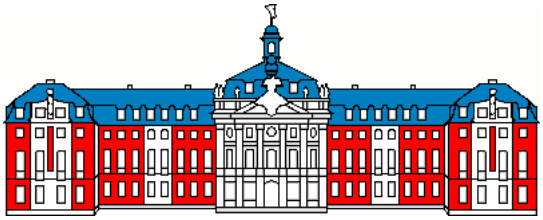


Learning à la Bayes

—From image reconstruction to inverse quantum theory —

Part 4: Inverse Quantum Theory

Jörg Lemm

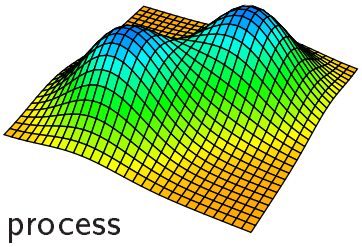
Institut für Theoretische Physik
Universität Münster

lemm@uni-muenster.de
http://pauli.uni-muenster.de/~lemm

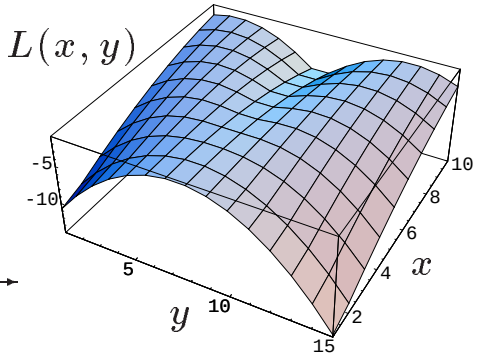
J.L. physics/9912005

Bayesian density estimation

prior density $p(L)$

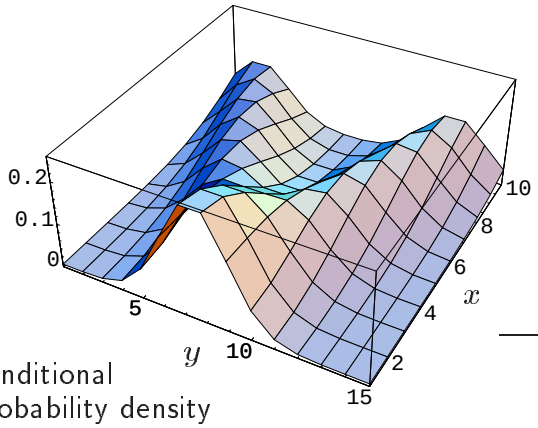


stochastic process
(e.g., mixture of Gaussians,
constraint on norm and positivity)



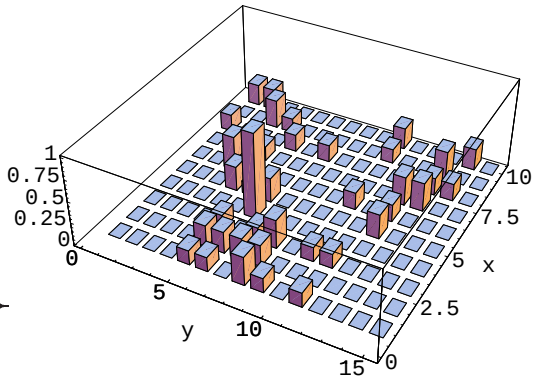
example
$L(x,y) = \ln p(y|x,L)$

likelihood model $p(y|x,L)$

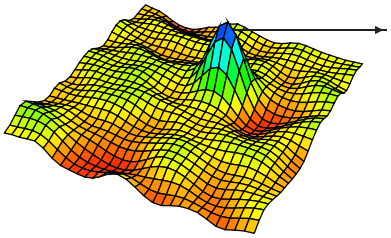


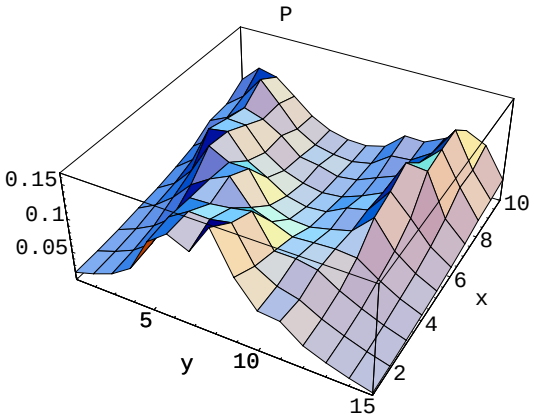
conditional
probability density

(training) data D



posterior density $p(L|D)$



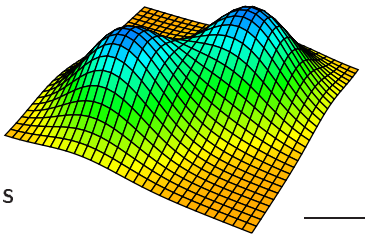


maximum posterior solution
for $p(y|x,L)$

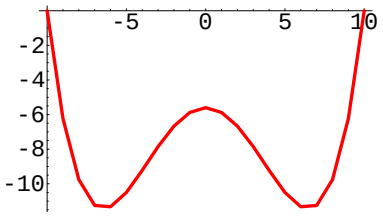
J.L., Uhlig, Weiguny, PRL 84 (2000)

Inverse Quantum Statistics à la Bayes

prior density $p(v)$



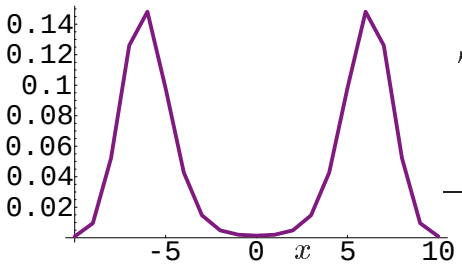
stochastic process (e.g., mixture of Gaussians)



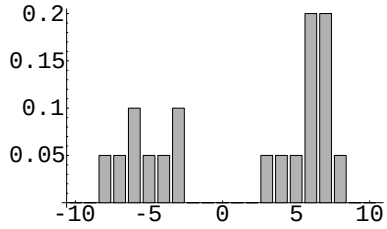
example of a local potential $v(x)$

likelihood model $p(x|\hat{x}, v)$

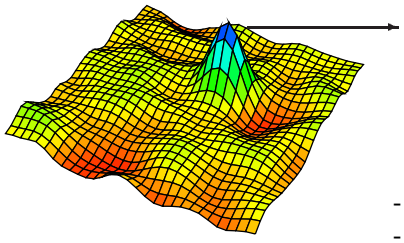
a possible realization of (training) data D

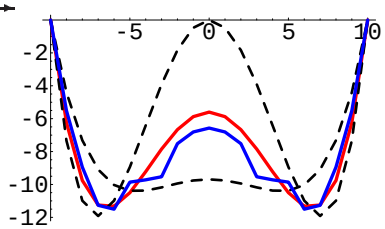


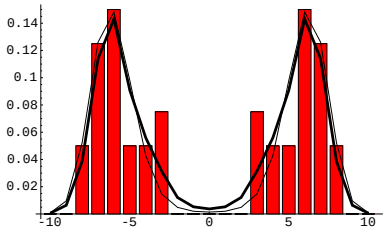
likelihood for $\beta = 1$



posterior density $p(v|D)$

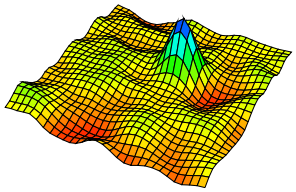




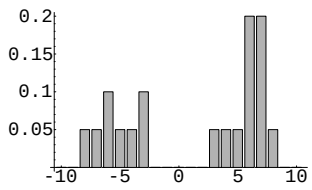


maximum posterior solution

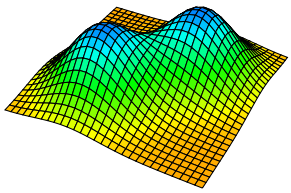
with



$\propto$



$\times$



The likelihood model of quantum statistics

Quantum system with Hamiltonian

$$H = T + V$$

e.g., with local potential

$$V(x, x') = \delta(x - x') \underbrace{v(x)}_{\text{to find!}}$$

The probability to find value x when measuring observable O at a quantum system in a state described by density operator ρ is given by

$$p(x|O, v) = \mathrm{Tr}\left[\pi(x, O)\ \rho(v)\right]$$

where $\pi(x, O) = \sum_\xi |x, \xi\rangle\langle x, \xi|$ denotes the projector in the space of eigenfunctions $|x, \xi\rangle$ of O with eigenvalues x. (The label ξ distinguishes degenerate eigenfunctions.)

For a canonical ensemble the density operator is given by

$$\rho = \frac{\exp(-\beta H)}{\mathrm{Tr}\ \exp(-\beta H)}$$

For position measurements $O = \hat{x}$

$$p(x|\hat{x}, v) = \sum_\alpha p_\alpha |\phi_\alpha(x)|^2 = \left\langle |\phi(x)|^2 \right\rangle$$

with $H|\phi_\alpha\rangle = E_\alpha |\phi_\alpha\rangle$, $p_\alpha = e^{-\beta E_\alpha}/Z$, $Z = \sum_\alpha e^{-\beta E_\alpha}$

J.L., Uhlig, Weiguny, PRL 84 (2000)

Functional derivative of likelihood

Functional derivative of likelihood with respect to $v(x)$

$$\delta_{v(x)} p(x_i|\hat{x}, v) = \frac{\delta}{\delta v(x)} \left(\frac{\sum_\alpha e^{-\beta E_\alpha} |\phi_\alpha(x_i)|^2}{\sum_{\alpha'} e^{-\beta E_{\alpha'}}} \right)$$

$$= \left\langle \phi^*(x_i) \delta_{v(x)} \phi(x_i) \right\rangle + \left\langle \delta_{v(x)} \phi^*(x_i) \phi(x_i) \right\rangle$$
$$-\beta \left[\left\langle \delta_{v(x)} E \, |\phi(x_i)|^2 \right\rangle - \left\langle \delta_{v(x)} E \right\rangle \left\langle |\phi(x_i)|^2 \right\rangle \right]$$

From the Schrödinger equation $H \, |\phi_\alpha\rangle = E_\alpha \, |\phi_\alpha\rangle$ follows

$$\left(\delta_{v(x)} H\right) |\phi_\alpha\rangle + H \delta_{v(x)} \, |\phi_\alpha\rangle$$

$$= \left(\delta_{v(x)} E_\alpha\right) |\phi_\alpha\rangle + E_\alpha \delta_{v(x)} \, |\phi_\alpha\rangle$$

and thus (for orthonormal, nondegenerate eigenfunctions)

$$\delta_{v(x)} E_\alpha = \left\langle \phi_\alpha \left| \delta_{v(x)} H \right| \phi_\alpha \right\rangle = |\phi_\alpha(x)|^2$$

$$\delta_{v(x)} \phi_\alpha(x') = \sum_{\gamma \neq \alpha} \frac{1}{E_\alpha - E_\gamma} \phi_\gamma(x') \phi_\gamma^*(x) \phi_\alpha(x)$$

with

$$\delta_{v(x)} H(x', x'') = \delta_{v(x)} V(x', x'') = \delta(x - x') \delta(x' - x'')$$

Functional derivative of Gaussian processes

For a Gaussian process

$$p(v) = \left(\det \frac{\lambda \mathbf{K}_0}{2\pi} \right)^{\frac{1}{2}} e^{-\frac{\lambda}{2} \langle v - v_0 \,|\mathbf{K}_0|\, v - v_0 \rangle}$$

the functional derivative with respect to the potential v is

$$\delta_v \ln p(v) = -\lambda \mathbf{K}_0 (v - v_0)$$

The equation is also valid for mixtures of Gaussian processes

$$p(v) = \sum_{k=1}^{M} p(k)\, p(v|k)$$

where

$$\begin{aligned} \mathbf{K}_0 &= \sum_k p(k|v)\, \mathbf{K}_k \\ v_0 &= \mathbf{K}_0^{-1} \sum_k p(k|v)\, \mathbf{K}_k v_k \end{aligned}$$

with $p(k|v) = p(v|k)p(k)/p(v)$.

Noisy energy measurements

Measurements of energy levels or the expectation of the energy at finite temperatures

$$U = \langle E \rangle = \sum_{\alpha} p_{\alpha} E_{\alpha}$$

can be useful to determine better the depth of a potential. For instance, a noisy measurement κ of U corresponds to

$$p_U \propto e^{-E_U}, \quad E_U = \frac{\mu}{2}(U - \kappa)^2$$

where $U \to \kappa$ for $\mu \to \infty$. With

$$\delta_{v(x)} U = \left\langle \delta_{v(x)} E \right\rangle - \beta \left\langle E \; \delta_{v(x)} E \right\rangle + \beta \left\langle E \right\rangle \left\langle \delta_{v(x)} E \right\rangle$$

one finds for the functional derivative of E_U

$$\delta_{v(x)} E_U = \mu \, (U - \kappa) \left\langle |\phi(x)|^2 \left[1 - \beta \, (E \; - U) \right] \right\rangle$$

Functional derivative of the posterior density

The stationarity equation for a posterior with Gaussian process prior and noisy energy measurement

$$0 = \delta_{v(x)} \ln p(v|D)$$

$$= \delta_{v(x)} \left(\sum_i \ln p(x_i|\hat{x}, v) - \frac{\lambda}{2} \langle v - v_0 \, |\mathbf{K}_0| \, v - v_0 \rangle - E_U \right)$$

can be obtained by collecting:

1. the functional derivative of the likelihood

$$\begin{aligned} &\delta_{v(x)} p(x_i|\hat{x}, v) = \\ &\quad \left\langle \left[\delta_{v(x)} \phi^*(x_i) \right] \phi(x_i) \right\rangle + \left\langle \phi^*(x_i) \delta_{v(x)} \phi(x_i) \right\rangle \\ &-\beta \left[\left\langle |\phi(x_i)|^2 |\phi(x)|^2 \right\rangle - \left\langle |\phi(x_i)|^2 \right\rangle \left\langle |\phi(x)|^2 \right\rangle \right] \end{aligned}$$

2. the functional derivative of the prior

$$\delta_v \ln p = -\lambda \mathbf{K}_0 (v - v_0)$$

3. the functional derivative of the energy term

$$\delta_{v(x)} E_U = \mu \, (U - \kappa) \left\langle |\phi(x)|^2 \left[1 - \beta \, (E \; - U) \right] \right\rangle$$

Iteration methods = learning algorithms

Choosing an initial guess $v^{(0)}$, step width η, and a positive definite matrix $\mathbf{A}$ the MAP stationarity equation can be solved by iteration

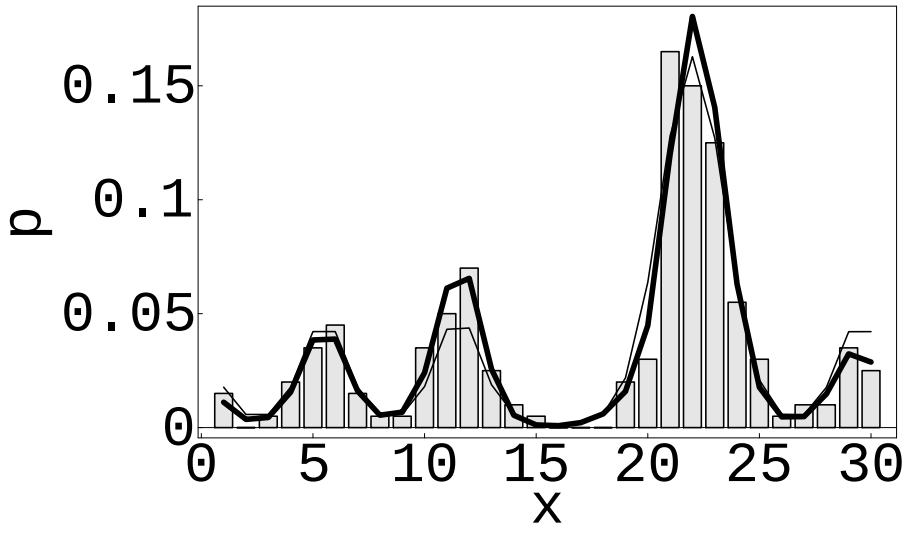
$$\begin{aligned} v^{(r+1)} &= v^{(r)} + \eta \mathbf{A}^{-1} \Big[\mathbf{K}_0^{(r)} (v_0 - v^{(r)}) \\ &\quad + \sum_i \delta_{v(x)} \ln p(x_i | \hat{x}, v^{(r)}) - \delta_{v(x)} E_U^{(r)} \Big] \end{aligned}$$

Typically, η and posssibly $\mathbf{A}$ will be adapted during iteration The simple choice $\mathbf{A} = \mathbf{K}_0$ often proved to be useful. Different initial guesses $v^{(0)}$ can lead to different results.

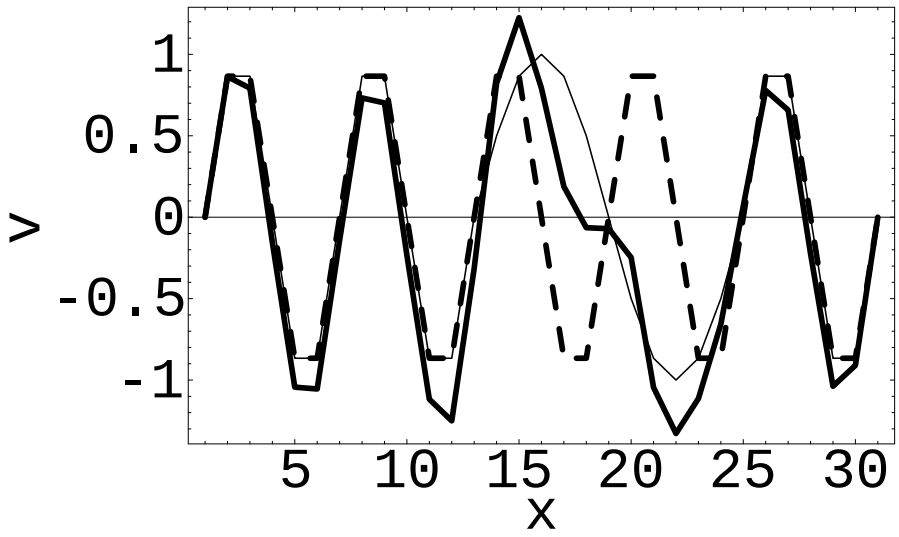
J.L., Uhlig, Weiguny, PRL 84 (2000)

Reconstruction of approximately periodic potentials

(a) LIKELIHOODS



(b) POTENTIALS

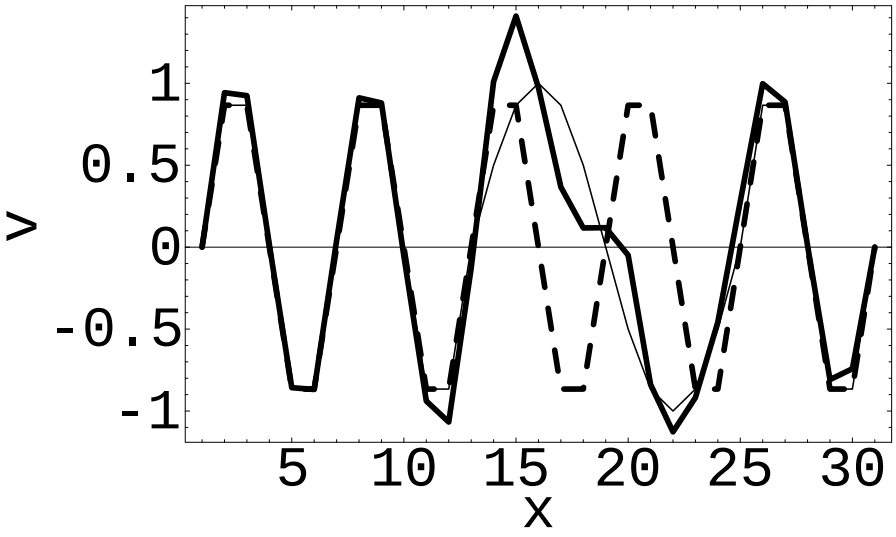


(a) relative frequencies of observations (bars), true (thin) and reconstructed (thick) likelihoods. (b) True potential $v_{\rm true}$ (thin), reference potential $v_0 = \sin(\pi x/3)$ (dashed), and reconstructed potential v (thick). (200 data points, mesh with 30 points, $m = 0.25$ with $\hbar = 1$, $\beta = 4$, $\mathbf{K}_0 = -\Delta$, $\lambda = 0.2$, $\mu = 0$, $U(v_{\rm true}) = -0.354$, $U(v) = -0.552$.)

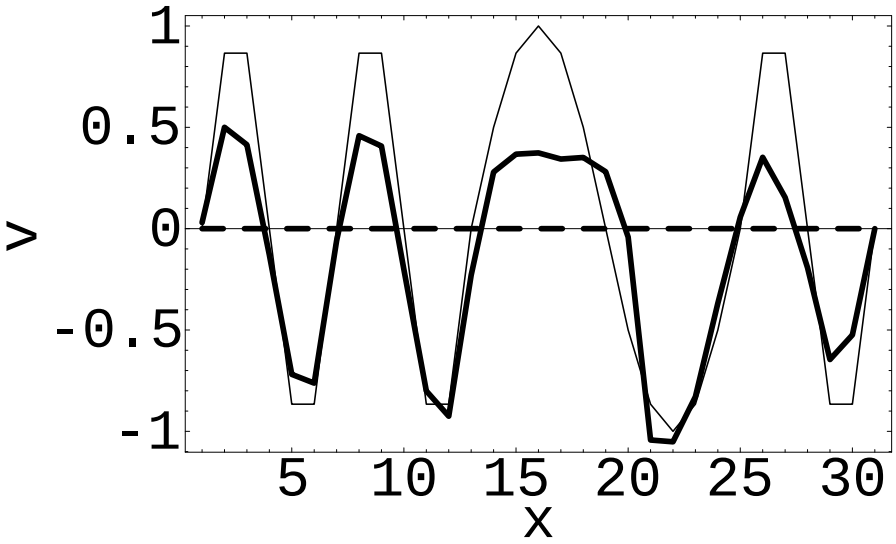
J.L., Uhlig, Weiguny, PRL 84 (2000)

Reconstruction of approximately periodic potentials

(a) With periodic reference potential



(b) With periodic prior covariance



Reconstruction including E_U with $\kappa = U(v_{\text{true}}) = -0.354$. (a) $\mathbf{K}_0 = -\Delta$, $v_0(x) = \sin(\pi x/3)$, $\mu = 1000$, $U(v) = -0.353$. (b) $\mathbf{K}_0 = -\Delta - \gamma\Delta_\theta$, $v_0 \equiv 0$, $\theta = 6$, $\gamma = 0.12$, $\lambda = 0.05$, $\mu = 10$, $U(v) = -0.351$.

J.L., Uhlig, Weiguny, quant-ph/0005122

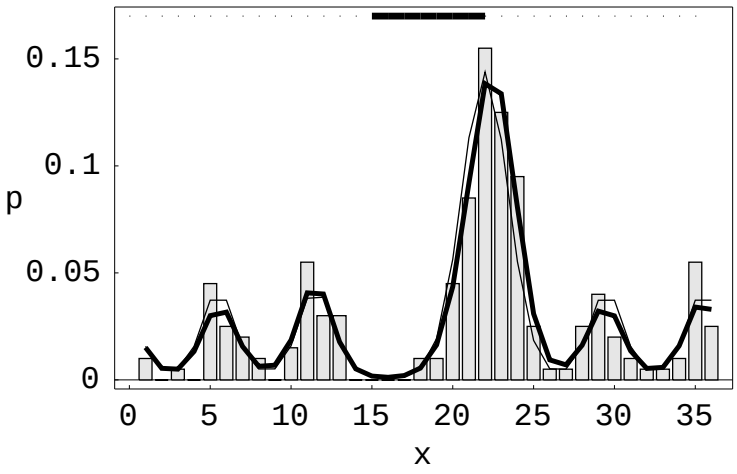
Reconstruction with local hyperfield

Local switching between different reference potentials $v_0(x;\theta) = [1-\theta(x)]v_1(x) + \theta(x)v_2(x)$ using a binary hyperfield $\theta(x)$

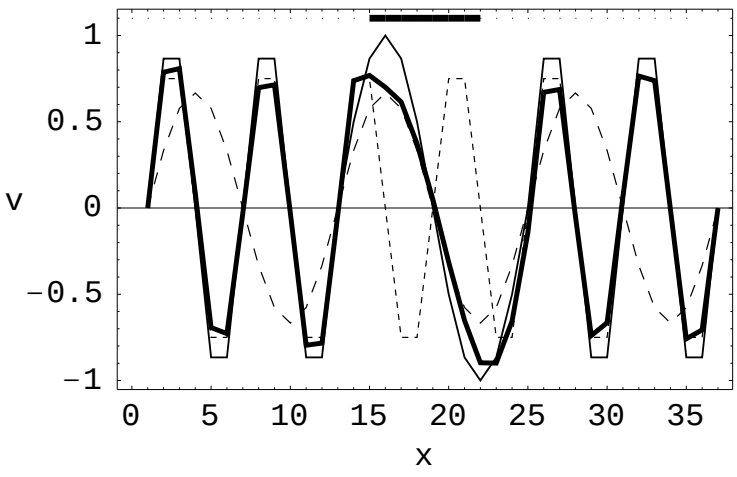
$$E_0(v,\theta) = \frac{\lambda_1}{2}\langle v - v_0(\theta)|v - v_0(\theta)\rangle - \frac{\lambda_2}{2}\langle v\,|\Delta|\,v\rangle - \ln p(\theta),$$

Additional hyperprior $p(\theta)$ to control number of discontinuities of $\theta(x)$. Hyperfield optimized by "simulated annealing".

(a) LIKELIHOODS

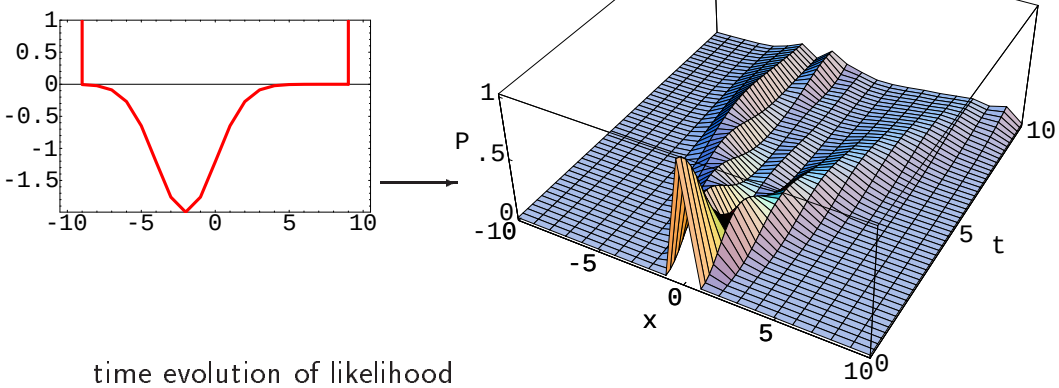


(b) POTENTIALS



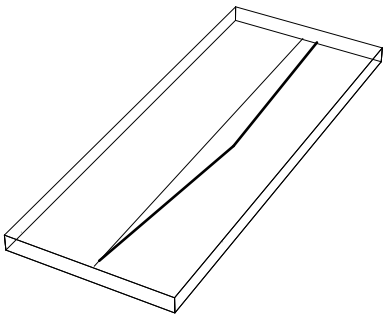
Non–stationary quantum systems

local potential $v(x)$

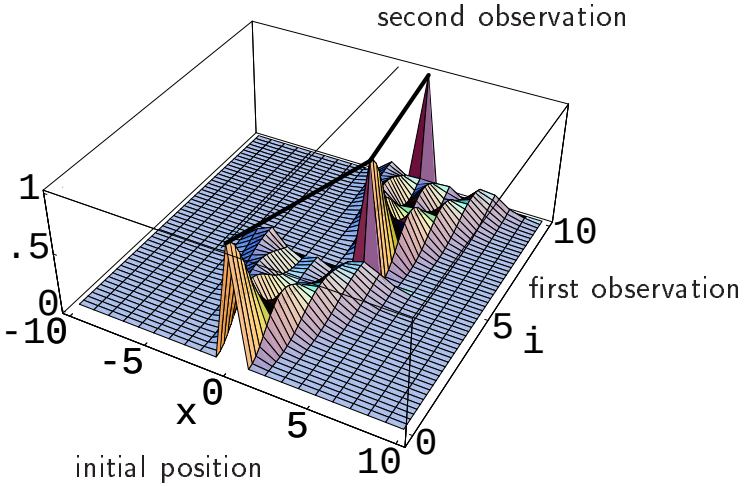


time evolution of likelihood
for a particle with initial position $x_0 = 0$

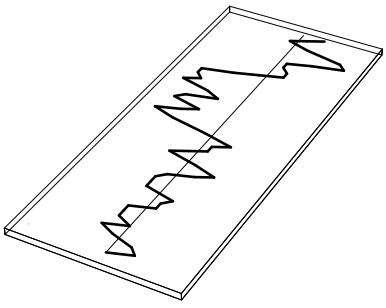
measurements of particle position
with time intervals $\Delta t = 5$.

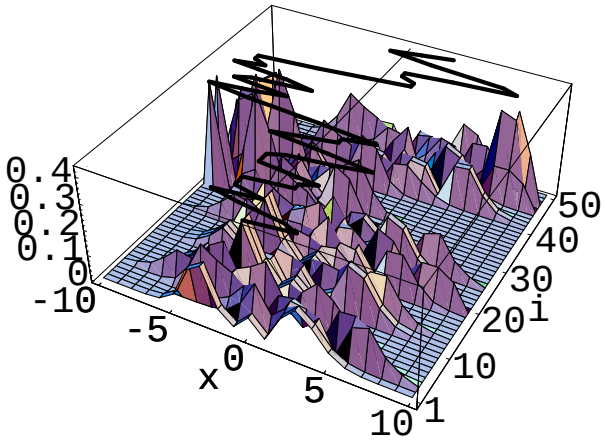


second observation



observed time series





J.L., quant-ph/0002010 (submitted)

Likelihoods for time–dependent systems

Probability to observe position x_i for a particle which have been at position x_{i-1} at time $t_i - \Delta_i$

$$p_i = p(x_i|\Delta_i, x_{i-1}, v) = |\phi_i(x_i)|^2$$

where $\phi_i(x_i) = \langle x_i|\phi_i\rangle = \langle x_i|U_i\, x_{i-1}\rangle$ and v–dependent time–evolution operator:

$$U_i = \exp\left(-i\Delta_i H\right)$$

With $H\psi_\alpha = E_\alpha\psi_\alpha$ and

$$\begin{aligned}
\delta_{v(x)}E_\alpha &= \left\langle \psi_\alpha \,\middle|\, \delta_{v(x)}H \,\middle|\, \psi_\alpha \right\rangle = |\psi_\alpha(x)|^2, \\
\delta_{v(x)}\psi_\alpha(x') &= \sum_{\gamma\neq\alpha} \frac{1}{E_\alpha - E_\gamma}\,\psi_\gamma(x')\psi_\gamma^*(x)\psi_\alpha(x)
\end{aligned}$$

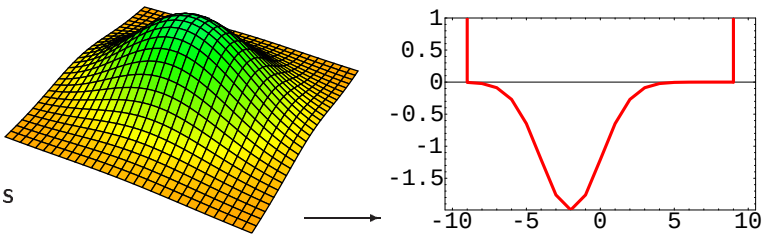
it follows

$$\begin{aligned}
\delta_{v(x)}\phi_i(x_i) \;=\; & \delta_{v(x)}\,\langle x_i|U_i\, x_{i-1}\rangle \;= \\
& \sum_\alpha e^{-i\Delta_i E_\alpha}\Big[\left(-i\Delta_i|\psi_\alpha(x)|^2\right)\psi_\alpha(x_i)\psi_\alpha^*(x_{i-1}) \\
& + \sum_{\gamma\neq\alpha}\frac{1}{E_\alpha - E_\gamma}\psi_\gamma(x_i)\psi_\gamma^*(x)\psi_\alpha(x)\psi_\alpha^*(x_{i-1}) \\
& + \sum_{\gamma\neq\alpha}\frac{1}{E_\alpha - E_\gamma}\psi_\gamma^*(x_{i-1})\psi_\gamma(x)\psi_\alpha^*(x)\psi_\alpha(x_i)\Big]
\end{aligned}$$

J.L., quant-ph/0002010

Time–dependent inverse quantum theory

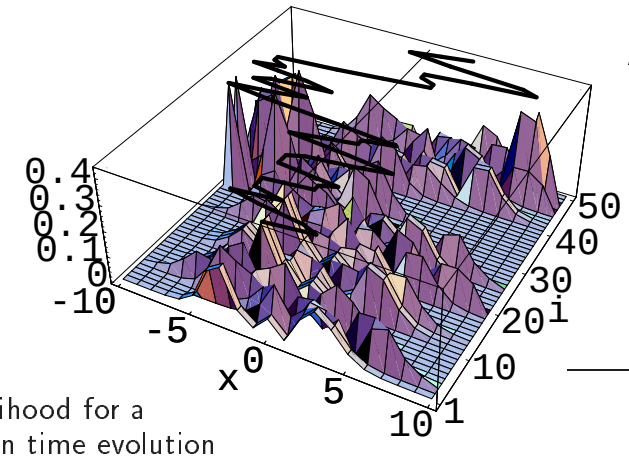
prior density $p(v)$



stochastic process

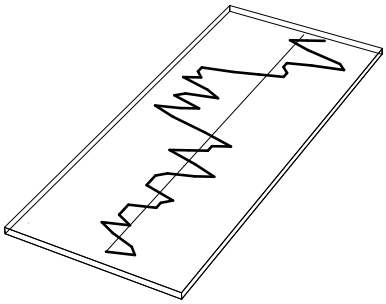
example of a
local potential $v(x)$

likelihood model $p(x|t_i, x_{i-1}, v)$

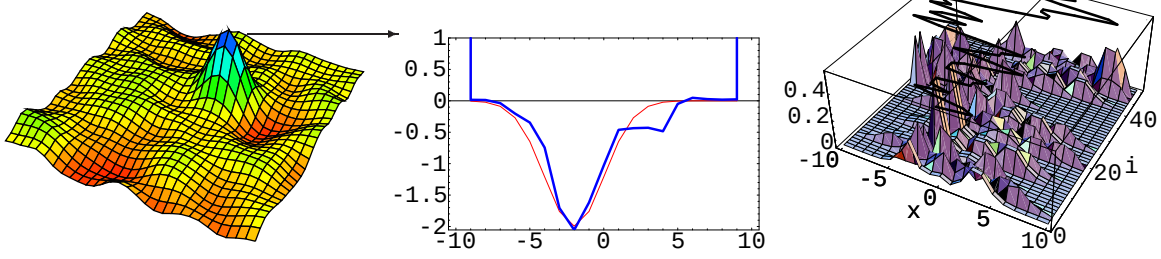


likelihood for a
given time evolution

a possible
realization of
(training) data D

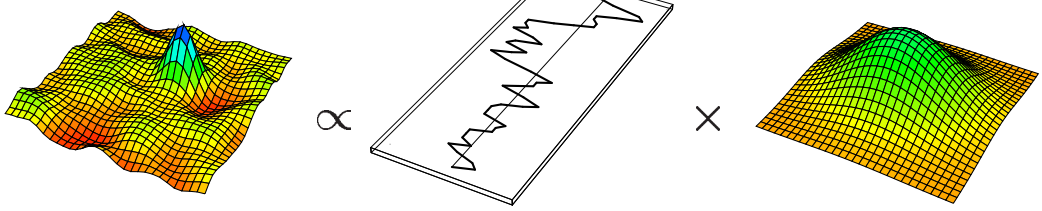


posterior density $p(v|D)$



maximum posterior solution

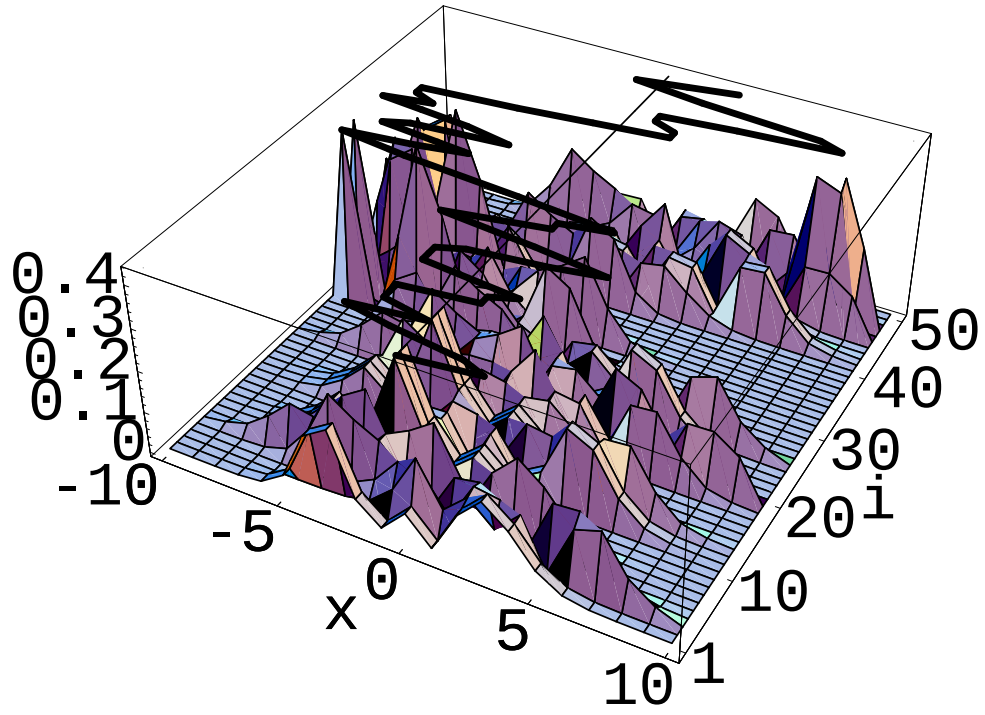
where



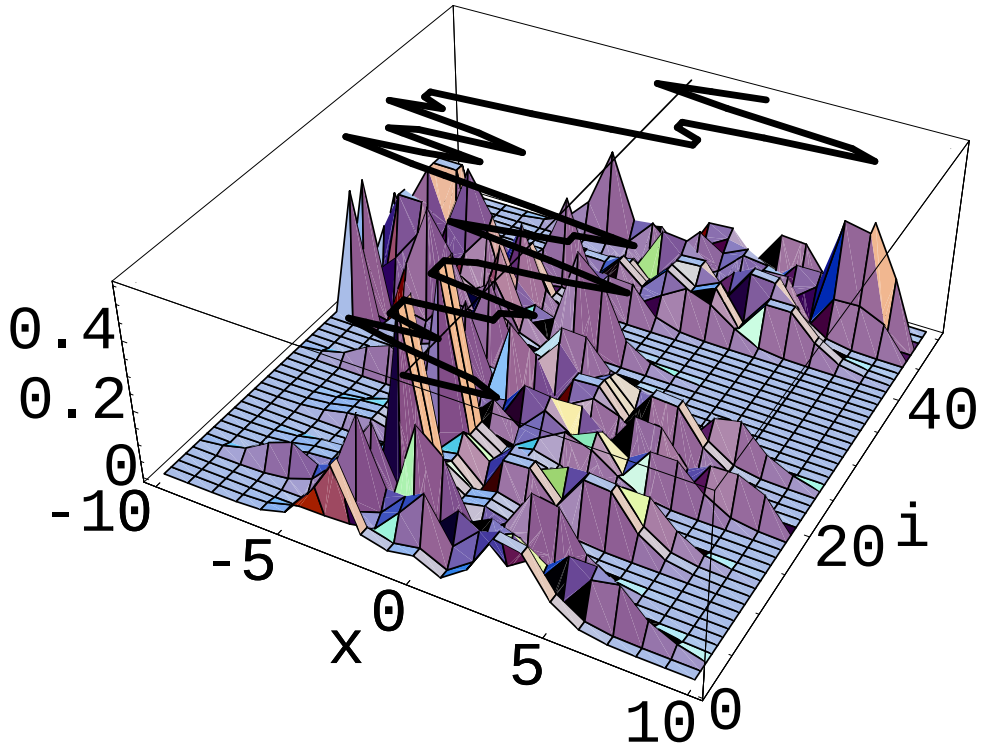
Time–dependent inverse quantum theory:

Time series data

original likelihoods



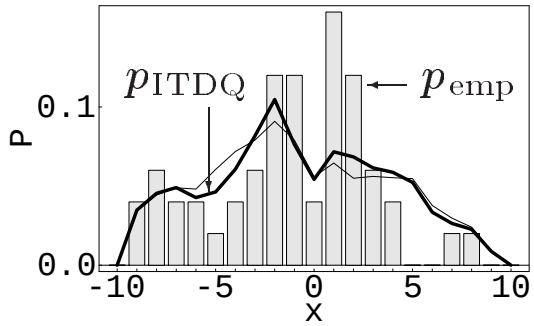
reconstructed likelihoods



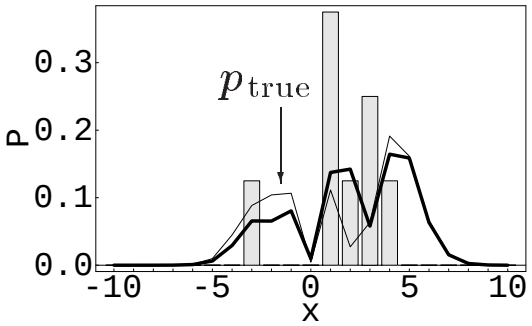
Time–dependent inverse quantum theory:

Time series data

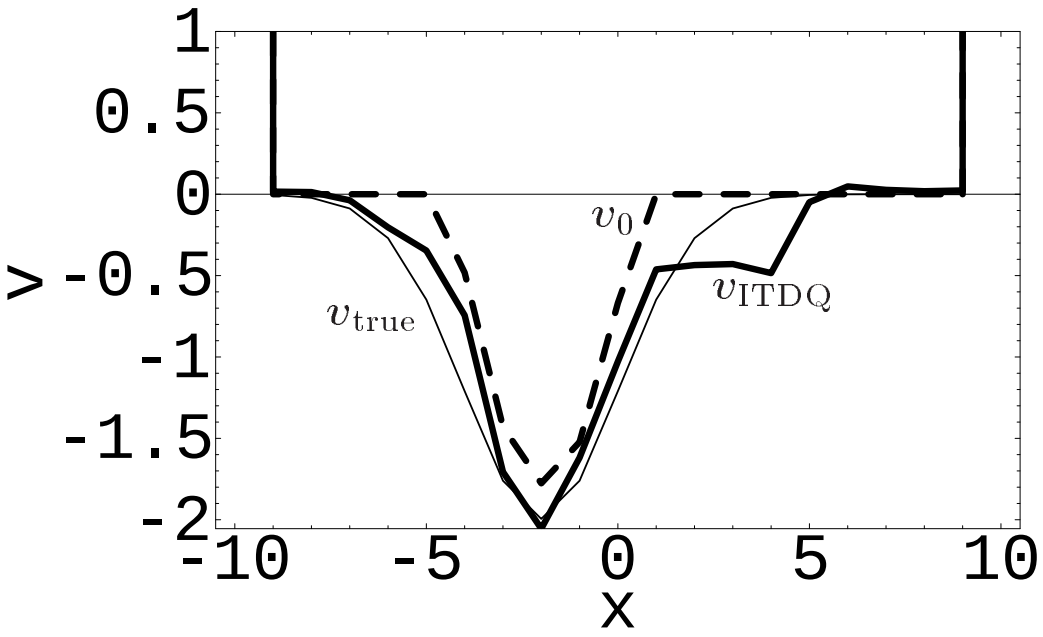
transition probabilities



sum over all x_{i-1}



for $x_{i-1} = 1$



J.L., Uhlig, PRL 84 (2000)

Many–body likelihood

Fermionic many–body Hamiltonian

$$H = \sum_{\alpha\beta} T_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

with local two–body–potential in $z = |x_{(1)} - x_{(2)}|$

$$V_{x_{(1)}x_{(2)}x'_{(1)}x'_{(2)}} = v(z)[\delta_{x_{(1)},x'_{(1)}}\delta_{x_{(2)},x'_{(2)}} - \delta_{x_{(1)},x'_{(2)}}\delta_{x_{(2)},x'_{(1)}}]$$

Hartree–Fock approximation: $h\varphi_k = \epsilon_k\varphi_k$ with

$$h_{xx'} = T_{xx'} + \sum_{k=1}^{N} \left\langle x\varphi_k \left| V \right| x'\varphi_k \right\rangle$$

HF ground state: $|\Phi_0\rangle = |\varphi_1, \cdots, \varphi_N\rangle$

Hartree–Fock likelihoods:
(**A**) 2–particle data: $p_{\rm HF}(\vec{x}_i|\hat{x}, v) = |\Phi_0(\vec{x}_i)|^2$
(**B**) 1–particle data: $p_{\rm HF}(x_i|\hat{x}, v) = \sum_{k=1}^{N} |\varphi_k(x_i)|^2$

Inverse HF equation:

$$\underbrace{|\delta_{v(z)}\varphi_k\rangle}_{\substack{\rm two--body\\ \rm equation}} = \sum_{l\neq k} \frac{1}{\epsilon_k - \epsilon_l} |\varphi_l\rangle \left\langle \varphi_l \left| \delta_{v(z)} h \right| \varphi_k \right\rangle$$

$$\delta_{v(z)} h_{xx'} = \sum_{j=1}^{N} \Big[\left\langle x\,\varphi_j \left| \delta_{v(z)} V \right| x'\,\varphi_j \right\rangle + \left\langle x\,\delta_{v(z)}\varphi_j \left| V \right| x'\,\varphi_j \right\rangle + \left\langle x\,\varphi_j \left| V \right| x'\,\delta_{v(z)}\varphi_j \right\rangle \Big]$$

$\Rightarrow$ 3 nested iteration procedures for v, $\delta_v\varphi_k$ and h

The Bayesian inverse Hartree–Fock algorithm

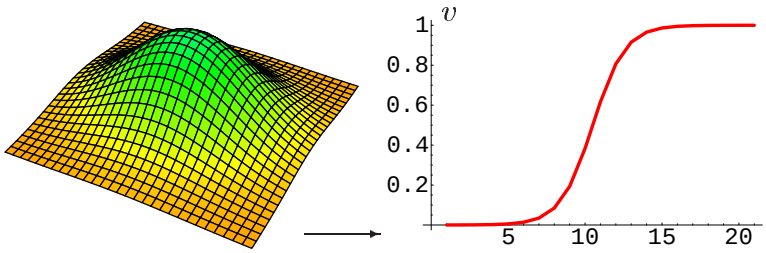
The reconstruction of a potential from observational data by means of the inverse Hartree–Fock approaches requires

1. the iterative solution of the Maximum–A–Posteriori stationarity equation for the Potential v. Each iteration step requires
2. the functional derivatives of the likelihoods, e.g., $\delta_{v(x)} \ln p(\vec{x}_i|\hat{x}, v)$ or $\delta_{v(x)} \ln p(x_i|\hat{x}, v)$. Those are obtained by solving the (two–particle–like) inverse Hartree–Fock equation for given
3. one–particle–orbitals φ_i, defined as solution of the self–consitent (one–body–)Hartree–Fock equation.

J.L., Uhlig, PRL 84 (2000)

Hartree–Fock approximation for inverse problems

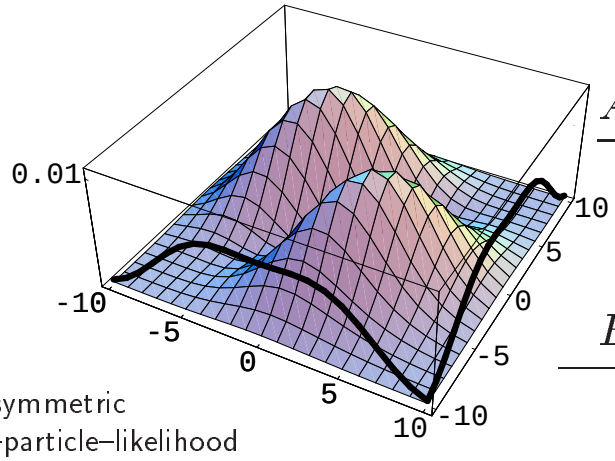
priori density $p(v)$



stochastic prozes

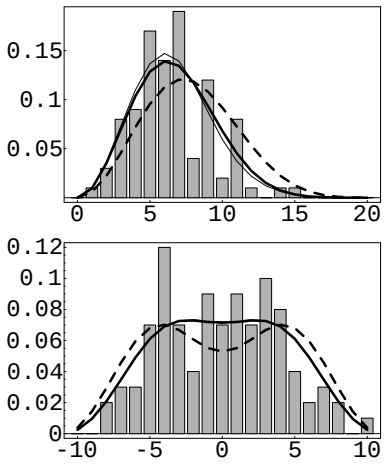
example of a
local potential $v(|x_{(1)} - x_{(2)}|)$

likelihood model $p(x_{(1)}, x_{(2)}|\hat{x}, v)$

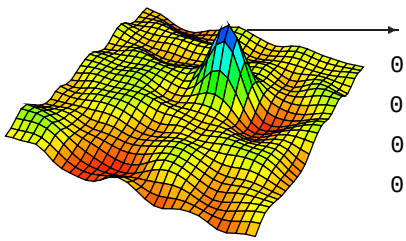


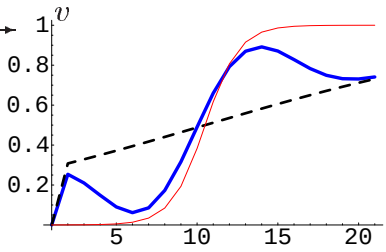
antisymmetric
two–particle–likelihood
and one–particle–likelihood/10

(training) data D

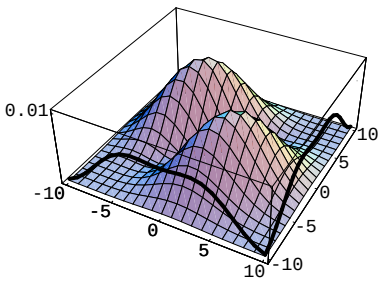


posterior density $p(v|D)$



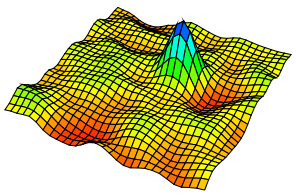


maximum–posterior solution

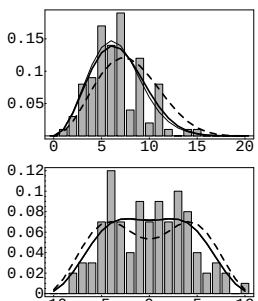


Hartree–Fock likelihood

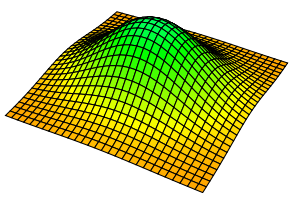
where



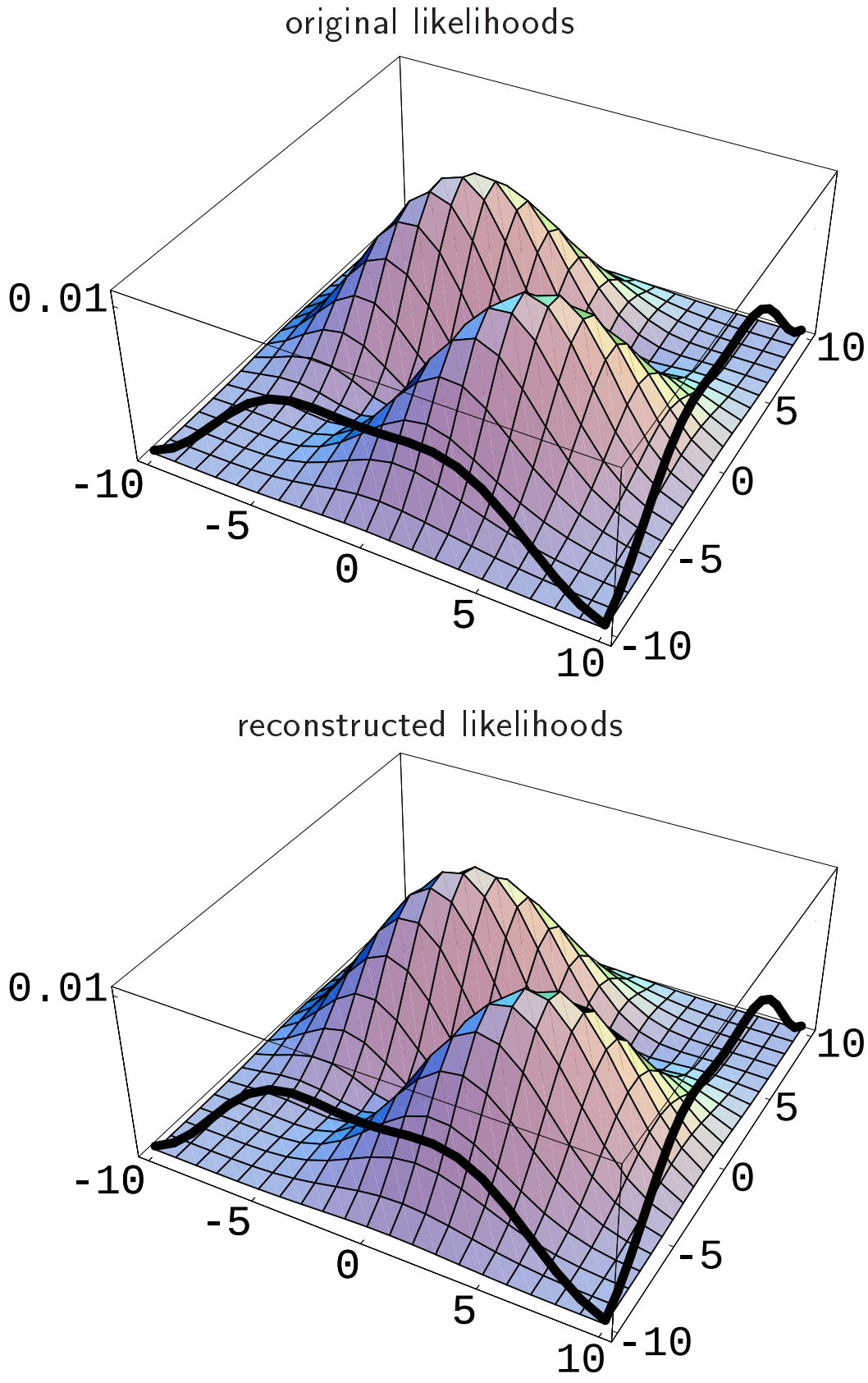
$\propto$



$\times$

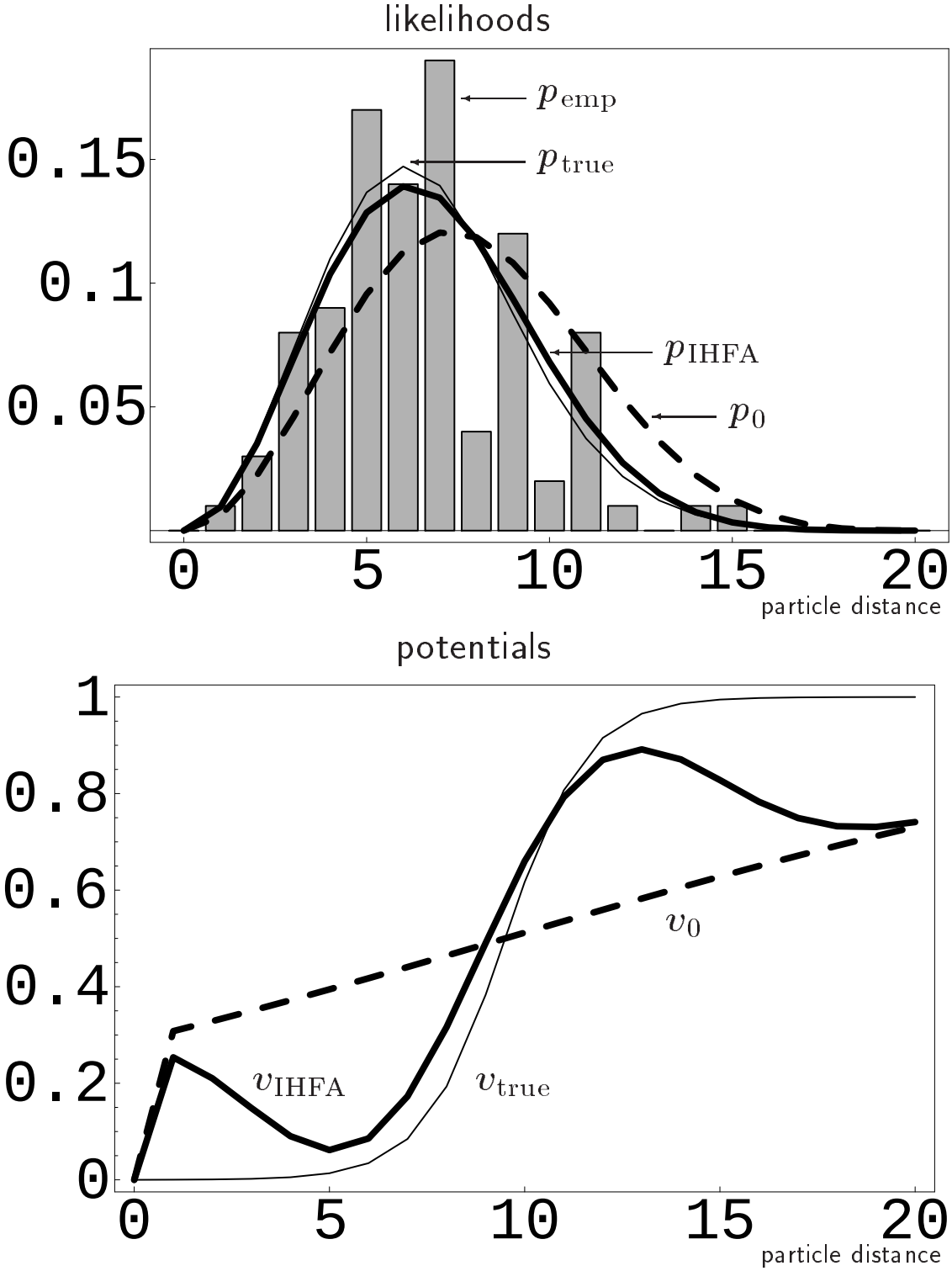


Bayesian inverse Hartree–Fock theory



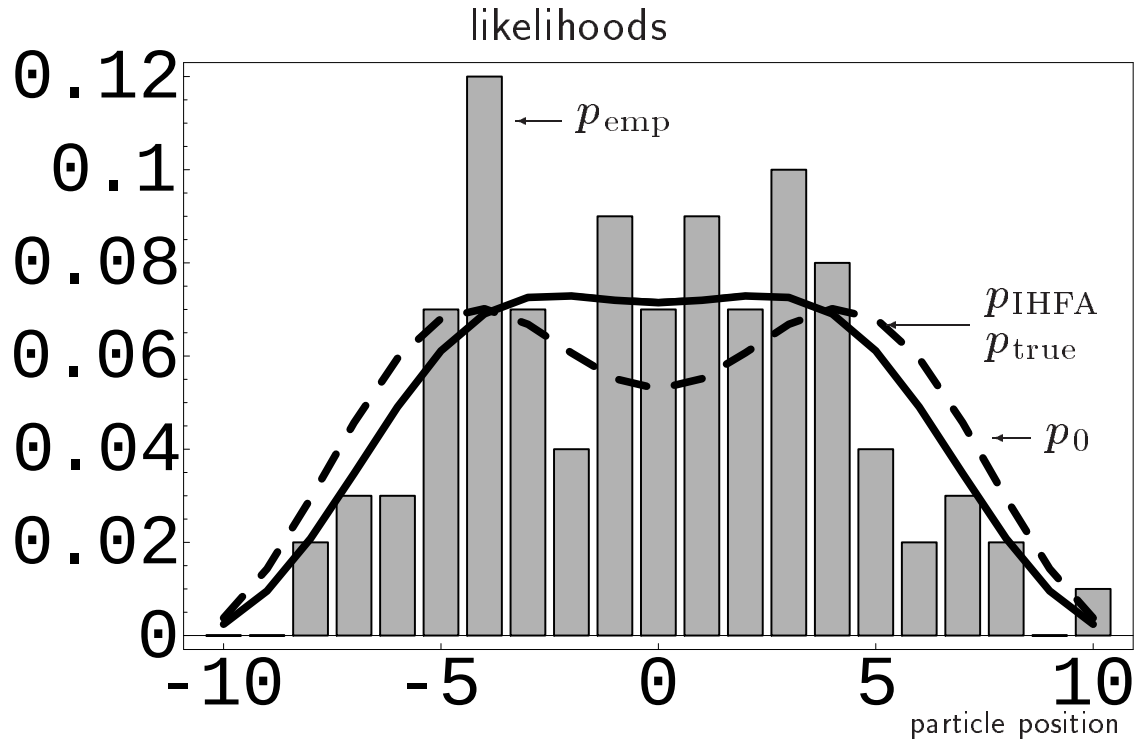
Bayesian inverse Hartree–Fock theory:

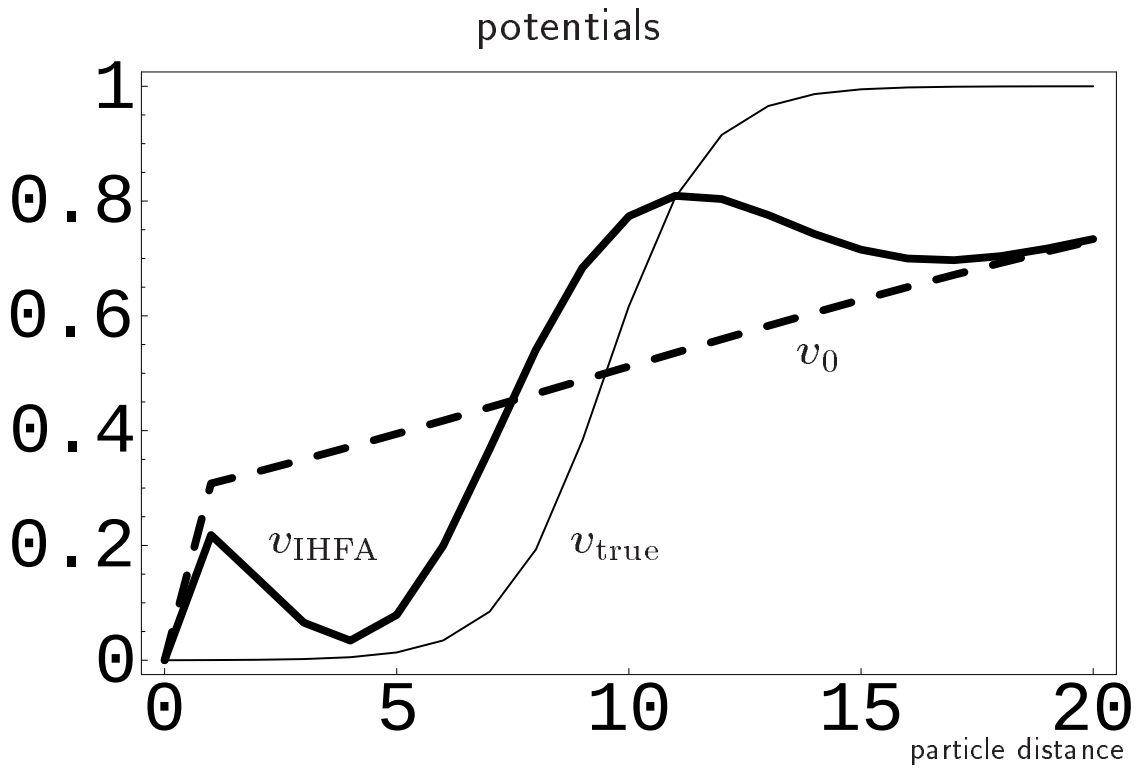
two–particle data



Bayesian inverse Hartree–Fock theory:

one–particle data





"Bayesian Field Theories"

likelihood $p(y\|x,h)$	problem type
$\frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{[y-h(x)]^2}{2\sigma^2}\right]$ (Gaussian, σ fixed)	regression J.L., ICANN99 (image reconstruction)
$\sum_k \frac{1}{\sigma_k\sqrt{2\pi}}\exp\left[-\frac{[y-h_k(x)]^2}{2\sigma_k^2}\right]$ (mixture of Gaussians)	clustering
discrete y	classification
of general form	density estimation J.L., physics/9912005
Trace$[\rho(h)\,\pi(x,y)]$	inverse quantum statistics J.L., Uhlig, Weiguny, PRL 84 (2000) inverse Hartree–Fock Theory J.L., Uhlig, PRL 84 (2000) inverse time–dependent QM J.L., quant-ph/0002010
$\langle\delta(y-x[x_{\rm cl},p_{\rm cl}])\rangle_{\rm cl}$	classical approx. of inv. QS J.L., Uhlig, to app. in Few Body Sys.

Nonparametric Bayesian methods

Advantages:

1. Based on realistic data assumptions: Only a finite number of noisy observational data is used. No expectation values or whole functions are needed as input.

2. Explicit and situation specific implementation of "a–priori" information is possible (mixture of Gausian prior processes, hyperparameter and hyperfields).

Disadvantage:

Numerically expensive