full Gaussian Integral

$$I_i\left(x_{i+1}, \ldots, x_N\right) = C \int_{-\infty}^{\infty} i_i\left(h_i\left(\tau_i\right)\right) \ldots \exp\left(-\omega \tau_i^2\right) \mathrm{d}\tau_i$$

Steepest Descent for Wavepackets

Final Quadrature

- Resolved nested integral

$$I = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f\left(\underline{h}(\underline{\tau})\right) \prod_{i=1}^{N} C_i \exp\left(-\omega \tau_i^2\right) \mathrm{d}\tau_1 \cdots \mathrm{d}\tau_N$$

- Apply Gauss-Hermite Quadrature $Q \approx I$

$$Q = \prod_{j=1}^{N} C_j \sum_{k_1}^{n} \cdots \sum_{k_N}^{n} f\left(h_1\left(x_{k_1}\right), \ldots, h_N\left(x_{k_N}\right)\right) \prod_{i=1}^{N} w_{k_i}$$

Sparse Quadrature Schemes

- Problem:
  - full tensor-product quadrature
    - with less nodes per direction
- Solution:
  - Sparse grid schemes
    - Smolyak rule

Sparse Quadrature Schemes

Smolyak Construction

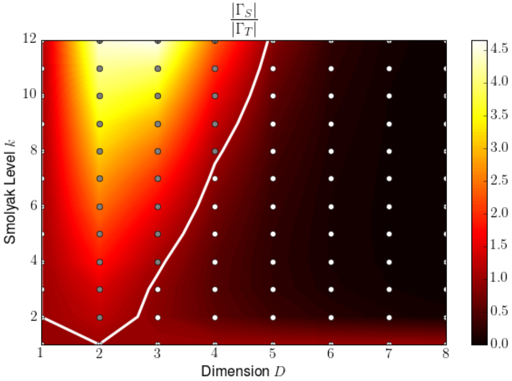
- Smolyak construction:

$$S_{D,k} := \sum_{q=k-D}^{k-1} (-1)^{k-1-q} \binom{D-1}{k-1-q} \sum_{\substack{\underline{l} \in \mathbb{N}^D \\ \|\underline{l}\|_1 = D+q}} \left(Q_{l_1} \otimes \cdots \otimes Q_{l_D} \right)$$

- Sum of many (smaller) tensor products

Sparse Quadrature Schemes

Construction with Gauss-Hermite rules



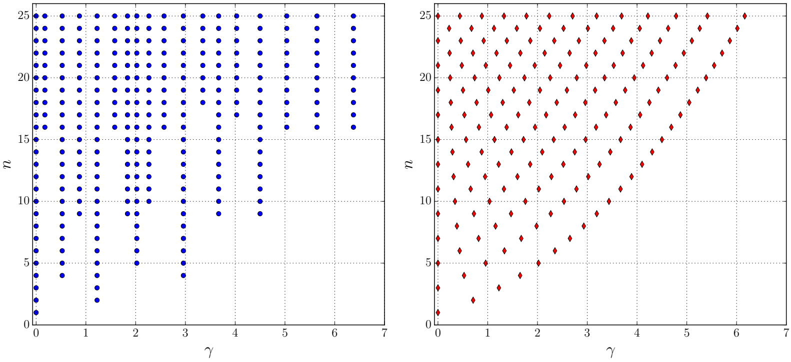
Sparse Quadrature Schemes

Smolyak Construction Issues

- Problem:
  - Gauss-Hermite points not nested
    - more points than full tensorproduct!
- Solution:
  - Search rules with nested nodes
  - For interval $(-\infty, \infty)$ with weight $\exp(-x^2)$
    - Iterative *Kronrod* extensions
    - *Genz-Keister* rules

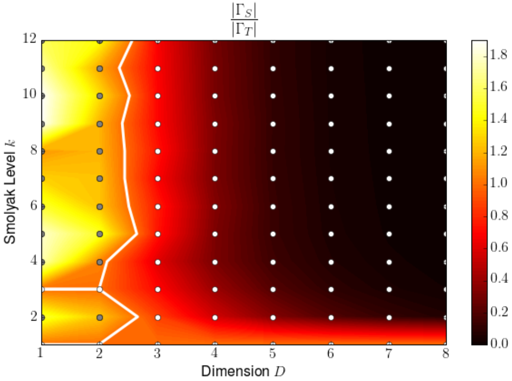
Sparse Quadrature Schemes

Genz-Keister Nodes



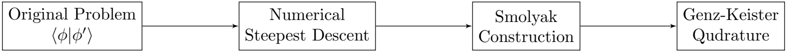
Sparse Quadrature Schemes

Construction with Genz-Keister nested rules



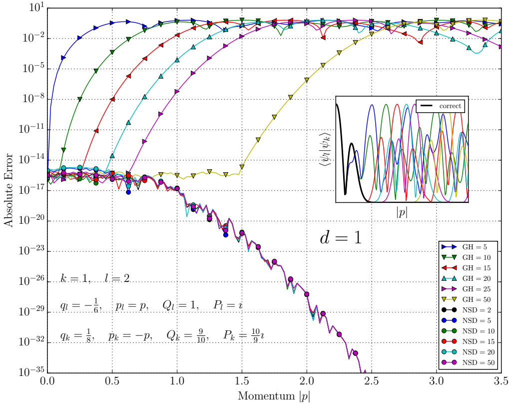
Final Solution for computing overlap Integrals

- Chain of Transformators
  - Steepest Descent: *remove oscillations*
  - Sparse Grid: *lessen curse of dimensionality*
  - Genz-Keister rules: *make nodes nested*



Numerical Experiments

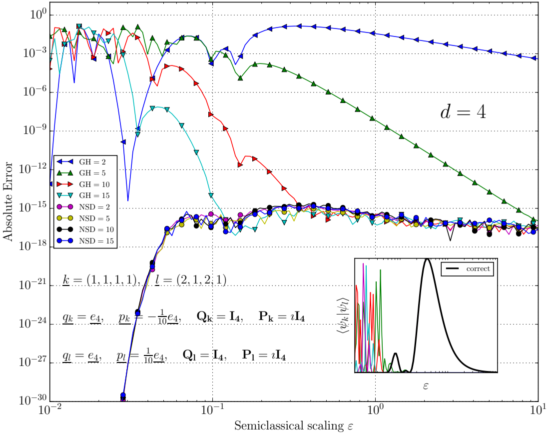
Convergence



Gauss-Hermite is wrong, Steepest Descent Transformation is perfect

Numerical Experiments

Convergence

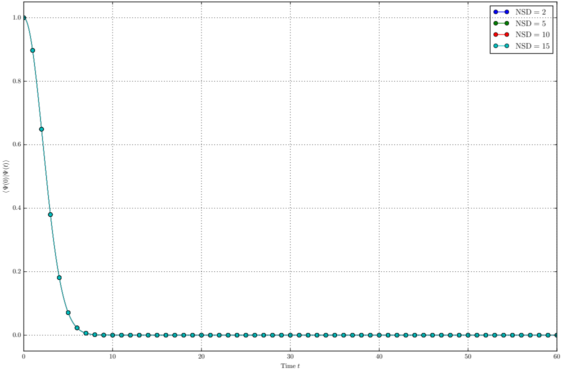


Gauss-Hermite is wrong, Steepest Descent Transformation is perfect

Real-world Example Hg_2

- Compute autocorrelation $|A(t)|$ by improved integrator

$$A(t) := \langle \Psi_0 \,|\, \Psi_t \rangle = \int \cdots \int_{\mathbb{R}^D} \overline{\Psi_0(\underline{x})} \Psi_t(\underline{x}) \mathrm{d}\underline{x}$$



Future Work and Open Topics

- Proof steepest descent technique for (semi-)infinite intervals
- Other integrals like $\langle \phi | V | \phi \rangle$
  - Potentials with non-polynomial or exponential parts
- Non-classical Smolyak constructions
  - Hyperbolic cut sections
  - Adaptive versions
- Proof (non-)existence of higher Kronrod Extensions
- Implement much larger Genz-Keister rules

Numerical Steepest Descent

Literature

A. Deaño and D. Huybrechs.
Complex Gaussian quadrature of oscillatory integrals.
Numerische Mathematik, 112:197–219, 2009.

D. Huybrechs and S. Vandewalle.
On the Evaluation of Highly Oscillatory Integrals by Analytic Continuation.
SIAM Journal on Numerical Analysis, 44(3):1026–1048, 2006.

D. Huybrechs and S. Vandewalle.
The Construction of Cubature Rules for Multivariate Highly Oscillatory Integrals.
Mathematics of Computation, 76(260):pp. 1955–1980, 2007.

H. Majidian.
Numerical approximation of highly oscillatory integrals on semi-finite intervals by steepest descent method.
Numerical Algorithms, pages 1–12, 2012.

The proof given by Majidian is wrong!

Hagedorn Wavepackets

Literature

R. Bourquin.
Wavepacket propagation in d-dimensional non-adiabatic crossings.
2012.
http://www.sam.math.ethz.ch/~raoulb/research/master_thesis/tex/main.pdf.

G. A. Hagedorn.
Raising and lowering operators for semiclassical wave packets.
Annals of Physics, 269(1):77–104, 1998.

Steepest Descent for Wavepackets

Literature

R. Bourquin.
Numerical steepest descent for overlap integrals of semiclassical wavepackets.
2014.
Unpublished.

Sparse Quadrature Schemes

Literature

R. Bourquin.
Exhaustive search for higher-order kronrod-patterson extensions.
2014.
Unpublished.

A. Genz and B. D. Keister.
Fully symmetric interpolatory rules for multiple integrals over infinite regions with gaussian weight.
1996.

S. Mehrotra and D. Papp.
Generating nested quadrature formulas for general weight functions with known moments.
ArXiv e-prints, Mar. 2012.
http://arxiv.org/abs/1203.1554.

Thanks for your Attention

Questions?