QUANTUM DYNAMICS IN TOMOGRAPHIC REPRESENTATION OF QUANTUM MECHANICS

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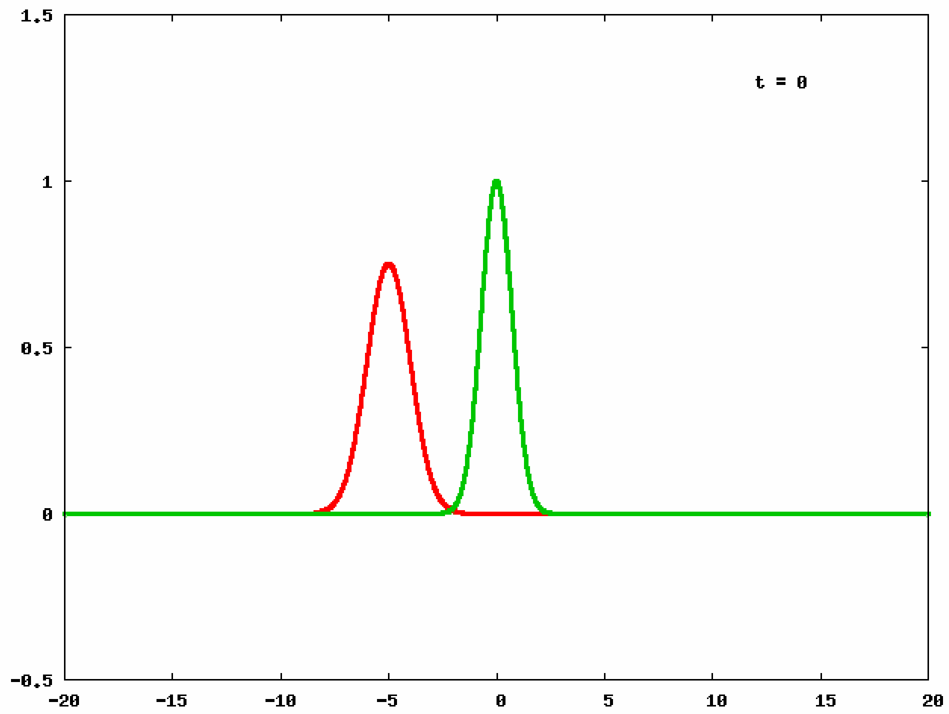
OUTLINE

- Schrodinger equation
- Approaches for quantum dynamics
- Wigner representation
- Tomographic representation
- Kolmogorov and Langevin equations
- Examples
- Conclusions

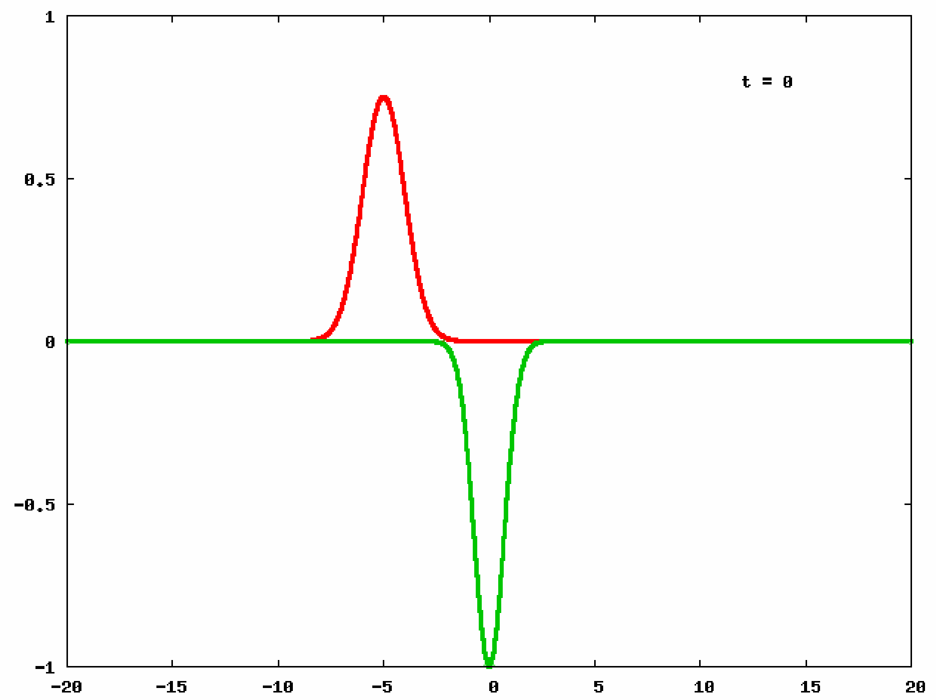
SCHRÖDINGER EQUATION

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

Tunneling through barrier



Scattering on well



APPROACHES TO QUANTUM DYNAMICS

- Wave packet molecular dynamics
  E.J. Heller J. Chem. Phys. **62,** 1544 (1975)
- DFT-MD
  R. Car, M. Parinello PRL 55, 2471 (1985)
- Quantum dynamics in Wigner representation
  Filinov V.S. Mol. Phys. **88**, 1517 (1996)
- Gaussian quantum dynamics
  Corney J.F., Drummond P.D. PRL **93**, 260401 (2004)

QUANTUM DYNAMICS IN WIGNER REPRESENTATION

Quasi-distribution function in phase space for the quantum case

Density matrix: $\rho(q',q'') = \psi^*(q')\psi(q'')$ $\quad \psi \in C$ $\quad i\frac{\partial \rho}{\partial t} = [\hat{H}, \rho]$

↓

Wigner function: $W^L(q,p) = \frac{1}{(2\pi)^{Nd}} \int \rho\left(q + \frac{\xi}{2}, q - \frac{\xi}{2}\right) e^{-ip\xi} d\xi$

$$\rho(q',q'') = \int W^L\left(\frac{q'+q''}{2}, p\right) e^{i(q'-q'')p} dp \qquad W^L \in R$$

Evolution equation: $\frac{\partial W^L}{\partial t} + \left\langle \frac{p}{m} \middle| \frac{\partial W^L}{\partial q} \right\rangle = \int ds W^L(p-s,q,t)\,\omega(s,q)\,ds$

$$\omega(s,q) = \frac{2}{(2\pi)^{Nd}} \int dq' U(q-q') \sin\left[\frac{2sq'}{\hbar}\right]$$

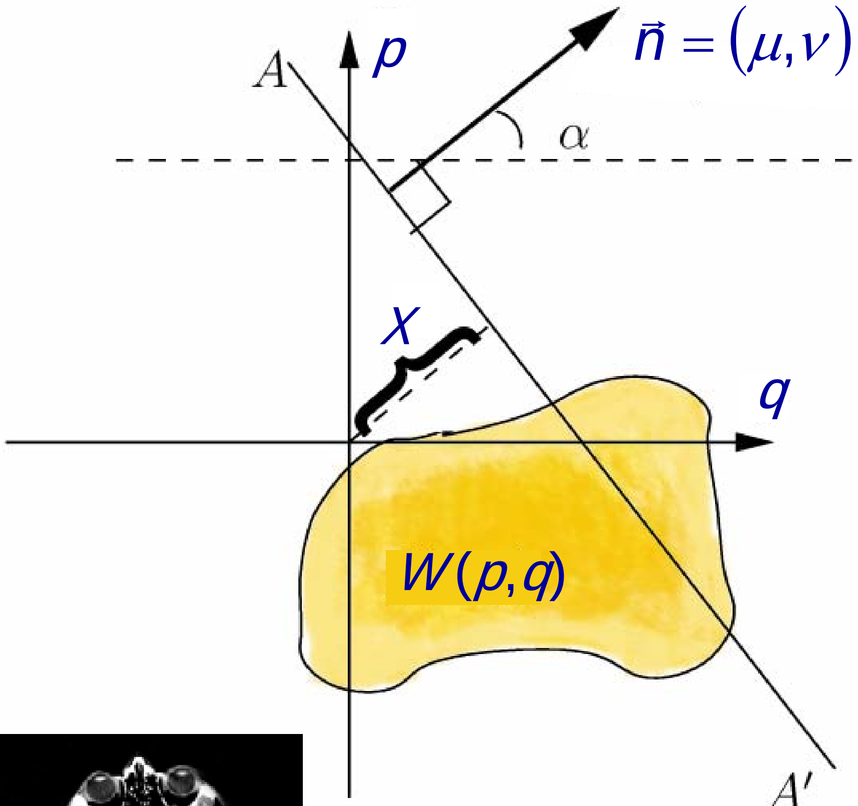
Classical limit $\hbar \to 0$:

$$\frac{\partial W^L}{\partial t} + \left\langle \frac{p}{m} \middle| \frac{\partial W^L}{\partial q} \right\rangle - \left\langle \frac{\partial U}{\partial q} \middle| \frac{\partial W^L}{\partial p} \right\rangle = 0$$

Characteristics (Hamilton equations):

$$\langle \dot{q} | = \left\langle \frac{p}{m} \right| \qquad \langle \dot{p} | = -\left\langle \frac{\partial U}{\partial q} \right|$$

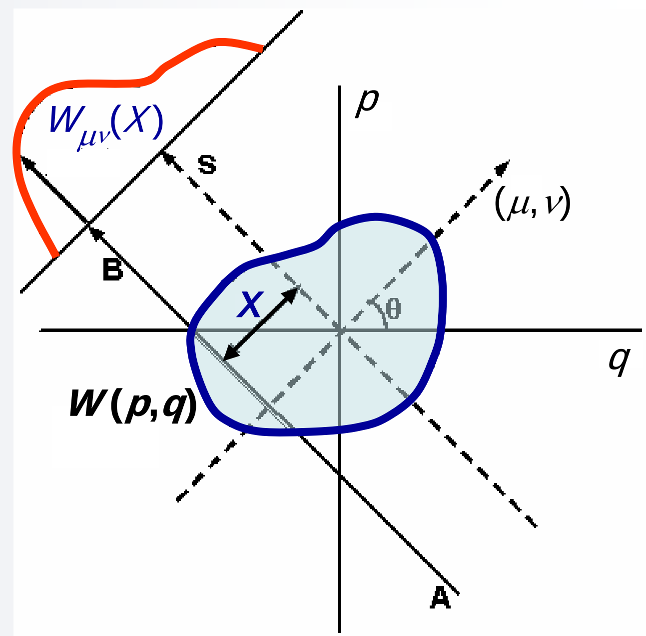
RADON TRANSFORMATION



$$X = \mu q + \nu p$$

$$W(X, \mu, \nu) = \int W(p,q)\,\delta(X - \mu q - \nu p)\,dq\,dp$$

$$W(p,q) = \int W(X, \mu, \nu)\, e^{-i(X - \mu q - \nu p)} \frac{dX\,d\mu\,d\nu}{(2\pi)^2}$$



- 3D (2D) object reconstruction using 2D (1D) images
- Quantum tomography

TOMOGRAPHIC REPRESENTATION

S. Mancini, V.I. Man'ko, P. Tombesi, Found. Phys. **27,** 801 (1997)

Radon transformation: $W^L(p,q) \Rightarrow W(X,\mu,\nu)$

$W \in R$

$W \geq 0$

Marginal distribution function:

$$W(X,\mu,\nu,t) = \int W^L(p,q,t)\,\delta\left(X - \langle \mu | q \rangle - \langle \nu | p \rangle\right) dp\,dq$$

$$W^L(p,q,t) = \int W(X,\mu,\nu,t)\, e^{-i\left(X - \langle \mu | q \rangle - \langle \nu | p \rangle\right)} \frac{dx\,d\mu\,d\nu}{(2\pi)^{2Nd}}$$

Evolution equation:

$$\frac{\partial W}{\partial t} - \left\langle \frac{\mu}{m} \middle| \frac{\partial W}{\partial \nu} \right\rangle = -\frac{1}{2}\int \frac{dX'\,ds\,dk}{2\pi} W(X', k\mu + s, k\nu)\, U(s)\, e^{i(X' - kX)} \sin\left[\frac{\langle k\nu | s \rangle}{2\hbar}\right]$$

Classical limit $\hbar \to 0$:

$$\frac{\partial W}{\partial t} - \left\langle \frac{\mu}{m} \middle| \frac{\partial W}{\partial \nu} \right\rangle + \frac{1}{4}\left\langle \nu \int ds\, |s\rangle U(s) \langle s| \,\middle|\, \frac{\partial W}{\partial \mu} \right\rangle + \frac{i}{4}\left\langle \nu \middle| \int ds\, U(s)\, |s\rangle\langle s| \right\rangle \frac{\partial W}{\partial X} = 0$$

Characteristic equations for X, μ, ν

PROPAGATORS AND KOLMOGOROV EQUATION

Formal solution:

$$W(X,\mu,\nu,t)=\int \Pi(X,\mu,\nu,t;X_0,\mu_0,\nu_0,t_0)W(X_0,\mu_0,\nu_0,t_0)dX_0 d\mu_0 d\nu_0$$

Properties:

$$\Pi(z_1,t_1;z_0,t_0)\geq 0 \qquad \int \Pi(z_1,t_1;z_0,t_0)dz=1$$

$$\Pi(z_3,t_3;z_1,t_1)=\int \Pi(z_3,t_3;z_2,t_2)\Pi(z_2,t_2;z_1,t_1)dz_2 \qquad t_1<t_2<t_3$$

(Chapman-Kolmogorov equation)

Kolmogorov equation for propagator:

$$\frac{\partial \Pi}{\partial t}+\sum_{j=1}^{n} a_j(z_1,t)\frac{\partial \Pi}{\partial z^j}+\frac{1}{2}\sum_{j=1}^{n}\sum_{l=1}^{n} b_{jl}(z_1,t)\frac{\partial^2 \Pi}{\partial z^j \partial z^l}=0$$

$$\frac{\partial \Pi}{\partial t}+\sum_{j=1}^{n}\frac{\partial}{\partial z^j}\left(a_j(z_2,t)\Pi\right)-\frac{1}{2}\sum_{j=1}^{n}\sum_{l=1}^{n}\frac{\partial^2}{\partial z^j \partial z^l}\left(b_{jl}(z,t)\Pi\right)=0$$

Langevin equation:

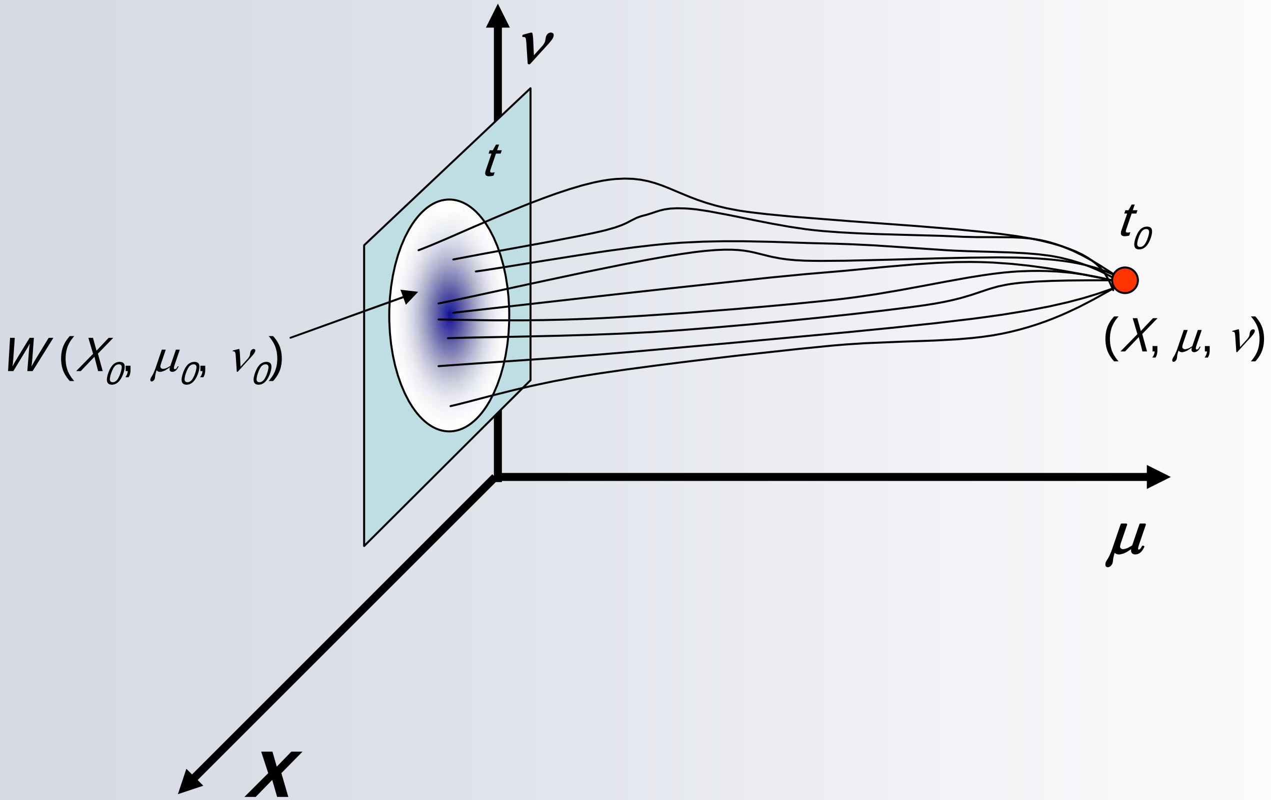
$$\frac{dz_j(t)}{dt}=\phi_j(z(t),t)+\sum_{l=1}^{2Nd+1} g_{jl}\xi_l(t)$$

$$\phi_j(z,t)=a_j(z,t)-\frac{1}{2}\sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial g_{jl}}{\partial z_k}g_{kl}$$

$$b_{jl}(z,t)=\sum_{k=1}^{n} g_{jk}g_{lk}$$

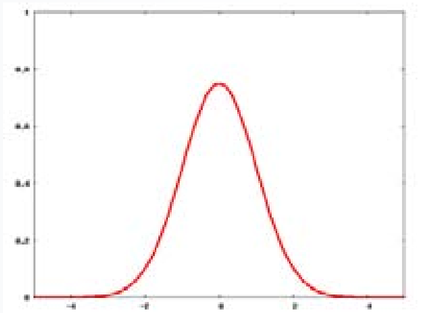
RECONSTRUCTION OF TOMOGRAPHIC FUNCTION

$$W(X,\mu,\nu,t)=\int \Pi(X,\mu,\nu,t_0;X_0,\mu_0,\nu_0,t)W(X_0,\mu_0,\nu_0,t_0)dX_0d\mu_0d\nu_0$$



CALCULATION OF AVERAGES

Initial wave function (1D):



$$\psi_0(q,p)=\left(\frac{A}{\pi}\right)^{1/4}\exp\left(-\frac{A}{2}(q-q_0)^2+ipp_0\right)$$

Average value:

$$\left\langle \hat{A}(t)\right\rangle=\int \exp(iX)W(X,\mu,\nu,t)A(\mu,\nu)dXd\mu d\nu$$

$$A(\mu,\nu)=\int A^W(q,p)\exp\left(-i\left(\langle\mu|q\rangle+\langle\nu|p\rangle\right)\right)\frac{dqdp}{(2\pi)^{2Nd}}$$

Two sets of initial conditions:

$\{X_1=0,\mu_1=1,\nu_1=0\}$ - coordinate

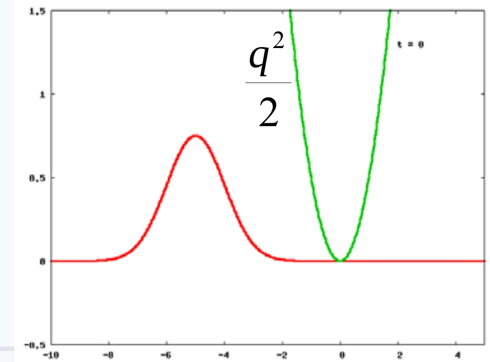
$\{X_2=0,\mu_2=0,\nu_2=1\}$ - momentum

$$\left\langle \hat{A}_q(t)\right\rangle=\int A_q(X)W(X,\mu_1=1,\mu_2=0,\nu_1=0,\nu_2=0,t)dX$$

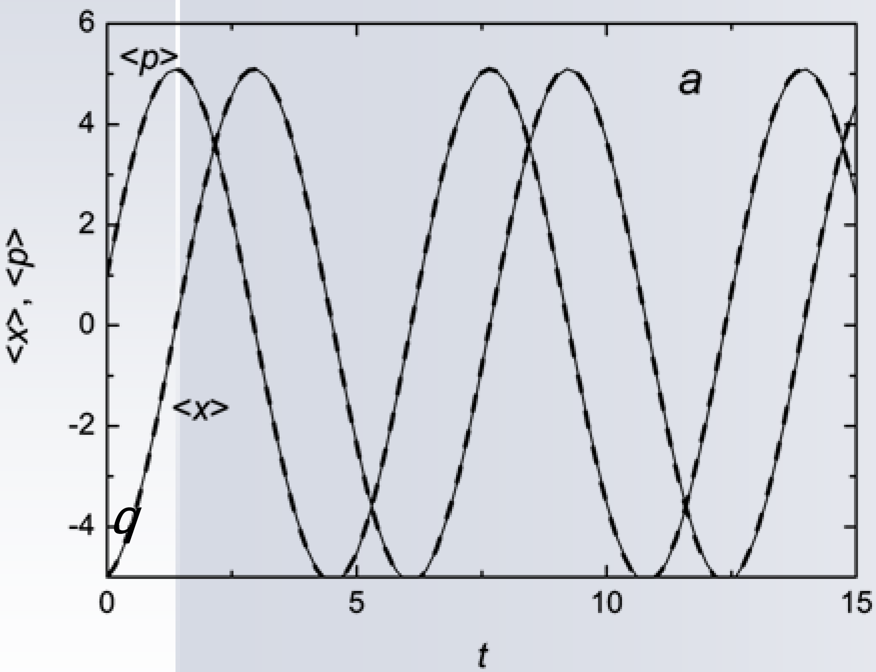
$$\left\langle \hat{A}_p(t)\right\rangle=\int A_p(X)W(X,\mu_1=0,\mu_2=0,\nu_1=1,\nu_2=0,t)dX$$

Energy and wave function are calculated similarly

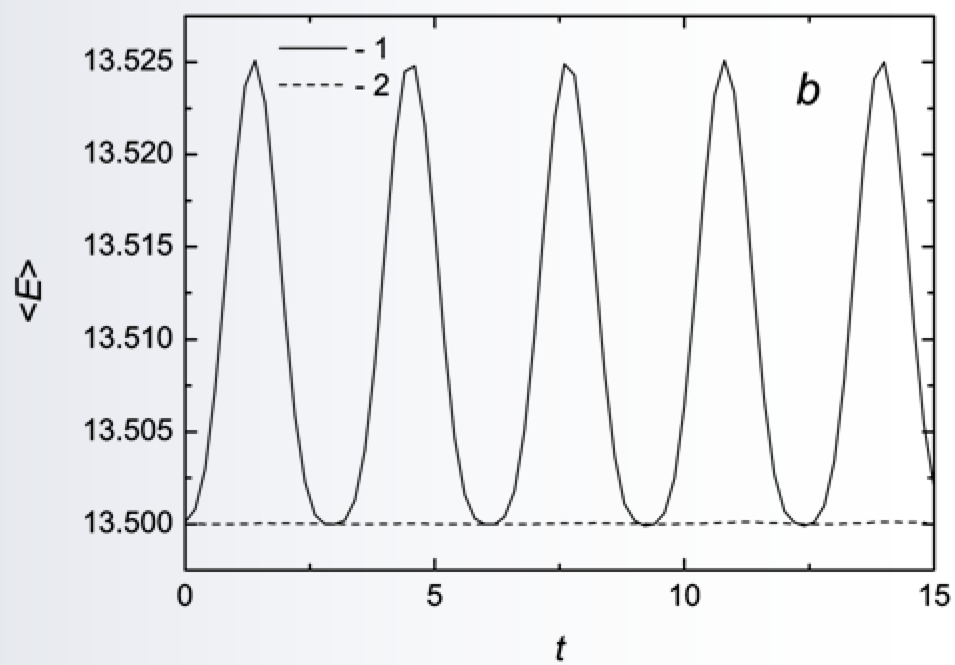
HARMONIC WELL: AVERAGE VALUES



Coordinate and momentum



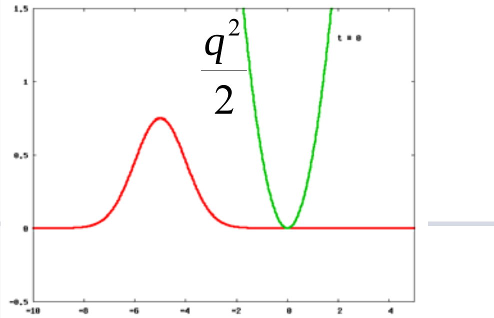
Total energy

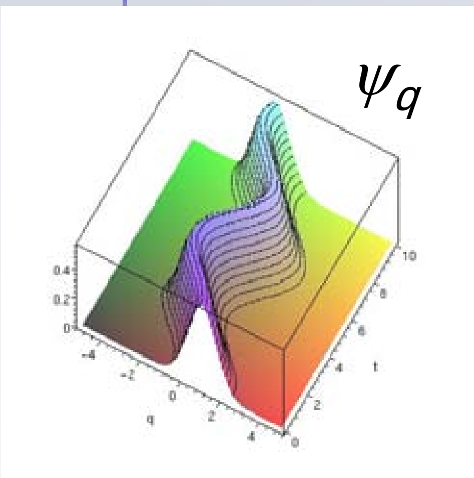


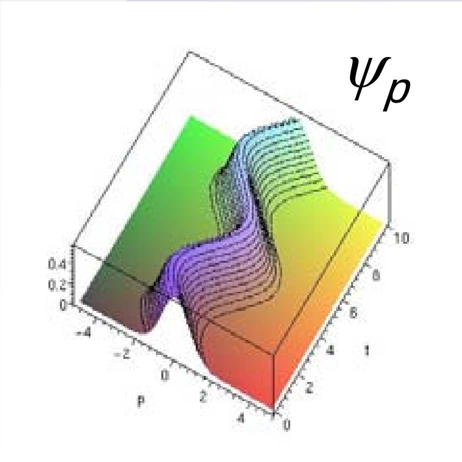
——— Schrödinger equation

- - - - - Tomographic representation

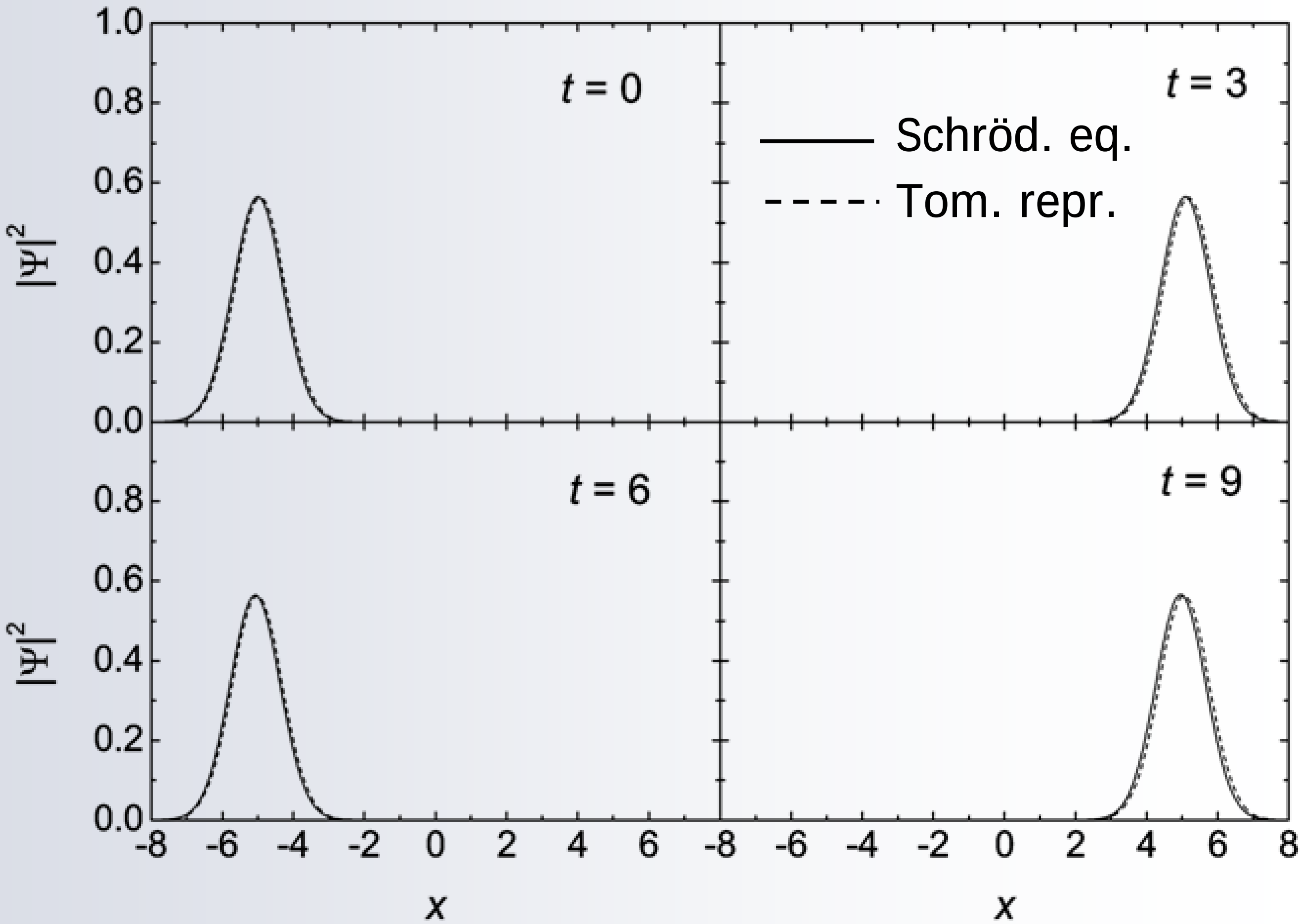
HARMONIC WELL: WAVE FUNCTIONS



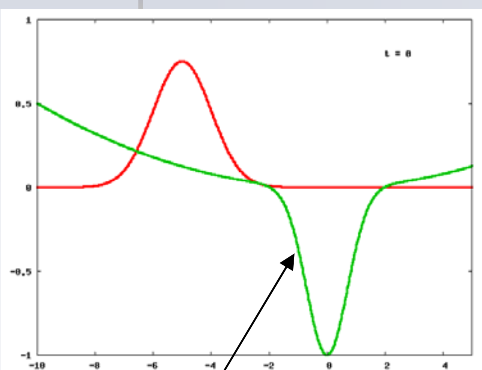




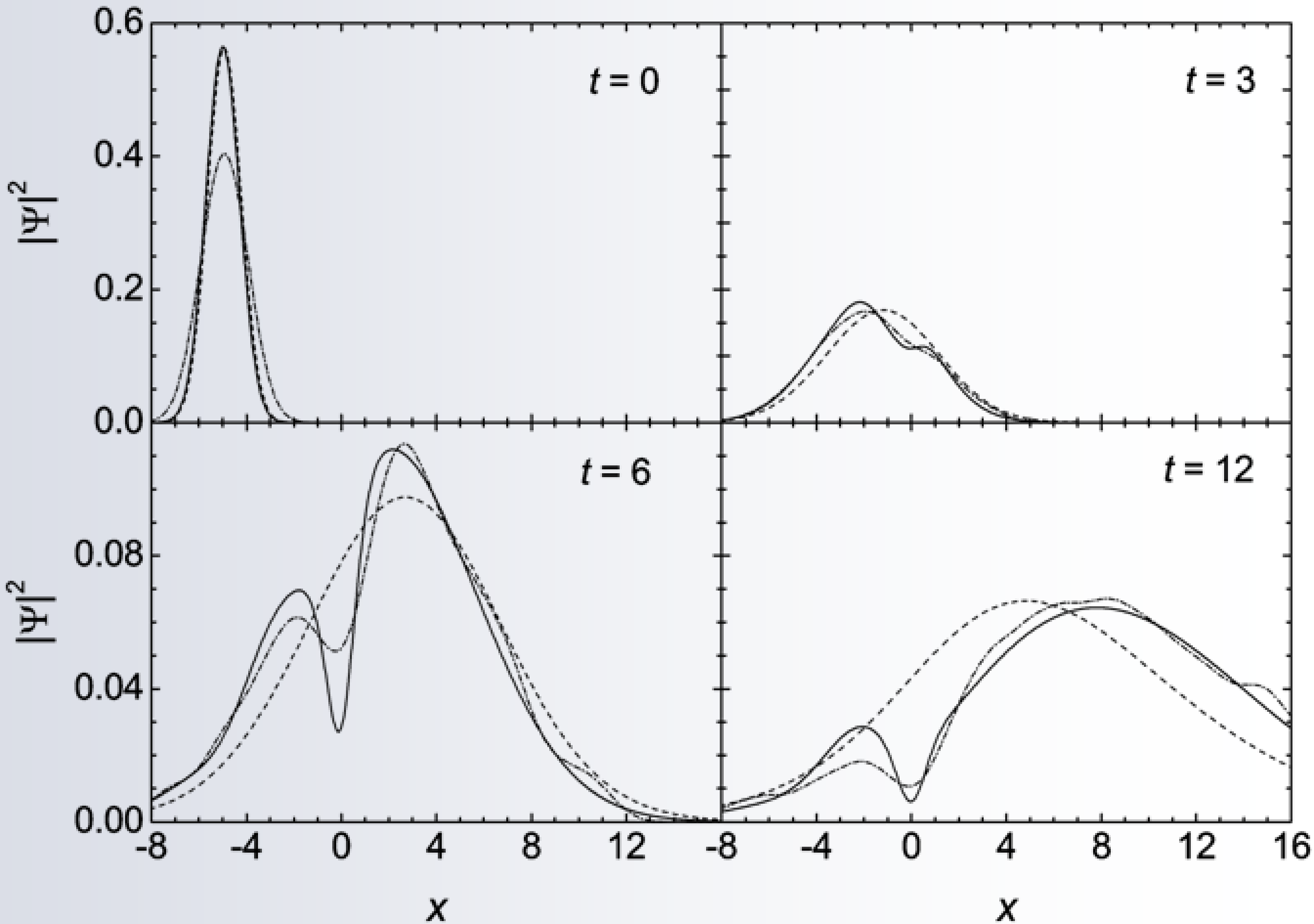
Harmonic well



GAUSSIAN WELL: WAVE FUNCTIONS



$$\frac{q^2}{200} - e^{-q^2}$$

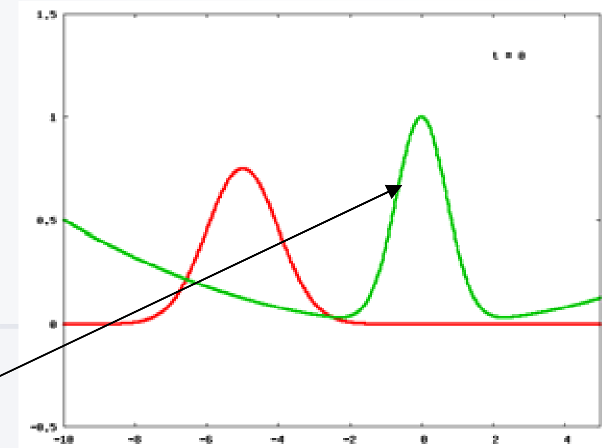


—— Schröd. eq.

- - - - Tom. repr.

—·— Wigner repr.

WAVE FUNCTION EVOLUTION

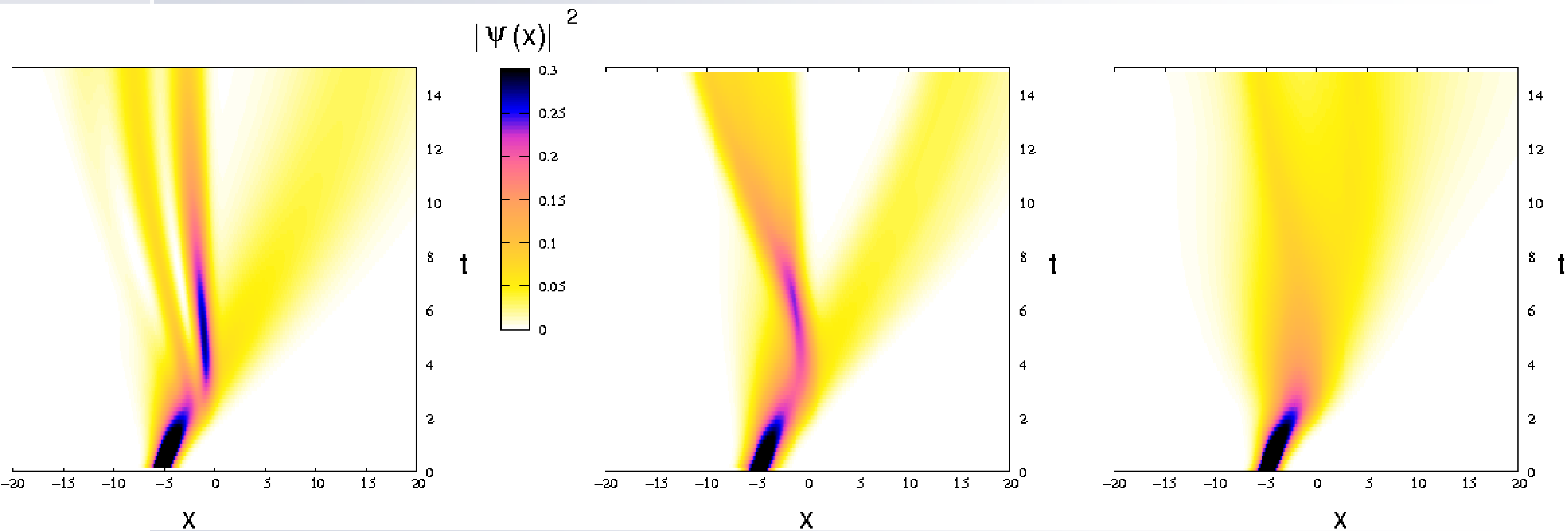


Gaussian barrier $\frac{q^2}{200} + e^{-q^2}$

Schrodinger equation

Wigner equation

Tomographic representation



CONCLUSIONS

- Dynamics of quantum particles is described by the Kolmogorov equation for the Green function in tomography representation (X, μ, ν)
- This is equivalent to the system of Langevin equations for (X, μ, ν) which can be solved by a combination of finite difference numerical scheme and random sampling
- Thus a quantum dynamics of particles is given by Markovian random processes
- The presented approach works very well for harmonic potential and satisfactory well for more complicated potentials
- The tomographic representation as well is a perspective tool for creation of quantum dynamics methods based upon Wigner formulation