Title: Simulating unitary dynamical maps on a quantum computer.

Date: Sep 12, 2007 02:00 PM

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Abstract: I will discuss an alternative approach to simulating Hamiltonian flows with a quantum computer. A Hamiltonian system is a continuous time dynamical system represented as a flow of points in phase space. An alternative dynamical system, first introduced by Poincare, is defined in terms of an area preserving map. The dynamics is not continuous but discrete and successive dynamical states are labeled by integers rather than a continuous time variable. Discrete unitary maps are naturally adapted to the quantum computing paradigm. Grover's algorithm, for example, is an iterated unitary map. In this talk I will discuss examples of nonlinear dynamical maps which are well adapted to simple ion trap quantum computers, including a transverse field Ising map, a non linear rotor map and a Jahn-Teller map. I will show how a good understanding of the quantum phase transitions and entanglement exhibited in these models can be gained by first describing the classical bifurcation structure of fixed points.

Simulating unitary dynamical maps on a quantum computer.

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Centre for Quantum Computer Technology,
The University of Queensland, Australia.

Jon Links, UQ
John Paul Barjaktarevic, UQ.
Melissa Duncan, UQ
Ross Mckenzie, UQ.

Outline of talk

- What is a unitary dynamical map?
- Fixed points and bifurcations.
- The Jahn-Teller unitary map.
- The transverse field-Ising unitary map.

Area preserving maps.

The King of Sweden and Professor Poincaré.

1885: Mathematical contest.

Is the solar system *dynamically stable* ?

Méthodes Nouvelles de la Mécanique Céleste.

First hints of chaos.

it may happen that small differences in the initial conditions produce very great ones in the final phenomena. A small error in the former will produce an enormous error in the latter. Prediction becomes impossible, and we have the fortuitous phenomenon.

Poincaré, "Science and Method", 1903.

Poincaré's method.

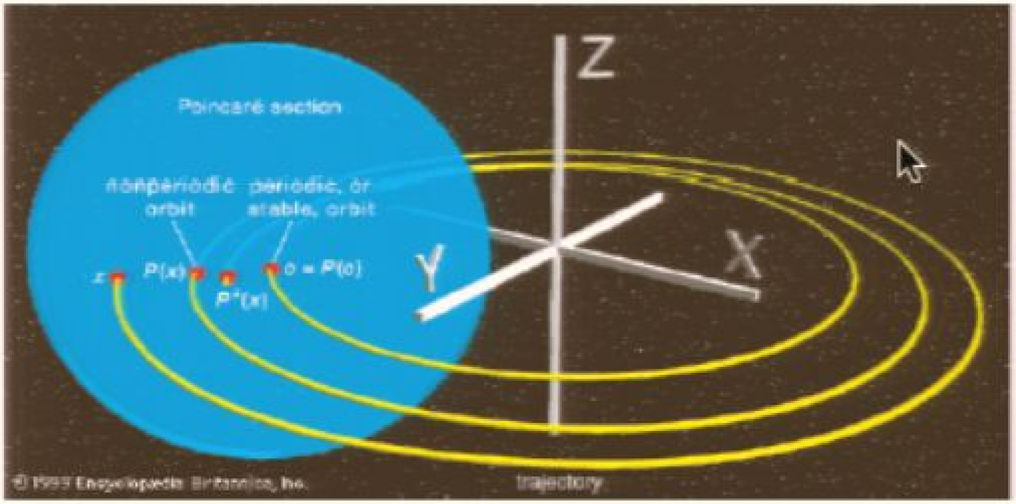
Beyond perturbation series to new geometric methods.

Not particular solutions but classes of solutions as a whole.

Interestingly, nothing about the three-body equations themselves had changed. Instead, using his new way of "viewing" differential equations, Poincaré could see something that was built into those equations all along but had previously escaped notice.

Ivars Peterson, MathTrek

Surface of section.



Studying the Poincaré map gives a complete characterization of the dynamics in a neighborhood of a periodic orbit.

The periodic orbit of the continuous dynamical system is stable if and only if the fixed point of the discrete dynamical system is stable.

Stroboscopic maps.

Periodically driven systems with a periodic Hamiltonian

$$H(t+T) = H(t)$$

Define discrete states

$$(q_n, p_n) = (q(t_0 + nT), p(t_0 + nT))$$

and *stroboscopic map*

$$(q_n, p_n) = F(q_{n-1}, p_{n-1})$$

Example: kicked rotor.

A free rotor subject to impulsive torques:

$$H(t) = \frac{L^2}{2} + k \cos\theta \sum_n \delta(t-n)$$

The Floquet map is then defined by

$$\begin{aligned} \theta_{n+1} &= \theta_n + L_{n+1} \\ L_{n+1} &= L_n + k \sin\theta_n \end{aligned}$$

Period-one fixed points:

$$\begin{aligned} \theta^* &= \theta^* + L^* \\ L^* &= L^* + k \sin\theta^* \end{aligned}$$

$$L^* = 0 \;\; \& \;\; \theta^* = 0, \pi$$

Example: kicked rotor.

Stability:

$$\begin{pmatrix} \delta\theta_{n+1} \\ \delta L_{n+1} \end{pmatrix} = \begin{pmatrix} 1 \pm k & 1 \\ \pm k & 1 \end{pmatrix} \begin{pmatrix} \delta\theta_n \\ \delta L_n \end{pmatrix}$$

$$+ : \theta = \pi$$

$$- : \theta = 0$$

1. $\theta = 0$

eigenvalues: $\lambda_\pm = (1 - k/2) \pm i\sqrt{1 - (1 - k/2)^2}$

stable: $0 < k < 4$

2. $\theta = \pi$

eigenvalues: $\lambda_\pm = (1 + k/2) \pm \sqrt{(1 + k/2)^2 - 1}$

unstable

Example: kicked rotor.

Area preserving?

$$\lambda_+ \lambda_- = 1$$

Bifurcation?

fixed point at $\theta^* = 0$ undergoes a change of stability for $k > 4$

This is a *period doubling* bifurcation.

Example: kicked rotor.

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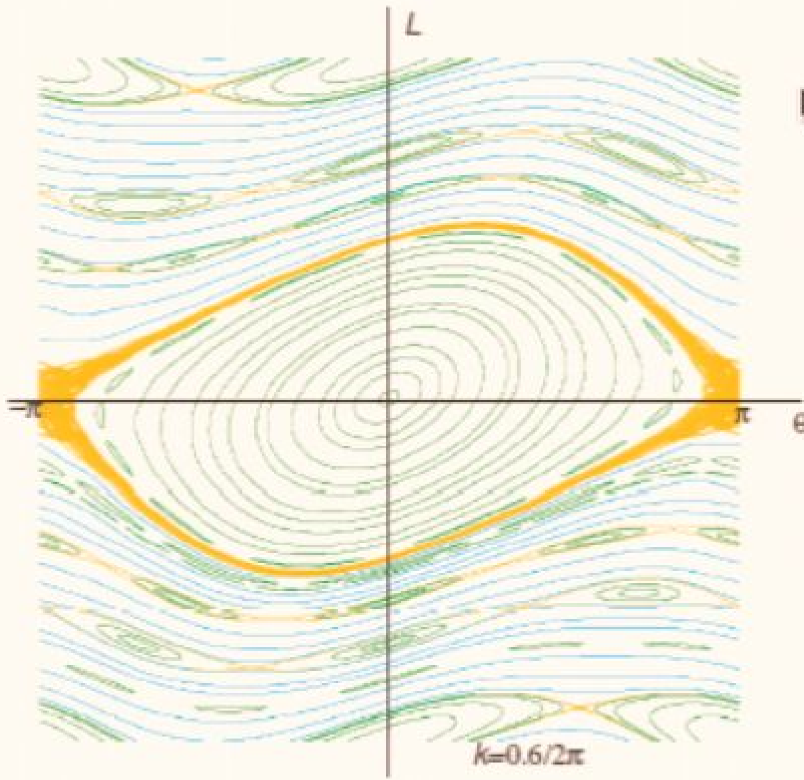
Example: kicked rotor.

very rich bifurcation dynamics



Example: kicked rotor.

Quantum description: unitary Floquet operator, $\hat{F}$, defines a *unitary dynamical map*:

$$|\psi_{n+1}\rangle = \hat{F}|\psi_n\rangle$$

$$\hat{F} = \exp\left(-\frac{i}{\hbar}k\cos\hat{\theta}\right)\exp\left(-\frac{i}{\hbar}\frac{\tau}{2}\hat{L}^2\right)$$

explicit kick period τ.

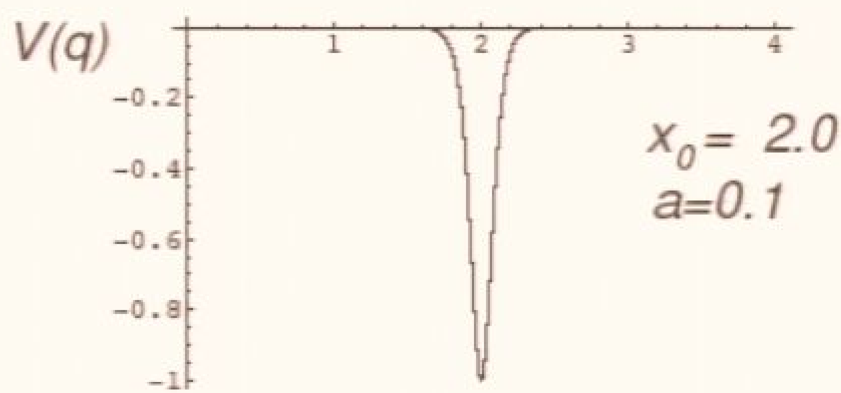
Kicked free particle: the Grover map

$$H = T(\hat{p}) + V(\hat{q}) \sum_n \delta(t-n)$$

Floquet map:

$$U = U_T . U_V = e^{-iT(\hat{p})} e^{-iV(\hat{q})}$$

Example: $V(q) = V_0 \left[\tanh^2\left(\frac{(q-q_0)}{a}\right) - 1\right]$ and $T(p) = p^2/2$.



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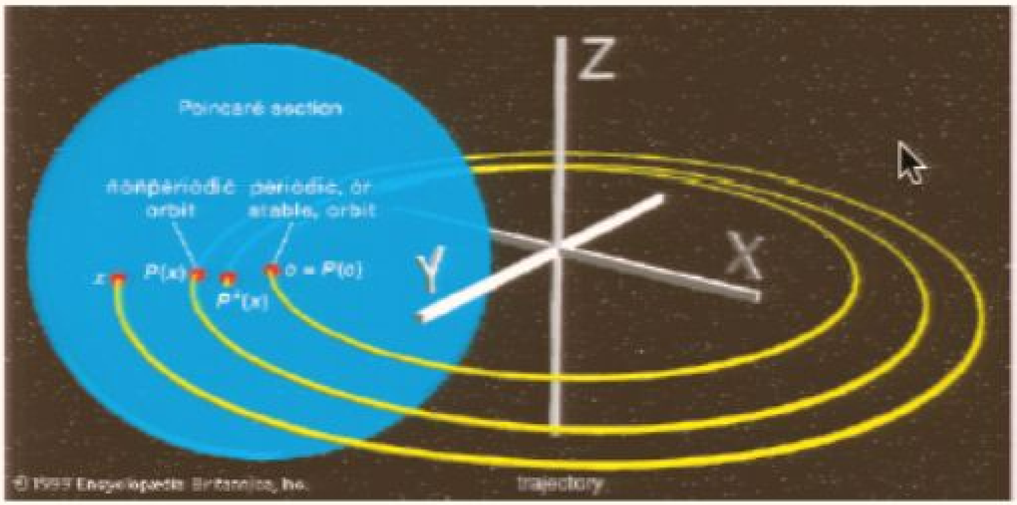

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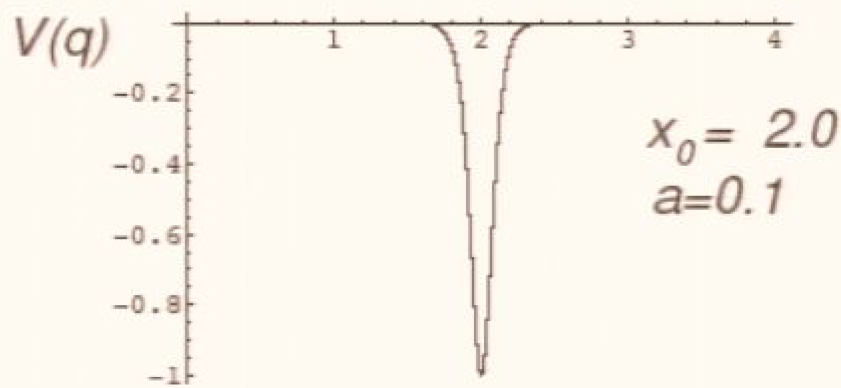
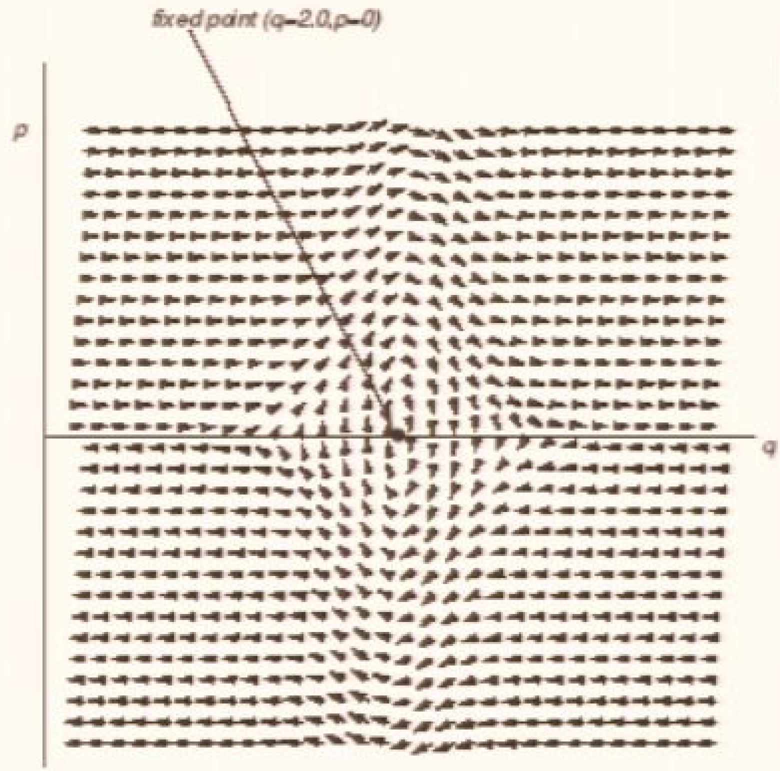


The flow version

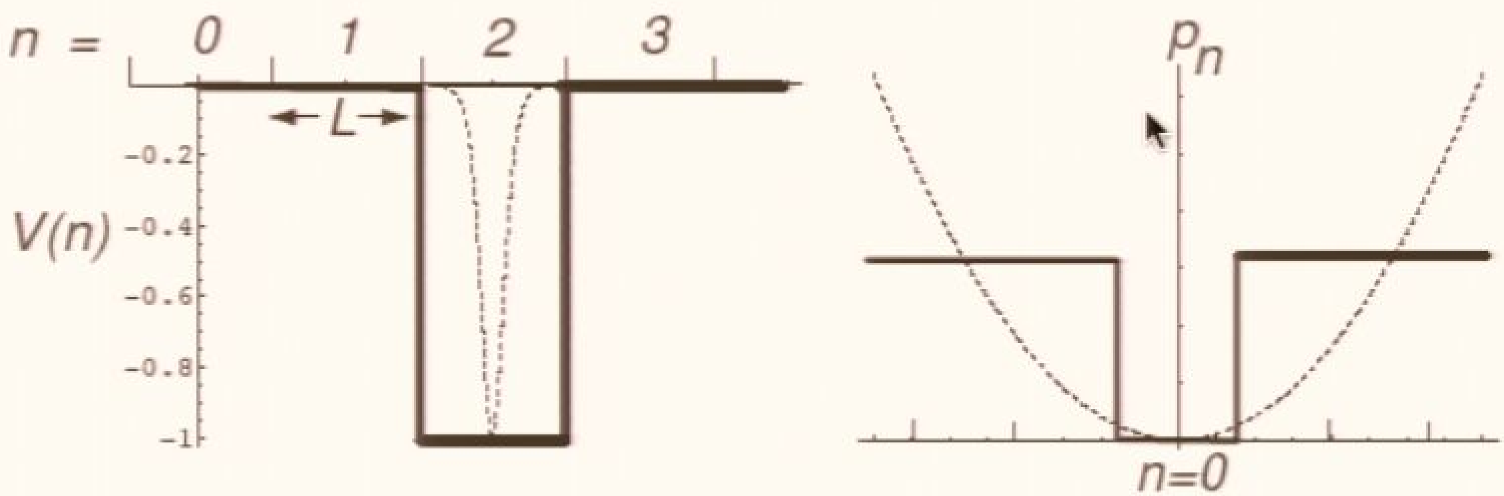
$$H = T(\hat{p}) + V(\hat{q})$$

Hamiltonian flow vector field:



Kicked free particle: the Grover map

Discretise position and momentum.



$$U_T = e^{-i\pi(1-|\bar{0}\rangle\langle\bar{0}|)}$$

$$U_V = e^{-i\pi|2\rangle\langle 2|}$$

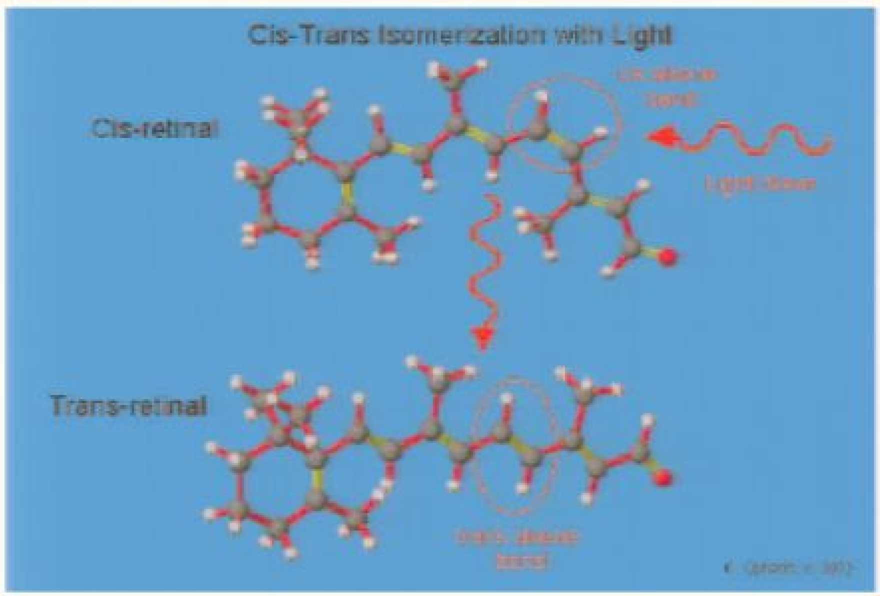
where $|\bar{0}\rangle = \mathcal{F}.\mathcal{T}.[|0\rangle] = |p_0\rangle$

Are there some physically interesting unitary maps that we can do right now?

Vision and quantum tunneling.

Cis-trans isomerization in rhodopsin.

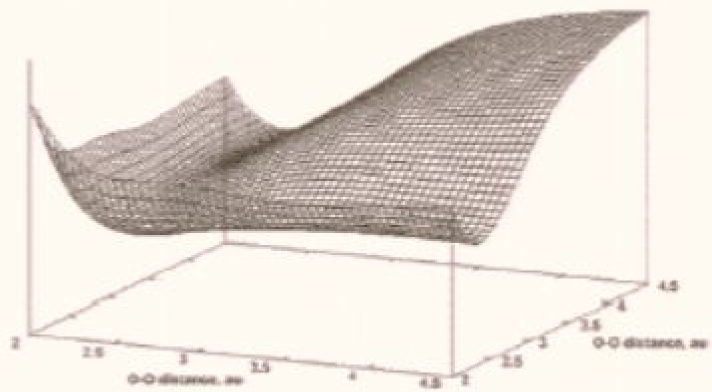
Absorption of a photon leads to a very fast (200 femtoseconds) isomerization of the molecule.



Potential surface

Triatomic molecule.

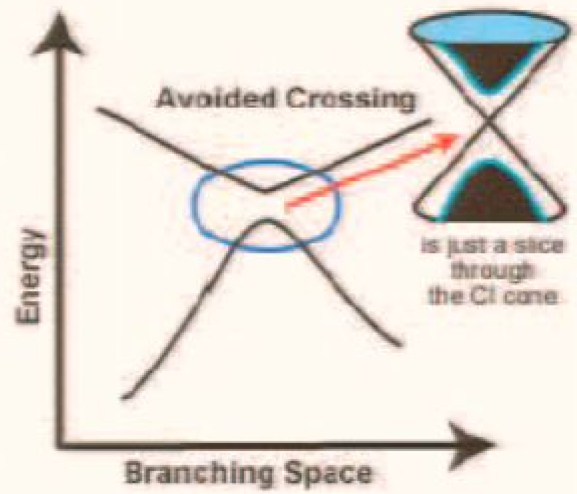
Plot electronic ground state energy as a function of internuclear separations X, Y



Ozone, ground electronic state.

Potential surface

Look at two electronic levels.
Find a two dimensional avoided crossing called a *conical intersection*



Minimal model

Use one two level system coupled to two oscillator coordinates: Jahn-Teller $E \otimes \epsilon$ model.

$$H = \tilde{\Delta}\sigma_z + \frac{1}{2m}(p_x^2 + p_y^2) + \frac{m\tilde{\omega}^2}{2}(q_x^2 + q_y^2) + \chi q_x \sigma_x + \chi q_y \sigma_y$$

Joel Gilmore, Ross H. McKenzie, *Criteria for quantum coherent transfer of excitons between chromophores in a polar solvent*, quant-ph/0412170

What is an ion trap?

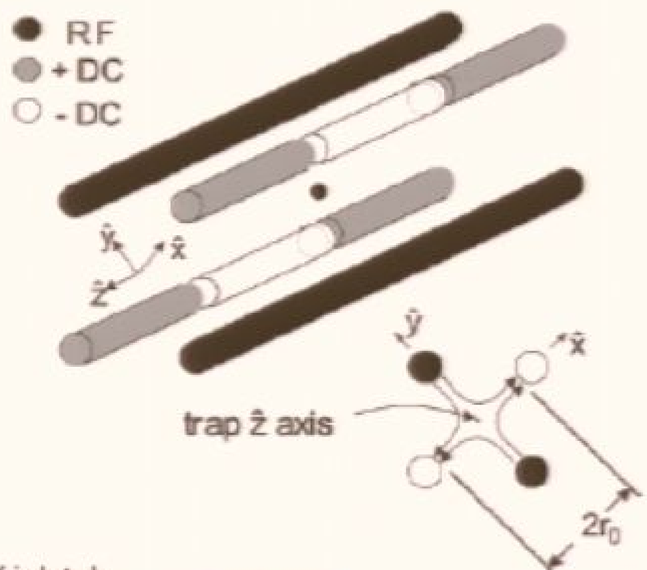
Objective: to harmonically trap a single ion in an electromagnetic trap, and cool to the vibrational ground state.

Problem: Laplace's equation $\rightarrow$ cannot make a stable electrostatic trap.

Solution: Time dependent potentials.

Examples.

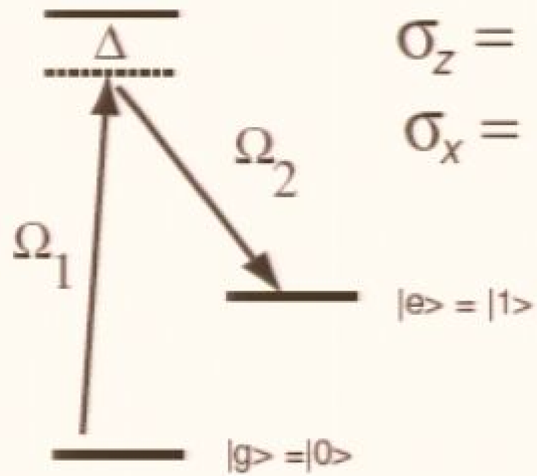
Linear RF trap.



Leibfried et al.
Rev. Mod. Phys. vol 75, 281 (2003)

Ion trap implementation.

Qubit states are electronic states of ions (typically metastable).



$\sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$

$\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|$

Effective two-photon Rabi frequency $\Omega = \Omega_1 \Omega_2 / \Delta$

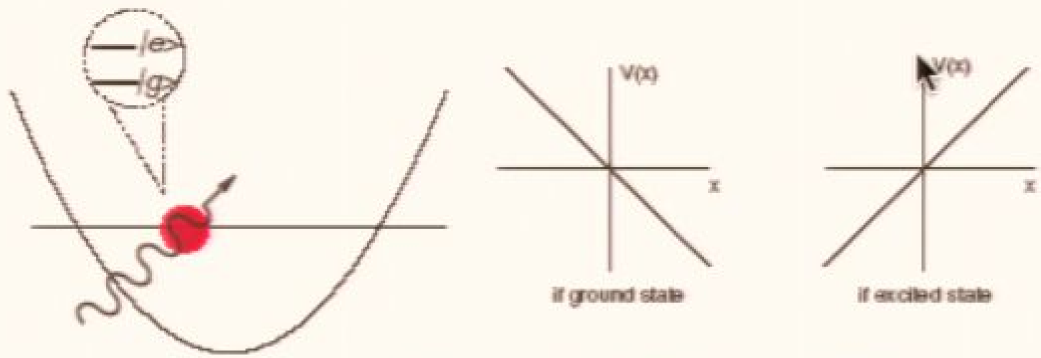
Single qubit rotations.

Tune Raman beams to the $|g\rangle \rightarrow |e\rangle$ transition, *carrier excitation*.

$$H_c = g\sigma_x$$

Conditional displacements.

Linear potential seen by atom depends on internal state.



Monroe et al. Science, 1996

Effective Hamiltonian

$$H_z = \frac{\hat{p}^2}{2m} + \frac{m\nu^2}{2}\hat{q}^2 + \chi(t)\hat{q}\sigma_z$$

a Jahn-Teller like interaction.

Conditional displacements.

Combine single qubit rotations and conditional displacements to give unitary kicks of the form

$$U_\alpha = e^{-i\chi\hat{x}\sigma_\alpha}$$

Two-dimensional ion trap.

Assume confinement is strong in $z-$direction and weaker in the $x, y-$direction. Use laser pulses for conditional displacements in orthogonal directions:

$$U = e^{-iH_0\tau}e^{-i\lambda H_x}e^{-i\lambda H_y}$$

$$H_0 = \tilde{\Delta}\sigma_z + \frac{1}{2m}(p_x^2 + p_y^2) + \frac{m\tilde{\omega}^2}{2}(q_x^2 + q_y^2)$$

$$H_\alpha = q_\alpha \sigma_\alpha \qquad \alpha = x, y$$

A Jahn-Teller map.

Semiclassical dynamics.

Step 1: quantum Heisenberg map,

$$\hat{A}_{n+1} = U^{\dagger} \hat{A}_n U$$

Step 2: take average values of both sides and factorise all moments, eg $\langle q_x \sigma_z \rangle = \langle q_x \rangle \langle \sigma_z \rangle$

Step 3: Assign classical variables,

$$\langle q_x \rangle \to q_x$$

$$\langle \sigma_\alpha \rangle \to s_\alpha$$

To get the classical map

$$(q_x, q_y, s_x, s_y, s_z)_{n+1} = M[(q_x, q_y, s_x, s_y, s_z)_n]$$

Fixed point analysis.

$$M[x^*] = x^*$$

When coupling is zero ($\lambda = 0$), fixed points are trivial

$$s_z = -1/2,\ s_x = s_y = q_x = q_y = p_x = p_y = 0$$

As λ is increased this point becomes unstable at

$$\lambda_b^2 = \frac{8\tan(\omega/2)}{\cot(\Delta/2) \pm 1}$$

$(\omega = \tilde{\omega}\tau,\ \Delta = \tilde{\Delta}\tau)$.

with $0, 1$ or 2 solutions depending on parameters.

Fixed points and bifurcations.

The smallest value for λ_b corresponds to a *pitchfork* bifurcation.

Fixed points correspond to solutions of,

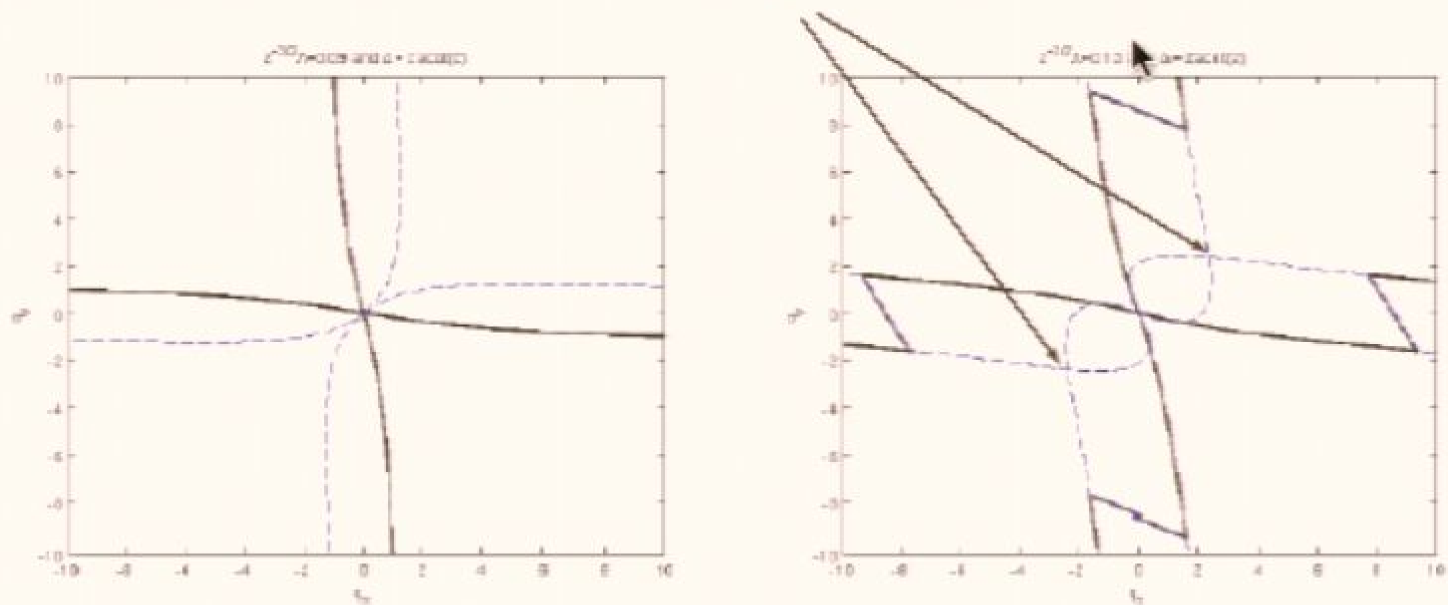
$$0 = \pm\frac{\lambda\cot(\omega/2)}{4\sqrt{4-Q^2}}(\cos\Delta\sin A+\sin\Delta\cos A\sin B+\sin A\cos B)+q_x$$

$$0 = \pm\frac{\lambda\cot(\omega/2)}{4\sqrt{4-Q^2}}(\cos\Delta\sin B+\sin\Delta\sin A\cos B+\cos A\sin B)+q_y$$

Consider as a zero contour of a two dimensional surface.

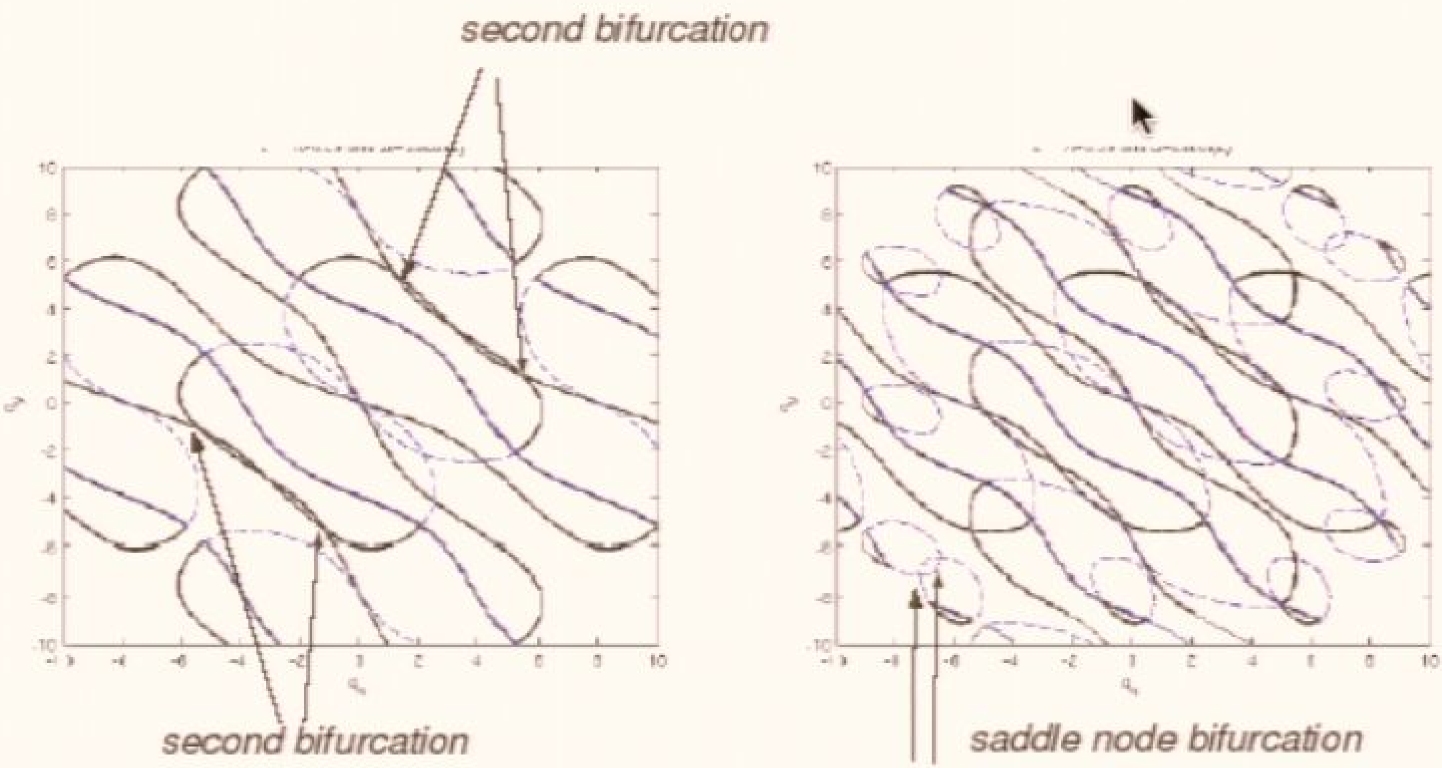
Fixed points and bifurcations.

first pitchfork bifurcation



New fixed points are on $q_x = q_y, \& p_\mu = -\tan(\omega/2) q_\mu$

Fixed points and bifurcations.



Quantum states and bifurcations.

At zero coupling, $\lambda = 0$, trivial fixed points correspond to ground states,

$$H_0 = \tilde{\Delta}\sigma_z + \frac{1}{2m}(p_x^2 + p_y^2) + \frac{m\tilde{\omega}^2}{2}(q_x^2 + q_y^2)$$

Designate ground state as $|\lambda = 0\rangle_e$.

Follow this ground state, as coupling is increased, $|\lambda\rangle_e$.

How does this state reflect the semiclassical bifurcations?

Phase-space representation for a quantum state.

Husimi function: project state onto oscillator coherent states (Bargmann rep.)

$$Q(\alpha) = |\langle\alpha|\psi\rangle|^2$$

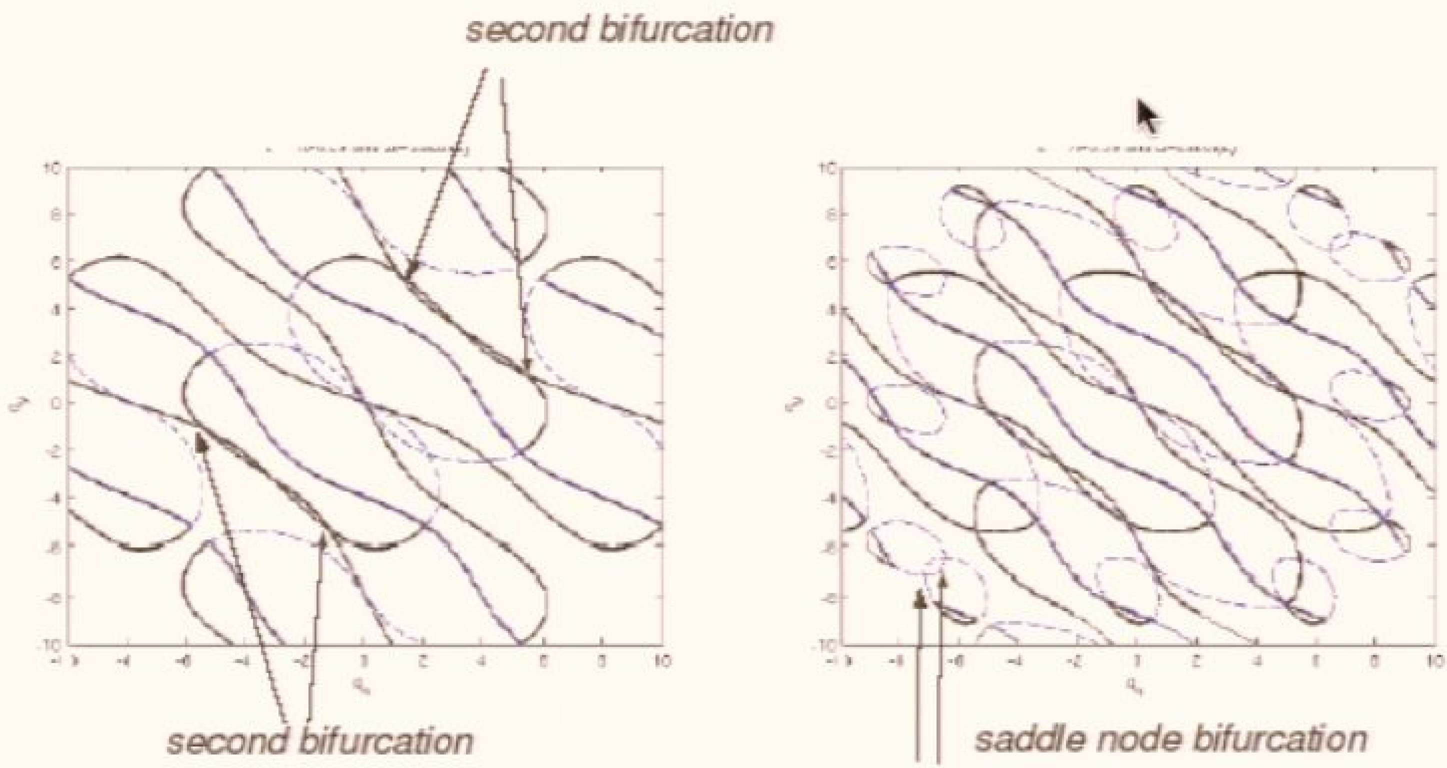
$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger}|0\rangle$$

$|0\rangle$ sho ground state and $\alpha = q + ip$

Plot Husimi function on the line of bifurcations:

$q_x = q_y, \qquad p_\mu = -\tan(\omega/2) q_\mu$

Fixed points and bifurcations.



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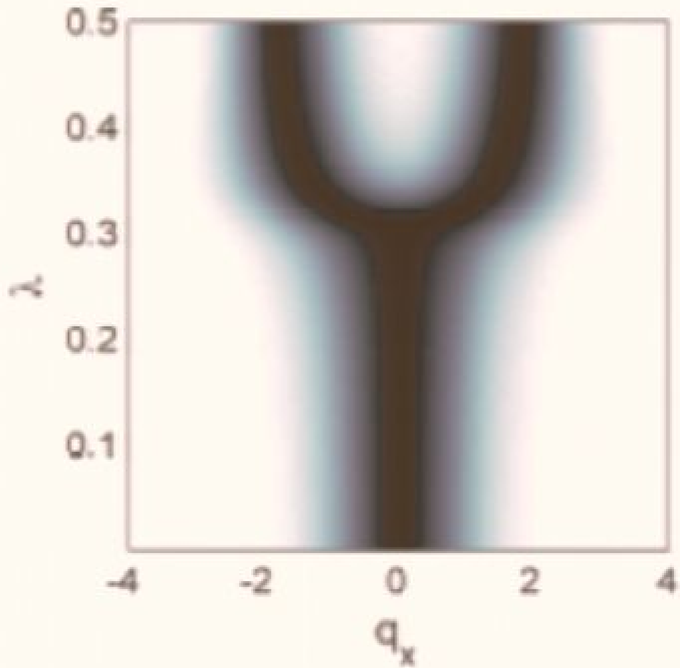
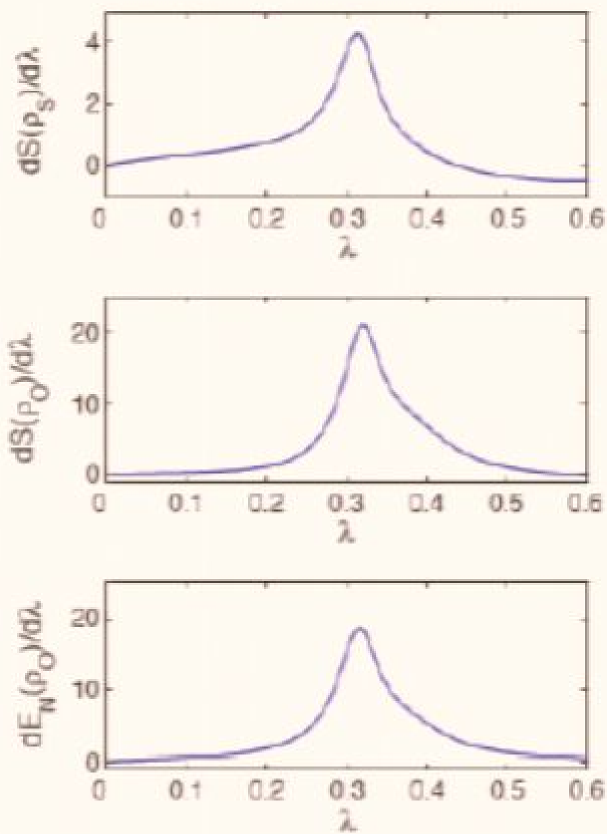
Quantum bifurcations.



$\lambda_b = 0.26$

Entanglement at the bifurcation.

$\lambda_b = 0.26$



vN entropy of qubit reduced state

vN entropy of qubit x one oscillator reduced state

log-neg of one oscillator

Suggestive of a quantum phase transition.

Are there interesting many-body unitary maps with a QPT?

Quantum phase transitions.

Quantum phase transition occurs at zero temperature as some other parameter is varied: pressure, magnetic field...

At $T = 0$ transition from the ordered phase to the disordered is driven purely by quantum-mechanical fluctuations.

At $T = 0$ we consider the ground state of a many body Hamiltonian.

Relate behavior of correlations at critical point to entanglement in the ground state.

Transverse field Ising model.

$$H = -h \sum_i \sigma_x^{(i)} - J \sum_i \sigma_z^{(i)} \sigma_z^{(i+1)}$$

Example: transverse Ising map.

$$U(\chi,\theta) = e^{-iH_\chi}e^{-iH_\theta} = U(\chi)U(\theta)$$

$$H_\chi = \chi \sum_{n=1}^{N} \sigma_z^{(n)}\sigma_z^{(n+1)} \qquad \text{two qubit gates}$$

$$H_\theta = \theta \sum_{n=1}^{N} \sigma_x^{(n)} \qquad \text{one qubit gates}$$

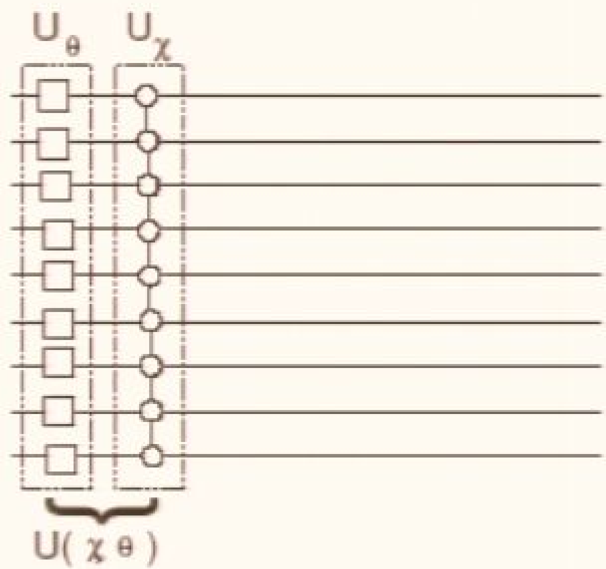
Iterated map:

$$[U(\chi)U(\theta)]^n$$

Example: transverse Ising map.

QC can implement

$$U(\chi, \theta) = e^{-iH_\chi} e^{-iH_\theta} = U(\chi)U(\theta)$$



Unitary Map versus Hamiltonian flow.

$$[U(\chi)U(\theta)]^n \neq e^{-inH_\theta - inH_\chi}$$

The iterated map is *not* an approximation to the transverse Ising dynamics.

Effective Hamiltonian and universality.

Find $\bar{H}$ where,

$$U(\chi, \theta) = e^{-iH_\chi} e^{-iH_\theta} = e^{-i\bar{H}}$$

Show that in the thermodynamic limit $\bar{H}$ is in the same universality class as the transverse field Ising model.

The effective Hamiltonian.

Use a Jordan-Wigner transformation on each unitary operator separately.

Step 1: define a_n,

$$\begin{aligned} \sigma_x^{(n)} &= 1 - 2a_n a_n^\dagger \\ \sigma_z^{(n)} &= a_n^\dagger + a_n \\ \sigma_y^{(n)} &= -i(a_n - a_n^\dagger) \end{aligned}$$

where

$$\{a_n^\dagger, a_n\} = 1, \qquad a_n^2 = 0, \qquad a_n^{\dagger 2} = 0,$$
$$[a_m^\dagger, a_n] = 0, \; [a_m^\dagger, a_n^\dagger] = 0, \; [a_m, a_n] = 0, m \neq n$$

The effective Hamiltonian.

Step 2.

$$
\begin{aligned}
c_n &= e^{i\pi \sum_{j=1}^{n-1} a_j^\dagger a_j} a_n \\
c_n^\dagger &= a_n^\dagger e^{-i\pi \sum_{j=1}^{n-1} a_j^\dagger a_j}
\end{aligned}
$$

which obey fermionic anti-commutation relations.

Effective Hamiltonian

$$\bar{H} = \Lambda_1 + \Lambda_2 + \Lambda_3$$

$$\begin{aligned}
\Lambda_1 &= \cos\theta\sin\chi[a_0(c_n^\dagger c_{n+1}^\dagger - c_n c_{n+1}) + \sum_{n,l}\frac{(a_{l+1}-a_{l-1})}{2}(c_n^\dagger c_{n+l}^\dagger - c_n c_{n+l})] \\
\Lambda_2 &= -i\sin\theta\sin\chi\sum_{n,l}[a_o(c_n^\dagger c_{n+1}^\dagger + c_n c_{n+1}) + \sum_{l}\frac{(a_{l+1}-a_{l-1})}{2}(c_n^\dagger c_{n+l}^\dagger + c_n c_{n+l})] \\
\Lambda_3 &= \sin\theta\cos\chi\sum_{l}[a_l(c_n^\dagger c_{n+l} - c_n c_{n+l}^\dagger)] + \cos\theta\sin\chi\sum_{n,l}[a_0(c_n^\dagger c_{n+1} - c_n c_{n+1}^\dagger) \\
&\quad + \frac{(a_{l+1}-a_{l-1}))}{2}(c_n^\dagger c_{n+l} - c_n c_{n+l}^\dagger)]
\end{aligned}$$

This has effective non-nearest neighbor interactions.

A quantum phase transition .

Does $\bar{H}$ fall into the same universality class as the transverse field Ising in thermodynamic limit?

YES !

can show,

$$a_l \leq ke^{-\mu l} \to 0 \quad \text{as} \quad l \to \infty$$

where $\mu = |\ln(\sin\theta \sin\chi)|$.

A quantum phase transition .

Ising criticality occurs for $\theta = \pm\chi$.

Find the ground state of the effective hamiltonian.

Look at second derivatives of the corresponding eigenvlaue (quasi-energy)

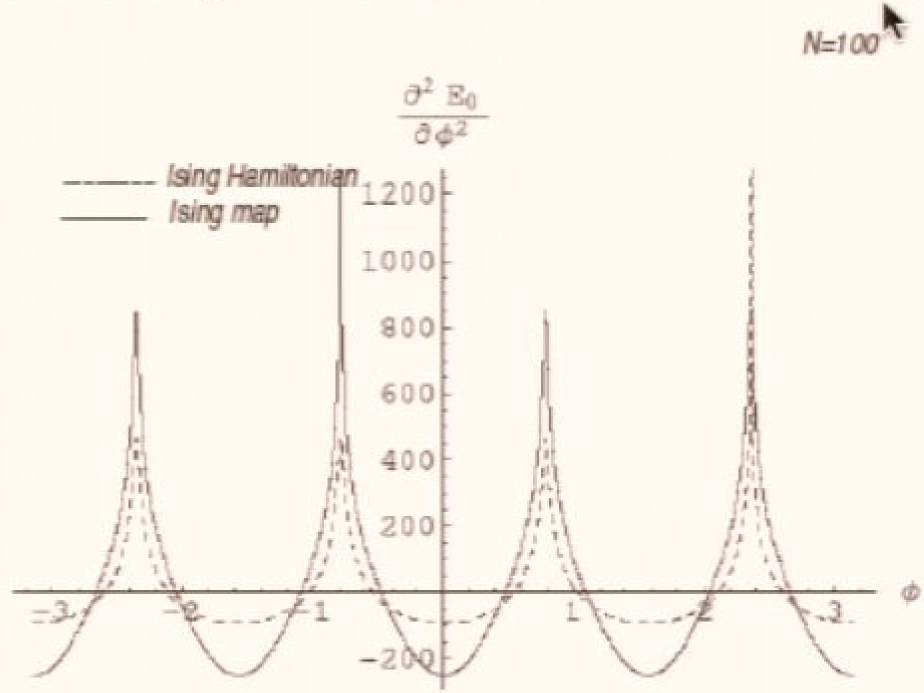
Singularities at Ising criticality points as N becomes large.

A many-body unitary map with a quantum phase transition, implemented on an ion trap QC.

Ground state quasi-energy.

$$\phi = \arctan(\theta/\chi)$$

Consider effective-ground state,



Conclusion.

- Realise quantum dynamical bifurcations on QC as iterated map.
- Realise QPT on QC as iterated map.
- Small scale simulation on an ion trap QC.
- New algorithms from iterated dynamical maps?
- Complexity of eigenstates of unitary maps and relationship to semiclassical dynamics?

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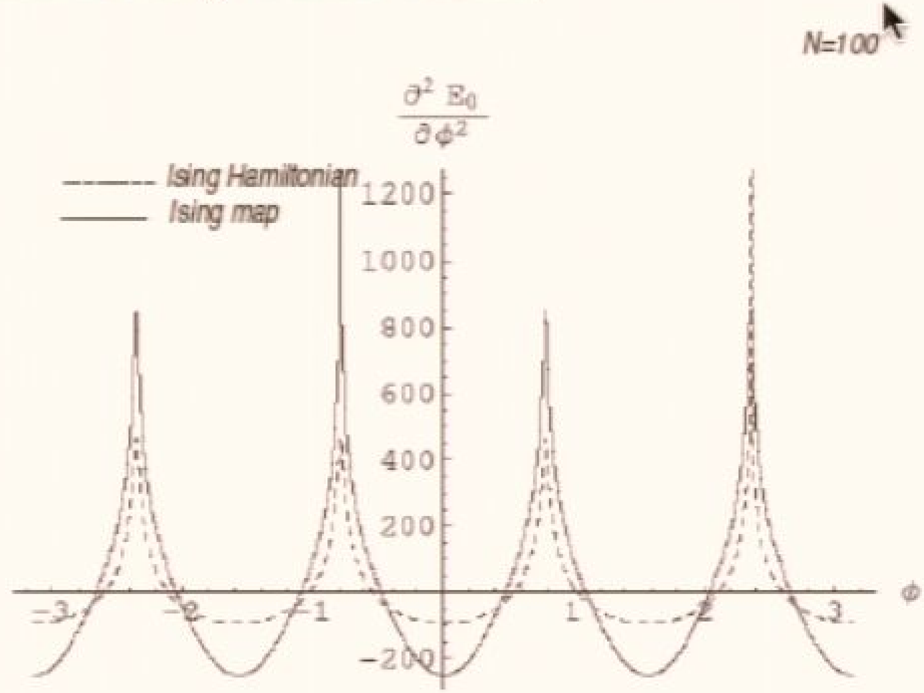

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$q_x = q_y, \qquad p_\mu = -\tan(\omega/2) q_\mu$

Phase-space representation for a quantum state.

Husimi function: project state onto oscillator coherent states (Bargmann rep.)

$$Q(\alpha) = |\langle\alpha|\psi\rangle|^2$$

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger}|0\rangle$$

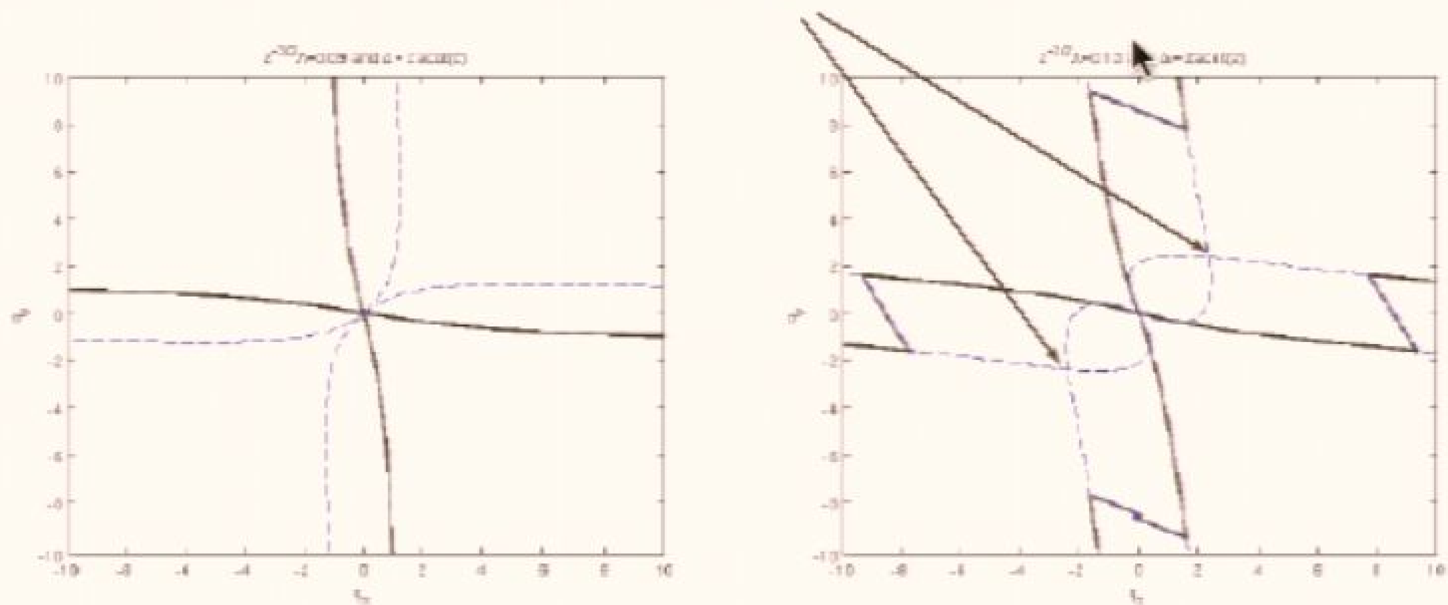
$|0\rangle$ sho ground state and $\alpha = q + ip$

Plot Husimi function on the line of bifurcations:

$q_x = q_y, \quad p_\mu = -\tan(\omega/2) q_\mu$

Fixed points and bifurcations.

first pitchfork bifurcation



New fixed points are on $q_x = q_y, \& p_\mu = -\tan(\omega/2) q_\mu$