How to deduce a physical dynamical model from expectation values

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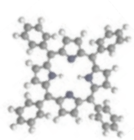
Operational ***D***ynamical ***M***odeling

theoretical framework to deduce *reduced-dimensional* and *computationally-efficient* models of complex quantum dynamics in *systematic fashion* from *observable* data

angstrom ⟷ **meter**

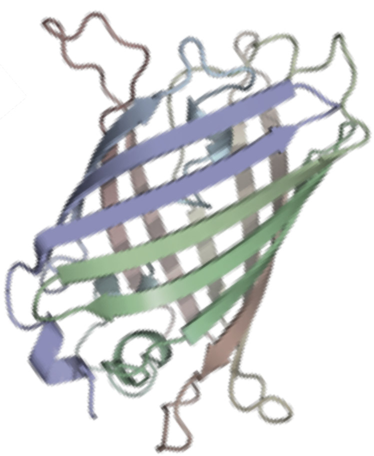
atom

molecule



material design

protein

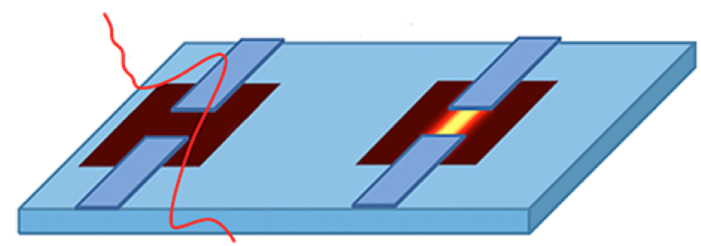


detection

superfluidity/BEC

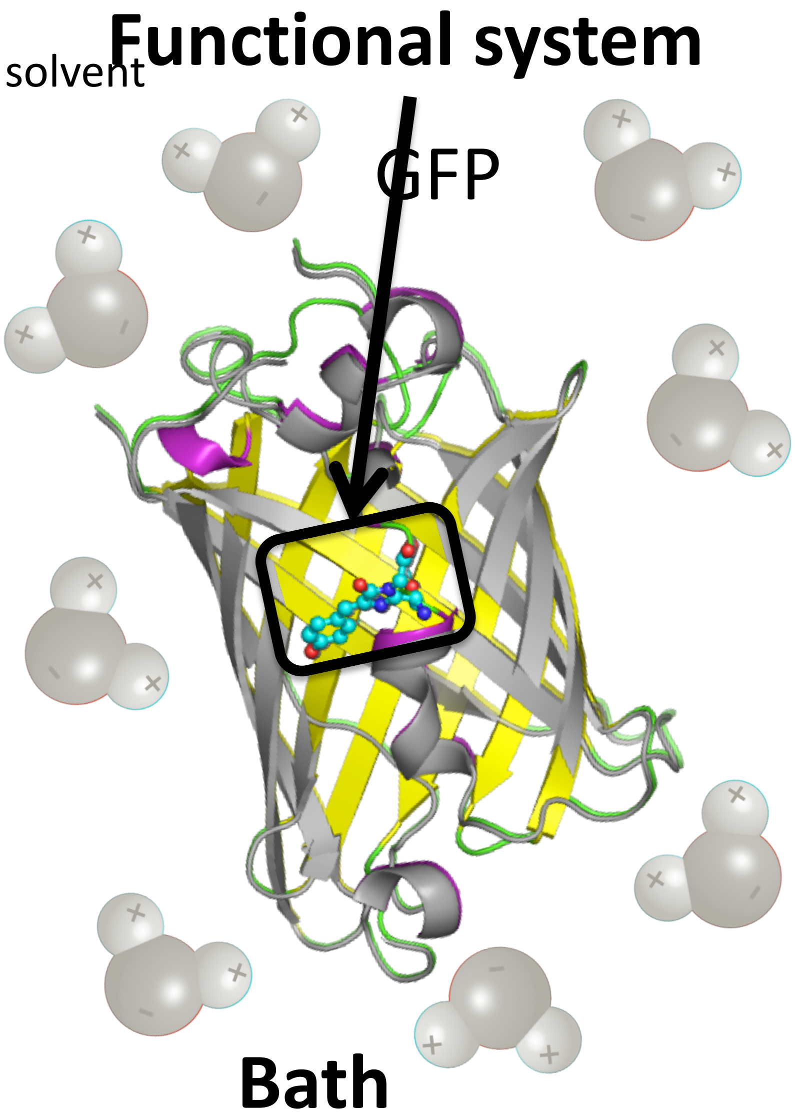
high precision metrology

ultrafast (picosecond) phase-switching materials

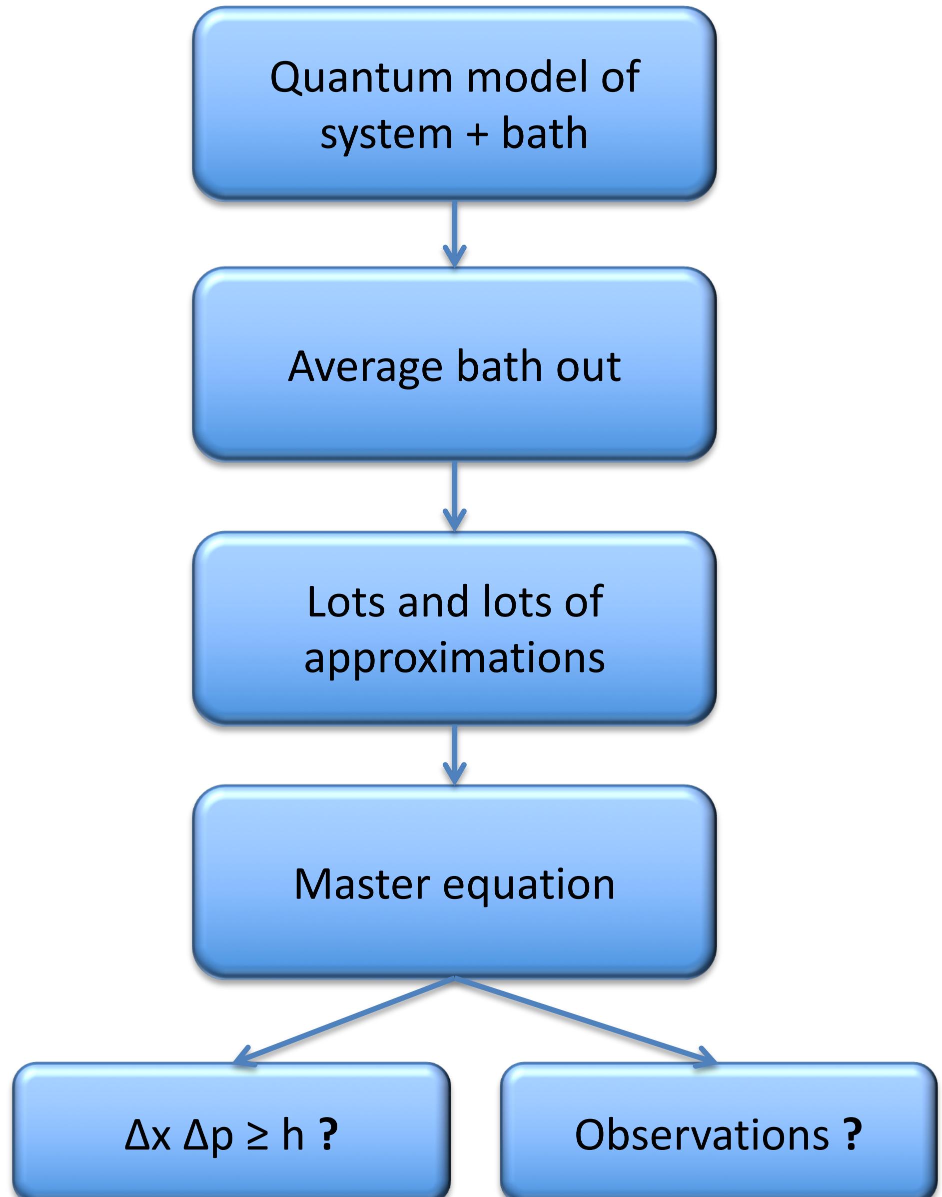


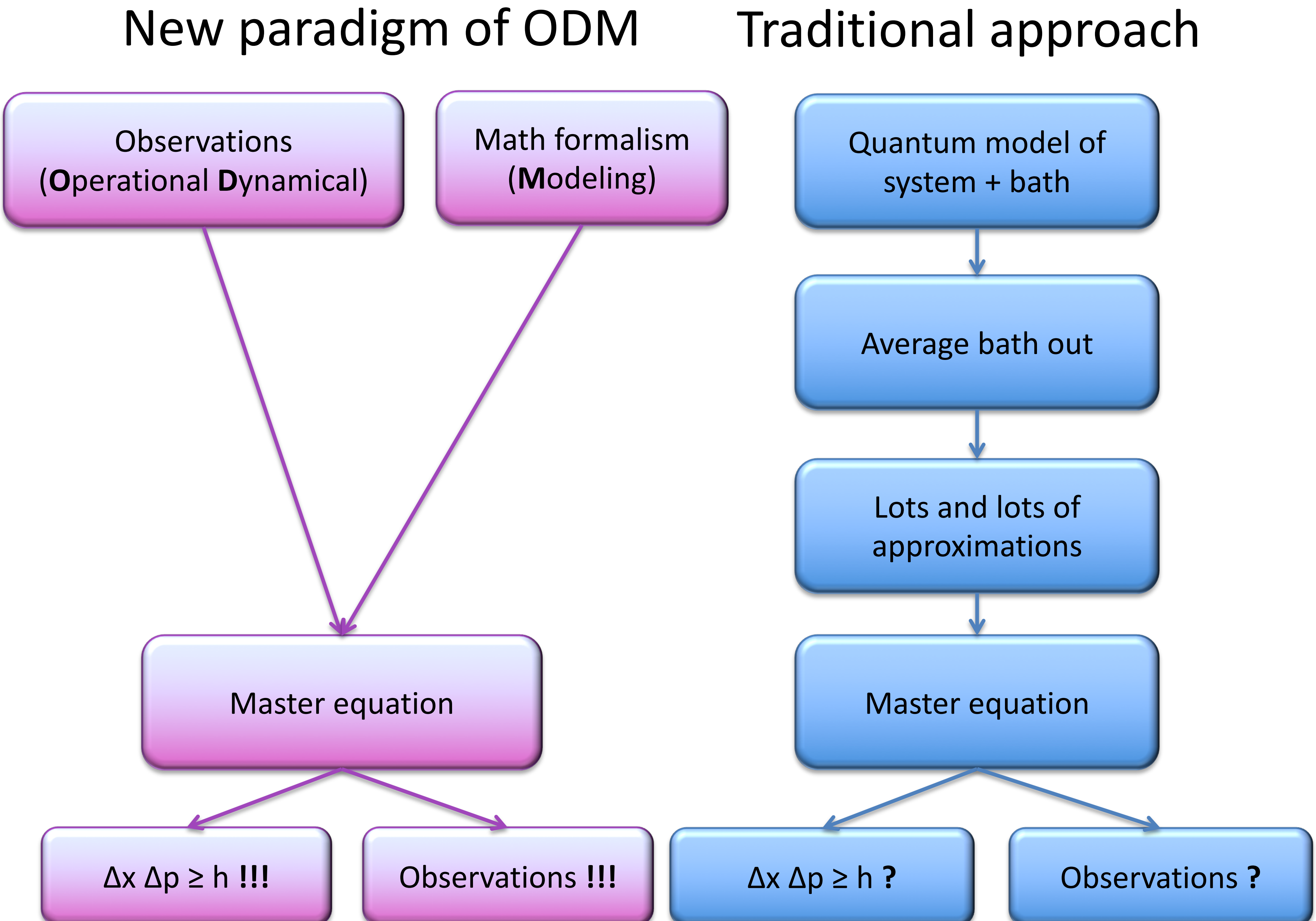
future generation of materials

Example: Model of molecular spectra



Traditional approach




New paradigm of ODM
Traditional approach
Observations
(**O**perational **D**ynamical)
Math formalism
(**M**odeling)
Master equation
Δx Δp ≥ h **!!!**
Observations **!!!**
Quantum model of
system + bath
Average bath out
Lots and lots of
approximations
Master equation
Δx Δp ≥ h **?**
Observations **?**

Outline

- Introduction to ODM
- Derive Schrodinger equation
- Quantum open system dynamics
  - Quantum reservoirs engineering
- Making *Pb* look like *Au*
- Conclusions

ODM: Consistency check

Observations are given by the following Ehrenfest theorems (aka, Drude model)

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$

$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

Note that

$$\Big\langle -U'(x)\Big\rangle = \Big\langle \sum_k c_k x^k \Big\rangle = \sum_k c_k \Big\langle x^k \Big\rangle$$

We want to represent dynamics in Hilbert space

$$\langle \hat{A}\rangle(t) = \langle \Psi(t)|\hat{A}|\Psi(t)\rangle$$

$$[\hat{x},\hat{p}] = i\hbar$$

$$i\hbar|d\Psi(t)/dt\rangle = \hat{H}|\Psi(t)\rangle$$

We get quantum generator of motion

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x})$$

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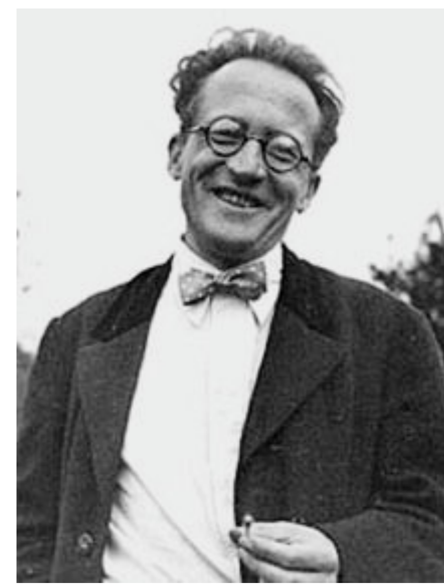
ODM: Quantum Mechanics

Ehrenfest is cooler than Schrödinger!

$$[\hat{x}, \hat{p}] = i\hbar$$

+

=



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We want to represent dynamics in Hilbert space

$$\langle \hat{A}\rangle(t) = \langle \Psi(t)|\hat{A}|\Psi(t)\rangle$$
$$[\hat{x},\hat{p}] = 0$$
$$i\hbar|d\Psi(t)/dt\rangle = \hat{H}|\Psi(t)\rangle$$

Koopman-von Neumann classical mechanics
i.e.
Newton mechanics

09, 190403]

ODM: Koopman-von Neumann Classical Mechanics

B. O. Koopman, PNAS USA **17**, 315 (1931)
J. von Neumann, Ann. Math. **33**, 587 (1932)

$$+ \quad [\hat{x},\hat{p}] = 0 \quad =$$

Liouvillian
Classical Mechanics

$$\bar{F} = \int dxdp\, \rho(x,p) F(x,p)$$

$$\left[\frac{\partial}{\partial t} + \frac{p}{m}\frac{\partial}{\partial x} - U'(x)\frac{\partial}{\partial p} \right] \rho(x,p;t) = 0$$

=

Koopman-von
Neumann
Classical Mechanics

$$[\hat{x}, \hat{p}] = 0$$

$$\bar{F} = \langle \Psi | F(\hat{x}, \hat{p}) | \Psi \rangle$$

$$\left[\frac{\partial}{\partial t} + \frac{p}{m}\frac{\partial}{\partial x} - U'(x)\frac{\partial}{\partial p} \right] \langle p\, x \,| \Psi(t) \rangle = 0$$

$$\rho(x,p;t) = |\langle p\, x \,| \Psi(t) \rangle\,|^2$$

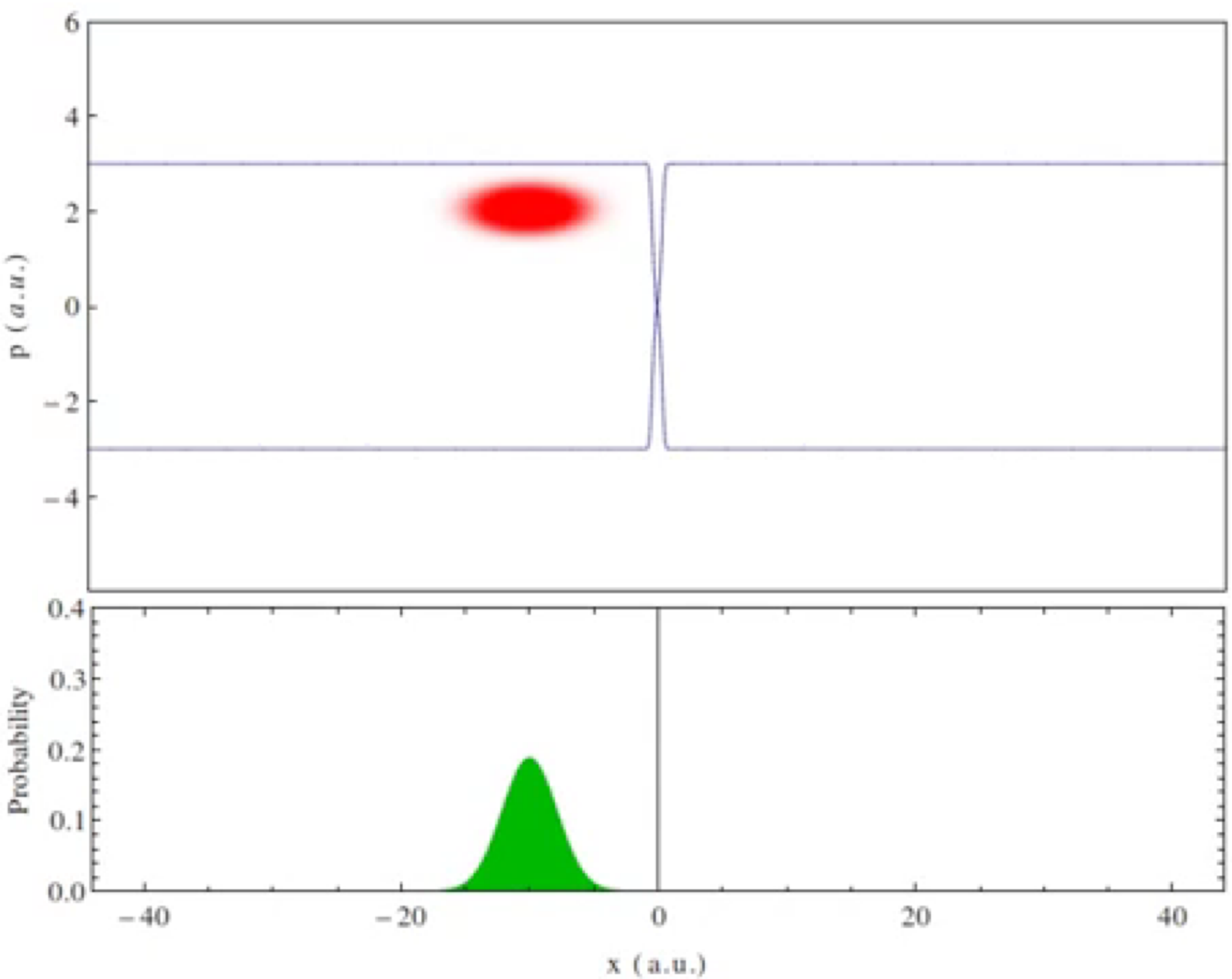
ODM: Reservoir engineering

- Tunneling is a quantum hallmark effect
- Coupling to bath destroys coherence, thereby ~~suppressing tunneling rates~~

Not so fast!

Let’s use ODM to find environment that enhance tunneling rates

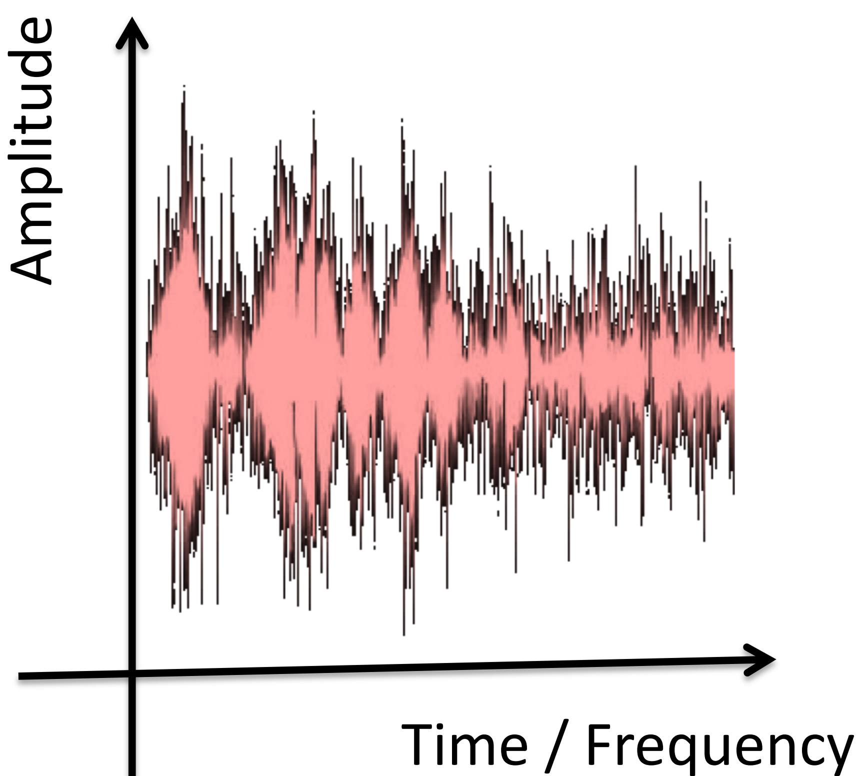
Wigner function for tunneling



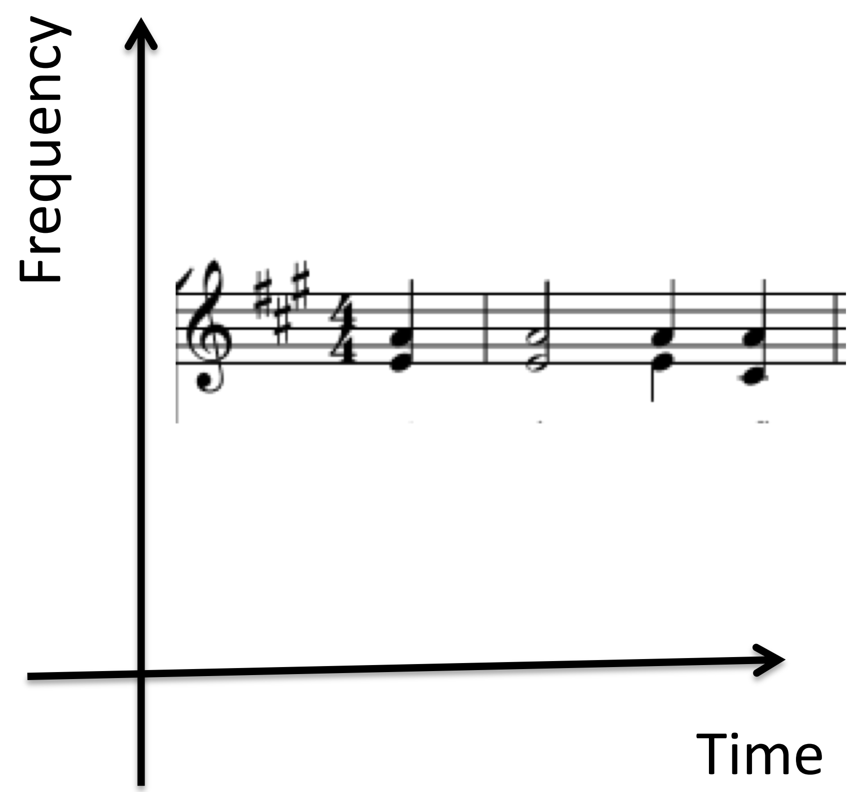
The Wigner quasi probability distribution

$$W(x,p) = \int \frac{d\lambda_p}{2\pi} \langle x - \hbar\lambda_p/2|\hat{\rho}|x + \hbar\lambda_p/2\rangle e^{ip\lambda_p}$$

(similar to density matrix)



(similar to Wigner function)



Quantum reserv

Particle ***feels*** potential barrier

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$
$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

We want our model to be Lindbladian, i.e.,

$$\langle \hat{O}\rangle = \mathrm{Tr}\,[\hat{O}\hat{\rho}(t)].$$
$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + D[\rho],$$
$$D[\hat{\rho}] = \frac{1}{\hbar}\left(\hat{A}\hat{\rho}\hat{A}^\dagger - \frac{1}{2}\hat{\rho}\hat{A}^\dagger\hat{A} - \frac{1}{2}\hat{A}^\dagger\hat{A}\hat{\rho}\right)$$
$$\hat{H} = \hat{p}^2/(2m) + U(\hat{x}).$$
$$[\hat{x},\hat{p}] = i\hbar.$$

We get unknown Lindbladian operator

$$A(x,p) = R(x)\exp\left(i\int^x \frac{U'(\xi)}{R^2(\xi)}d\xi\right)$$

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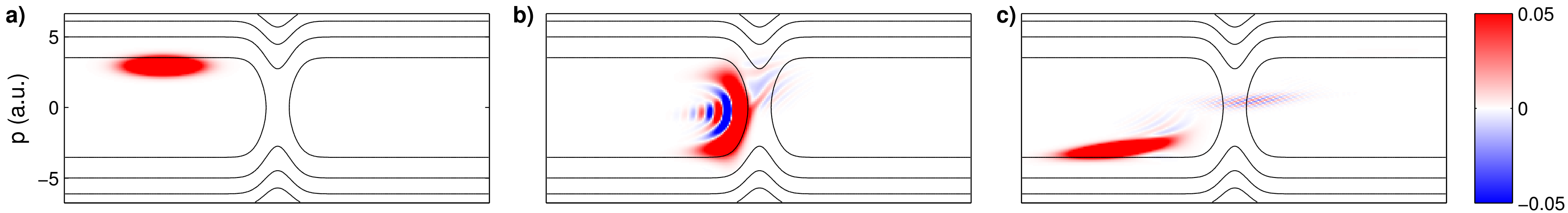
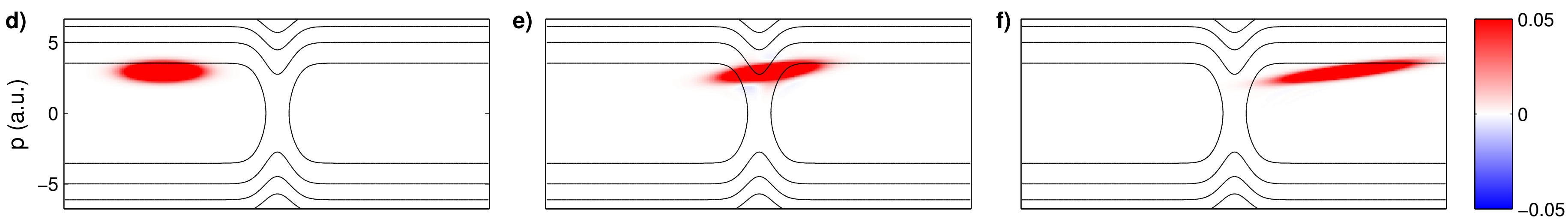
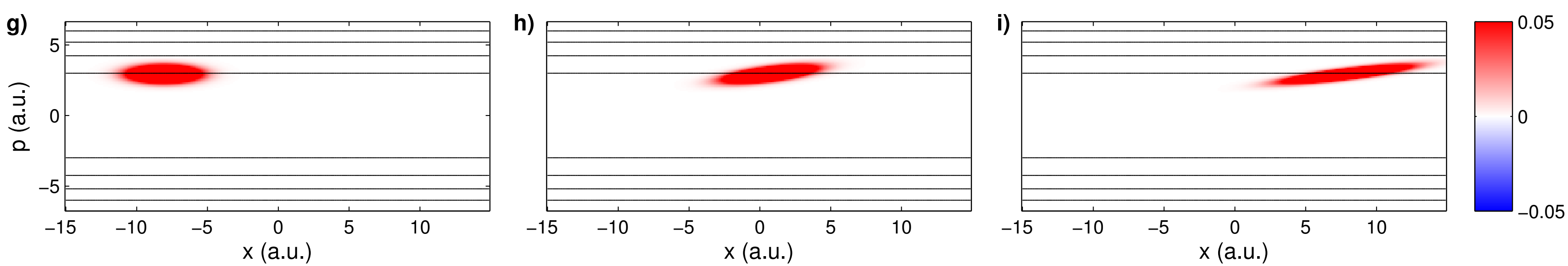
Closed system



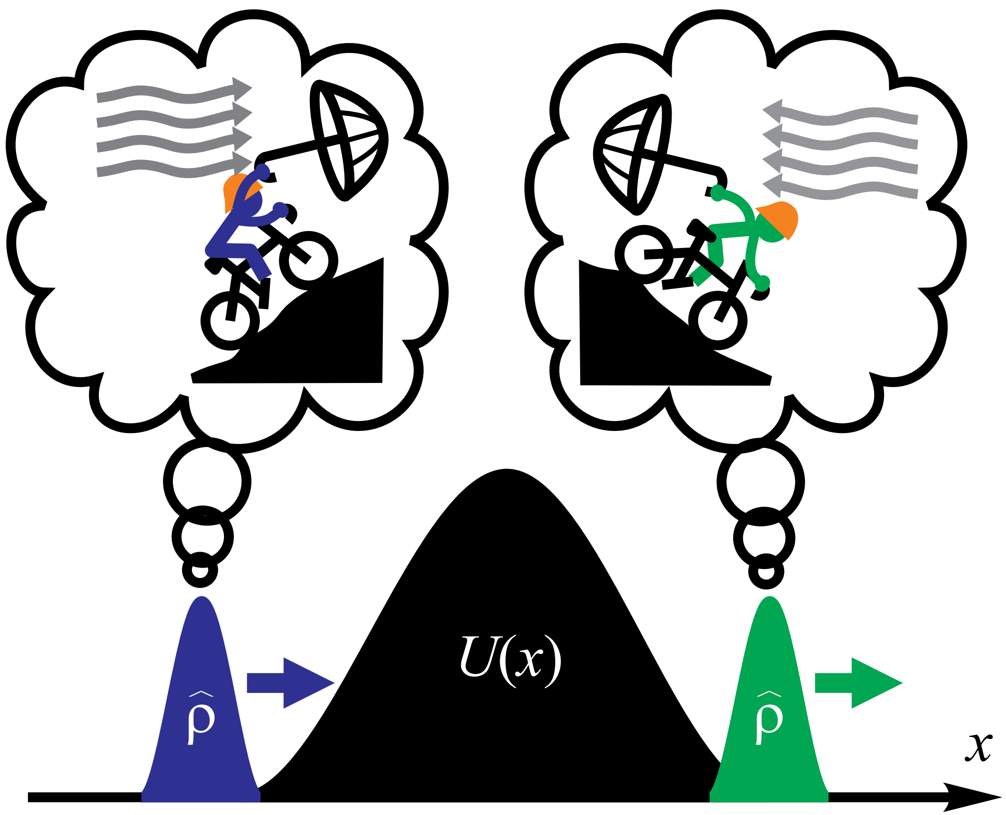
Designed open system



Coherent free particle evolution



What is the mechanism?



Quantum reservoirs engineering

using open system interactions

$$\langle \hat{O} \rangle = \mathrm{Tr}\,[\hat{O}\hat{\rho}(t)].$$

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \sum_{k=1}^{K} \mathcal{D}_{\hat{A}_k}[\hat{\rho}] + \sum_{n=1}^{N} \mathcal{D}_{\hat{B}_n}[\hat{\rho}]$$

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + U(\hat{x})$$

$$\mathcal{D}_{\hat{A}}[\hat{\rho}] = \frac{1}{\hbar}\left(\hat{A}\hat{\rho}\hat{A}^\dagger - \frac{1}{2}\hat{\rho}\hat{A}^\dagger\hat{A} - \frac{1}{2}\hat{A}^\dagger\hat{A}\hat{\rho}\right)$$

We want general dynamics

$$\frac{d}{dt}\langle \hat{x} \rangle = \langle G(\hat{p}) \rangle$$

$$\frac{d}{dt}\langle \hat{p} \rangle = \langle F(\hat{x}) \rangle$$

Can we make it a frie

frenemy?

[PRL **120,** 230404]

$$A_k(x) = R_k(x)\exp\left(i\int \frac{f_k(x)}{R_k^2(x)}\,\mathrm{d}x\right) \quad B_n(p) = S_n(p)\exp\left(-i\int \frac{g_n(p)}{S_n^2(p)}\,\mathrm{d}p\right)$$

Application 2: Dissipative Traps

Environment can trap a particle

Isolated particle is free

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle = \frac{1}{m}\langle\hat{p}\rangle;$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = 0.$$

Open particle is trapped

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$
$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

Quantum Reservoir Engineering

We want general dynamics

$$\frac{d}{dt}\langle\hat{x}\rangle = \langle G(\hat{p})\rangle$$

$$\frac{d}{dt}\langle\hat{p}\rangle = \langle F(\hat{x})\rangle$$

Modification of G cannot be done by conservative forces

using open system interactions

$$\langle\hat{O}\rangle = \mathrm{Tr}\,[\hat{O}\hat{\rho}(t)].$$

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \sum_{k=1}^{K}\mathcal{D}_{\hat{A}_k}[\hat{\rho}] + \sum_{n=1}^{N}\mathcal{D}_{\hat{B}_n}[\hat{\rho}]$$

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + U(\hat{x})$$

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[PRL **120,** 230404]

$$A_k(x) = R_k(x)\exp\left(i\int\frac{f_k(x)}{R_k^2(x)}\,\mathrm{d}x\right) \quad B_n(p) = S_n(p)\exp\left(-i\int\frac{g_n(p)}{S_n^2(p)}\,\mathrm{d}p\right)$$

Application 3: Channing mass

Environmental effective mass

Isolated particle

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$
$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

$\rightarrow$

Open particle

$$\frac{d}{dt}\langle x\rangle = \frac{1}{M}\langle p\rangle$$
$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

Application 4: Pseudo-relativistic dynamics

Isolated particle

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$
$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

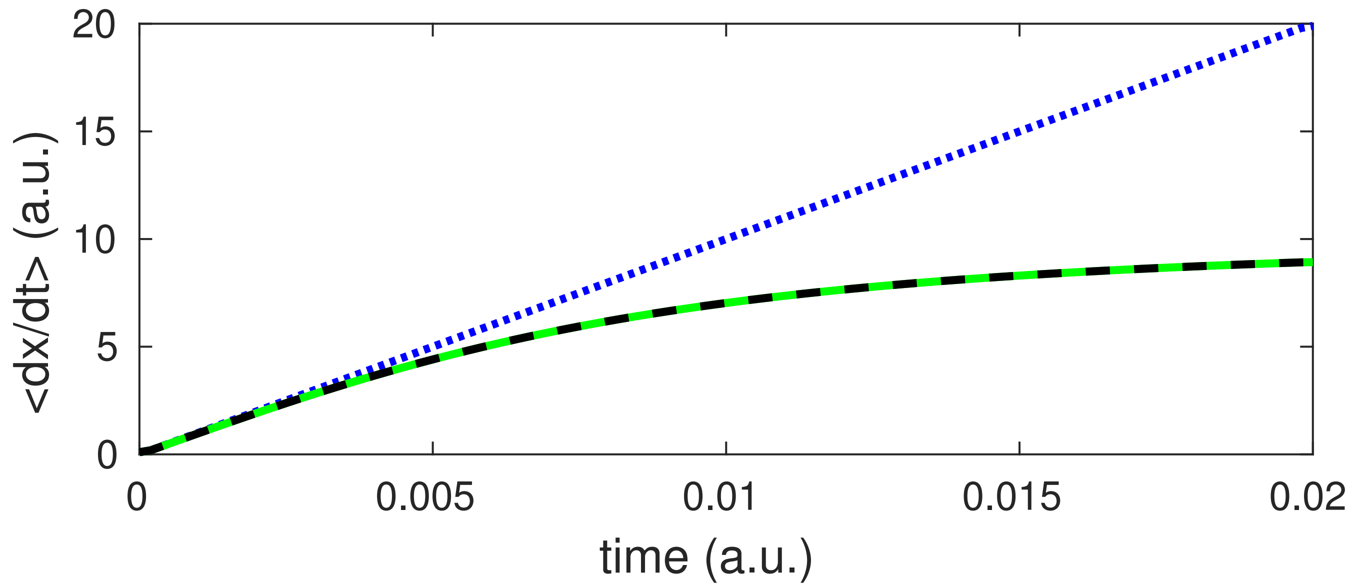
Open particle

$$\frac{d}{dt}\langle x\rangle = \left\langle \frac{p}{\sqrt{m^2 + p^2/c^2}} \right\rangle$$
$$\frac{d}{dt}\langle p\rangle = -\langle U'(x)\rangle$$

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + U(\hat{x}) \longrightarrow \hat{H}_{\mathrm{rel}} = \sqrt{c^2\hat{p}^2 + c^4} + U(\hat{x})$$

Application 4: Pseudo-relativistic dynamics

Numerical verification



How to Make Distinct Dynamical Systems Appear Spectrally Identical

i.e.

Making  ***Pb*** looks like  *Au*

Polarizability **Driving laser field**

Is it possible to find external laser field that drives an arbitrary optical response?

Yes!

[PRL **118**, 083201]

Making *A* looks like *B*

Main idea:

Polarizability (known)

system

Driving laser field (unknown)

$$\frac{d^2}{dt^2}\left\langle \sum_{k=1}^{N} \hat{x}_k \right\rangle = \left\langle \sum_{k=1}^{N} F_k(\hat{x}_k) \right\rangle + N E(t)$$

electrons

Therefore, if we want $Y(t) = \frac{d^2}{dt^2}\left\langle \sum_{k=1}^{N} \hat{x}_k \right\rangle$ then $E(t) = \frac{Y(t)}{N} - \frac{1}{N}\left\langle \sum_{k=1}^{N} F_k(\hat{x}_k) \right\rangle (t)$

Known

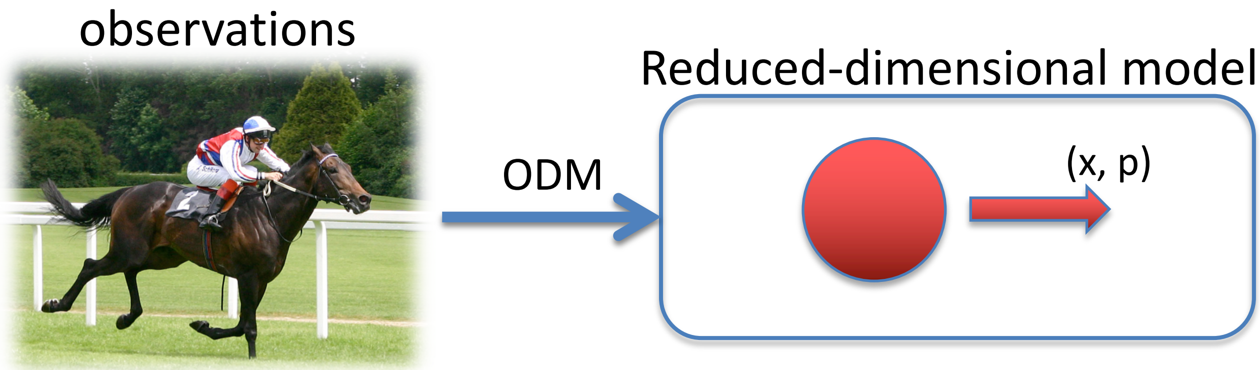
Unknown,
but can be estimated

ODM: Tracking control of optical response

Optical responses

Driving laser fields

Conclusions (3D of ODM)



- **D**erive new physical models
  - QED as open system dynamics
  - engineering environments with “paradoxical” behavior
  - Evolution in topologically nontrivial configuration spaces
- **D**arn inconsistencies in old models
  - conditions when averages incompatible with formalism
- **D**esign numerical methods
  - propagators for open system dynamics in Wigner phase-space formalism

Bonus: What was before the periodic table?

Story of $\hbar$

- $\hbar$ denotes lead in alchemy
- $\hbar$ denotes Saturn in astrology
- *Ħ (ħ)* is character in Maltese alphabet
- $\hbar$ is also known as Dirac constant (Dirac may have introduced it)