Lecture 3 Classical and quantum dynamics

First recall the general structure once again:–

To summarize: The phase space rep is defined by the Weyl-Wigner transform:

$$A = \mathcal{W}(\hat{a}) \qquad \hat{a} = \mathcal{W}^{-1}(A)$$

$$\mathcal{T} \xrightarrow{\mathcal{W}} \mathcal{K} \qquad \mathcal{K} \xrightarrow{\mathcal{W}^{-1}} \mathcal{T}$$

In $\mathcal{T}$: $((\hat{a}, \hat{b})) = \mathrm{Tr}(\hat{a}^\dagger \hat{b})$. In $\mathcal{K}$: $(A, B) = \frac{1}{2\pi\hbar} \int A(q,p)^* B(q,p)\, dq\, dp\,.$

$$A \star B = \mathcal{W}(\hat{a}\hat{b}) \neq \mathcal{W}(\hat{b}\hat{a}) = B \star A$$

$$\boxed{A(q,p) = \int a_K(q - y/2, q + y/2)\, e^{ipy/\hbar}\, dy}$$

$$\boxed{a_K(x,y) = \frac{1}{2\pi\hbar} \int A(\tfrac{x+y}{2}, p)\, e^{ip(x-y)/\hbar}\, dp}$$

Now to classical and quantum dynamics:–

Recall that in the Schrödinger picture, the dynamics of a closed quantum system is given by

$$i\hbar\frac{\partial\hat{\rho}(t)}{\partial t} = [\hat{H}, \hat{\rho}]$$

and that this is mapped by the Weyl-Wigner transform into

$$i\hbar\frac{\partial W(q,p,t)}{\partial t} = H(q,p) \star W(q,p,t) - W(q,p,t) \star H(q,p)$$

where

$W = \mathcal{W}(\frac{1}{2\pi\hbar}\hat{\rho})$ — the Wigner function.

Next recall that

$$A \star B = \mathcal{W}(\hat{a}\hat{b}) = \mathcal{W}\left(\mathcal{W}^{-1}(A)\mathcal{W}^{-1}(B)\right) \; .$$

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We find

$(A \star B)(q, p)$

$$= \frac{1}{(\pi\hbar)^2} \int A(q', p')B(q'', p'')\, e^{-2i(p[q'-q'']+p'[q''-q]+p''[q-q'])/\hbar}\, dq'\, dp'\, dq''\, dp''$$

— interesting form, but not very useful.

To proceed, we use again

$$e^{i(\alpha\hat{q}-\beta\hat{p})} = e^{-i\alpha\beta\hbar/2} e^{i\alpha\hat{q}}\, e^{-i\beta\hat{p}} = e^{i\alpha\beta\hbar/2}\, e^{-i\beta\hat{p}}\, e^{i\alpha\hat{q}}$$

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If $\hat{a} = e^{i(\alpha\hat{q}-\beta\hat{p})}$, $\hat{b} = e^{i(\gamma\hat{q}-\theta\hat{p})}$, then

$$\hat{a}\hat{b} = e^{i(\alpha\theta-\gamma\beta)\hbar/2}\, e^{i([\alpha+\gamma]\hat{q}-i[\beta+\theta]\hat{p})}$$

so

$$\mathcal{W}(\hat{a}\hat{b}) = e^{i(\alpha\theta-\gamma\beta)\hbar/2}\, e^{i([\alpha+\gamma]q-i[\beta+\theta]p)}\,.$$

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But in this case,

$$A(q,p) = e^{i(\alpha q-\beta p)}\,, \qquad B(q,p) = e^{i(\gamma q-\theta p)}\,,$$

and so

$$(A \star B)(q,p) = e^{i(\alpha\theta-\gamma\beta)\hbar/2}\, e^{i([\alpha+\gamma]q-i[\beta+\theta]p)} = e^{i(\alpha\theta-\gamma\beta)\hbar/2}\, A(q,p)B(q,p)\,. \quad (**)$$

We now introduce the 'Janus' operator in phase space:

$$J = \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}$$

and the associated *Poisson bracket*

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$$\{A, B\}_{PB} = A\,J\,B\,.$$

This enables us to express the star product in a more useful way.

In our special case we have

$$(A\,J\,B)(q,p) = (\alpha\theta - \gamma\beta)A(q,p)B(q,p)$$

and therefore, from $(**)$,

$$(A \star B)(q,p) = (A\,e^{i\hbar J/2}\,B)(q,p) = (B\,e^{-i\hbar J/2}\,A)(q,p)\,.$$

But then we see that this must be true also for all $A(q,p)$, $B(q,p)$ that can be expanded in such exponential functions (Fourier transforms!).

In this way we arrive at the much more useful form for the star product:

$$\boxed{A \star B = A\, e^{i\hbar J/2}\, B = B\, e^{-i\hbar J/2}\, A}$$

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$$A \star B = A\, e^{i\hbar J/2}\, B = A\, (1 + i\hbar J/2 + (i\hbar J/2)^2/2 + \ldots)\, B$$

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Note that the series terminates if either A or B is a polynomial in q and p.

For practical purposes, we regard the expansion as valid for all A and B of interest.

Next notice that

$$\mathcal{W}([\hat{a},\hat{b}]) = A\star B - B\star A = A\,e^{i\hbar J/2}\,B - A\,e^{-i\hbar J/2}\,B = 2iA\,\sin(\hbar J/2)\,B$$

or

$$\mathcal{W}(\tfrac{1}{i\hbar}[\hat{a},\hat{b}]) = \tfrac{2}{\hbar}A\,\sin(\hbar J/2)\,B$$

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This is the famous Moyal or star bracket,

$$\boxed{\{A,B\}_\star = \tfrac{2}{\hbar}\,A\,\sin(\hbar J/2)\,B}$$

which we also use mainly in expanded form as

$$\boxed{\{A,B\}_\star \sim A\,J\,B - \frac{\hbar^2}{24}\,A\,J^3\,B + \frac{\hbar^4}{1920}\,A\,J^5\,B\ldots}$$

Note that the leading term is the Poisson bracket.

Returning to the quantum dynamics, we now have

$$\hat{\rho}_t = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] \quad \xrightarrow{\mathcal{W}} \quad W_t = \{H, W\}_\star$$

and so

$$W_t = \{H, W\}_{PB} - \frac{\hbar^2}{24} H\, J^3\, W + \frac{\hbar^4}{1920} H\, J^5\, W + \dots$$

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The leading term is the classical, Liouvillean evolution. We can say that quantum dynamics is a deformation of classical dynamics with deformation parameter $\hbar$, where the Poisson bracket is replaced by the star bracket in phase space, or equivalently, by $(1/i\hbar)\times$ the commutator in Hilbert space.

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Wigner's idea was to use this expansion to define quantum corrections to the evolution of the classical Liouvillean density in phase space.

From that point of view, it defines one of many versions of semiclassical mechanics.

Note that if

$$H = p^2/2m + V(q)\,,$$

then the evolution of the Liouville density $\rho(q,p,t)$ is

$$\rho_t = \{H,\rho\}_{PB} = V'(q)\frac{\partial \rho}{\partial p} - \frac{p}{m}\frac{\partial \rho}{\partial p}\,.$$

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Then, to get semiclassical approximations:-

- 'expand' the star bracket in powers of $\hbar$.

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$$= \frac{1}{2\pi\hbar}\int A([x+y]/2,p)\, e^{ip(x-y)/\hbar}\, dp$$

or simply,

$$\boxed{\hat{A} = \mathcal{W}^{-1}(A)}$$

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In particular, given a Liouville density $\rho(q, p, t)$, set

$$\hat{G}(t) = 2\pi\hbar\, \mathcal{W}^{-1}\,(\rho(t))$$

- the Groenewold operator.

We find that

$$\langle A\rangle(t)\left[\equiv\int A(q,p)\rho(q,p,t)\,dq\,dp\right]=\mathrm{Tr}\left(\hat{G}(t)\hat{A}\right)$$

and

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but

$\hat{G}(t)$ is not positive definite — a quasidensity operator.

For a Gaussian density

$$\rho(q,p,t) \equiv \rho(q,p) = \frac{1}{\pi\beta\gamma}\, e^{-(q^2/\beta^2+p^2/\gamma^2)}\,,$$

with classical uncertainty product

$$\Delta q \Delta p = \beta\gamma/2$$

we find for the spectrum of G,

$$\lambda_n = \frac{2\hbar}{\beta\gamma+\hbar}\left(\frac{(\beta\gamma-\hbar)}{(\beta\gamma+\hbar)}\right)^n\,.$$

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Note that if $\beta\gamma < \hbar$ (so that $\Delta q\Delta p < \hbar/2$), then some of these eigenvalues are negative and some are greater than 1.

Consider $$\mathcal{W}^{-1}(AB) = \mathcal{W}^{-1}(\mathcal{W}(\hat{a})\mathcal{W}(\hat{b}))$$

We find that $\left(\mathcal{W}^{-1}\left(A\,B\right)\right)_K(x,y)$

$$= \int A_K\left(\frac{3x+y-2u}{4}, \frac{x+3y+2u}{4}\right) B_K\left(\frac{3x+y+2u}{4}, \frac{x+3y-2u}{4}\right) du$$

$$= \left(\mathcal{W}^{-1}\left(B\,A\right)\right)_K(x,y)$$

or simply

$$\boxed{\mathcal{W}^{-1}\left(A\,B\right) = \hat{A}\odot\hat{B} = \hat{B}\odot\hat{A}}$$

— commutative odot product.

Question:-

$$\rho_t = \{H, \rho\}_{PB} \quad \xrightarrow{\mathcal{W}^{-1}} \quad \hat{G}_t = \quad ?$$

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Not hard to see that

$$\mathcal{W}^{-1}(A_q) = [\hat{A}, \hat{p}]/(i\hbar) = \hat{A}_q\,, \quad \text{say}\,,$$
$$\mathcal{W}^{-1}(A_p) = [\hat{q}, \hat{A}]/(i\hbar) = \hat{A}_p\,, \quad \text{say}\,.$$

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Then

$$\mathcal{W}^{-1}\left(A_q\, B_p - A_p\, B_q\right) = \hat{A}_q \odot \hat{B}_p - \hat{A}_p \odot \hat{B}_q = \frac{1}{i\hbar}[\hat{A}\,, \hat{B}]_{\odot}\,, \quad \text{say}\,,$$

so we have

$$i\hbar \hat{G}_t = [\hat{H}\,, \hat{G}]_{\odot}$$

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- multiply operators (observables) using the commutative odot product
- evolve the Groenewold operator using the odot bracket rather than the commutator

Finally, to get semiquantum approximations:-

- 'expand' the odot bracket in powers of $\hbar$.

How do we do this?

Setting $Q = \frac{2}{\hbar}\sin(\hbar J/2)$, so that $A\,J\,B = A\,\frac{\hbar J/2}{\sin \hbar J/2}\,Q\,B$,

we use $\theta/\sin(\theta) = 1 + \theta^2/6 + 7\theta^4/360 - \ldots$ for $|\theta| < \pi$

to see that as $\hbar \longrightarrow 0$,

$$A\,J\,B \sim A\,Q\,B + \hbar^2 A\,J^2\,Q\,B/24 + 7\hbar^4 A\,J^4\,Q\,B/5760 - \ldots$$

$$\sim A\,Q\,B + \hbar^2(A_{qq}\,Q\,B_{pp} - 2A_{qp}Q\,B_{qp} + A_{pp}\,Q\,B_{qq})/24 + \ldots.$$

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Then, using $\mathcal{W}^{-1}\,(E\,Q\,F) = [\hat{E}, \hat{F}]$, we get

$$[\hat{A}, \hat{B}]_{\odot} \sim [\hat{A}, \hat{B}] + \hbar^2\left([\hat{A}_{qq}, \hat{B}_{pp}] - 2[\hat{A}_{qp}, \hat{B}_{qp}] + [\hat{A}_{pp}, \hat{B}_{qq}]\right)/24 + \ldots$$

So we have, finally,

$$i\hbar\hat{G}_t \sim [\hat{H}, \hat{G}] + \hbar^2 \left([\hat{H}_{qq}, \hat{G}_{pp}] - 2[\hat{H}_{qp}, \hat{G}_{qp}] + [\hat{H}_{pp}, \hat{G}_{qq}] \right) /24 + \dots$$

— the analogue of the evolution equation for the Wigner function.

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Note that we now get the quantum evolution plus a series of classical corrections.

This then is semiquantum mechanics — the quantum-classical interface can be explored starting from the quantum side!

We see that we can also view classical mechanics as a deformation of quantum mechanics – again $\hbar$ is the deformation parameter.

Compare:

$$W_t \sim \{H, W\}_{PB} - \hbar^2 \,(H\, J^3\, W)/24 + \ldots$$

$$i\hbar \hat{G}_t \sim [\hat{H}, \hat{G}] + \hbar^2 \left([\hat{H}_{qq}, \hat{G}_{pp}] - 2[\hat{H}_{qp}, \hat{G}_{qp}] + [\hat{H}_{pp}, \hat{G}_{qq}] \right) /24 + \ldots \, .$$

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If $H = p^2/2m + V(q)$, $\quad \hat{H} = \hat{p}^2/2m + V(\hat{q})$, then

$$W_t \sim \{H, W\}_{PB} - \hbar^2 V'''(q)\, W_{ppp}/24 + \hbar^4 V'''''(q) W_{ppppp}/1920 + \ldots$$

$$i\hbar \hat{G}_t \sim [\hat{H}, \hat{G}] + \hbar^2 [V''(\hat{q}), \hat{G}_{pp}]/24 + 7\hbar^4 [V''''(\hat{q}), \hat{G}_{pppp}]/5760 - \ldots .$$

To illustrate, consider Hamiltonians of the form

$$H_n = E\,(H_1/E)^n\,, \quad n = 1,\, 2,\, \ldots$$

$$H_1 = p^2/(2m) + m\omega^2 q^2/2 \qquad \text{(SHO)}$$

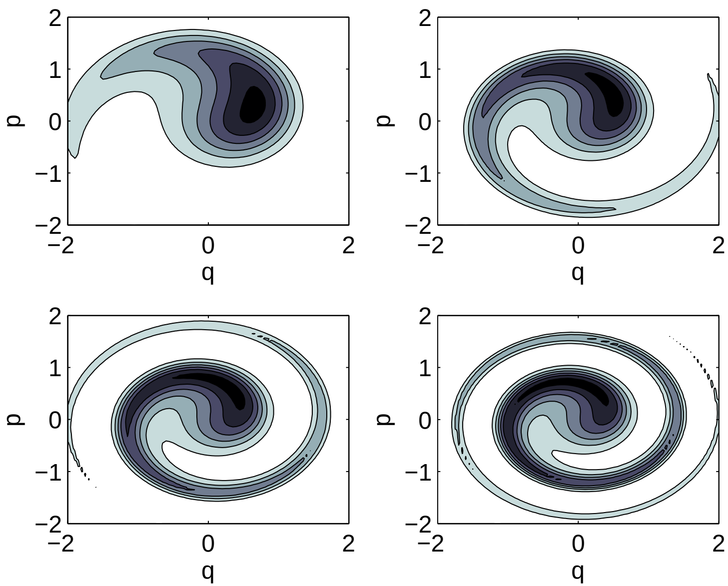
where E has dimensions of energy. Set $\mu = \hbar\omega/E$.

Take as initial Liouville density a Gaussian

$$\rho_{\kappa,\alpha_0}(q,p,0) = \frac{\kappa}{2\pi\hbar}\, e^{-\kappa|\alpha-\alpha_0|^2}$$

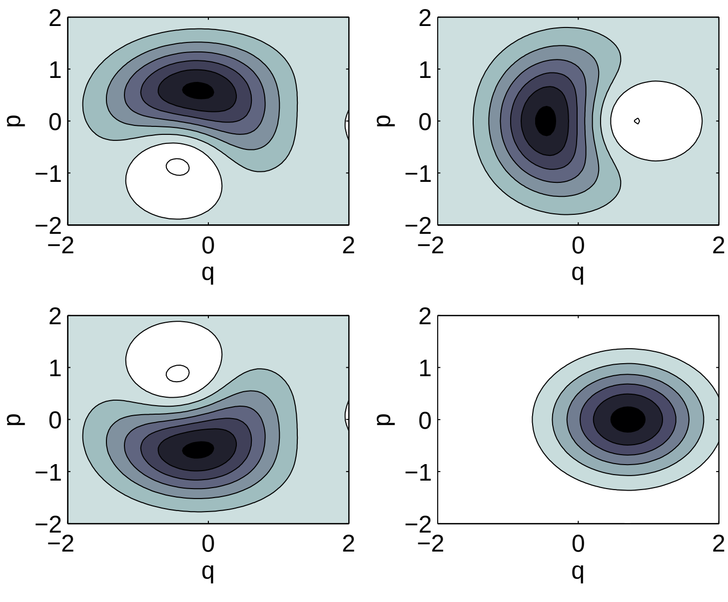
$\alpha = \left(\sqrt{m\omega}\, q + ip/\sqrt{m\omega}\right)/\sqrt{2\hbar}, \qquad \kappa = \hbar\omega/\epsilon$

where ϵ also has dimensions of energy.



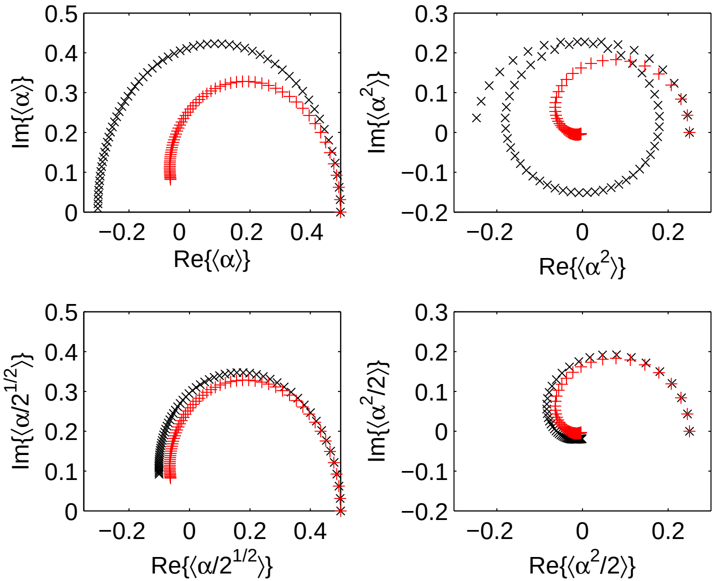
2
1
0
−1
−2
p
−2
0
2
q

Density plots showing the classical evolution of an initial Gaussian density centered at $\alpha_0 = q_0 = 0.5$ with $\kappa = 2$, as generated by the Hamiltonian $H_2 = H_1^2/E$. The parameters m, ω, E have been set equal to 1. The times of the plots are (a): $t = \pi/4$, (b): $t = \pi/2$, (c): $t = 3\pi/4$ and (d): $t = \pi$.

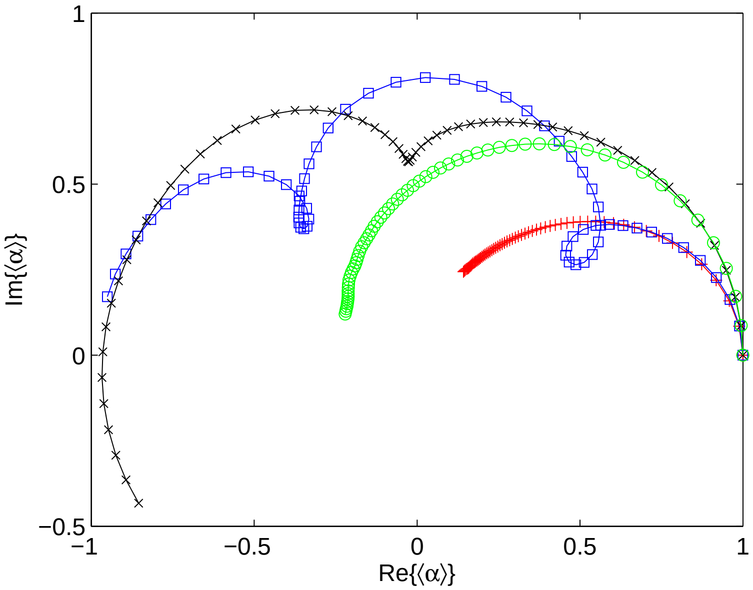


p
q
2
1
0
−1
−2
−2
0
2

Quantum evolution of an initial gaussian density, with the same parameter values used in Figure 1, with also $\mu = 1$, and shown at the same times.

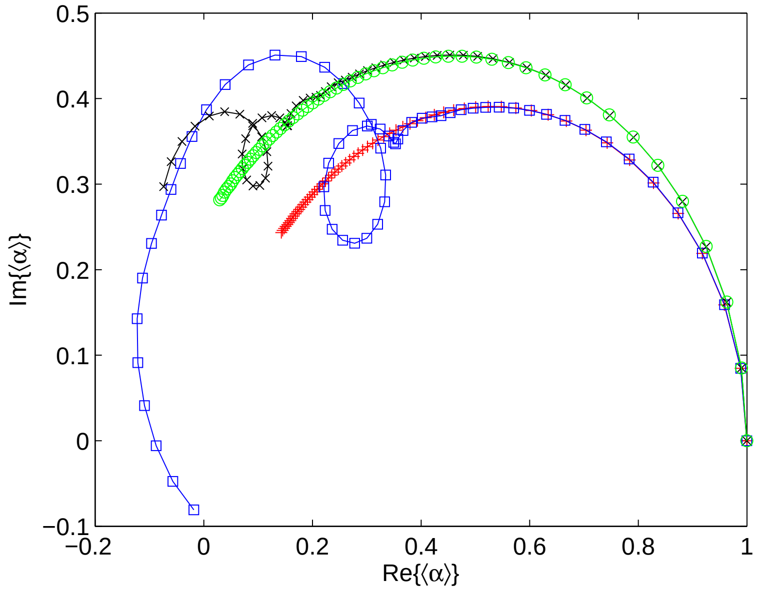

Im{⟨α⟩}
Re{⟨α⟩}
Im{⟨α^2⟩}
Re{⟨α^2⟩}
Im{⟨α/2^1/2⟩}
Re{⟨α/2^1/2⟩}
Im{⟨α^2/2⟩}
Re{⟨α^2/2⟩}

Classical and Quantum time evolution of the first and second moments of $(q+ip)/\sqrt{2}$ as generated by $H_2 = H_1^2/E$. Points on the classical curves are marked $+$ (red) and points on the quantum curve are marked $\times$ (black). The first moments are graphed on the left and the second moments on the right. In the two upper graphs, $\kappa = 2, \mu = 1/2, \alpha_0 = 0.5$ and in the lower two graphs, $\kappa = 1, \mu = 1/4, \alpha_0 = 1/\sqrt{2}$.



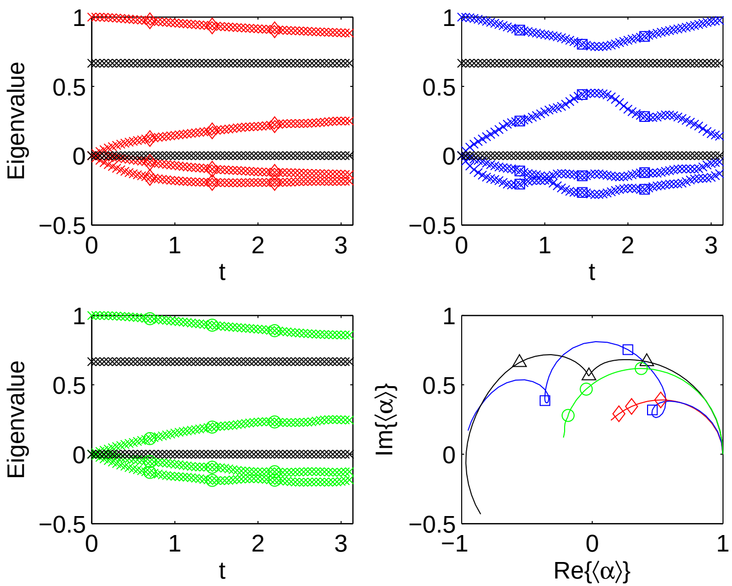
1
0.5
0
−0.5
−1
−0.5
0
0.5
1
Im{⟨α⟩}
Re{⟨α⟩}

Comparison of first moments of $(q+ip)/\sqrt{2}$ for classical (+, red), semiquantum (□, blue), quantum (×, black) and semiclassical (o, green) evolutions generated by the Hamiltonian $H_3 = H_1^3/E^2$ over the time-interval $[0,\pi]$. Here $\kappa = 2$, $\mu = 1/2$, $\alpha_0 = 1$.



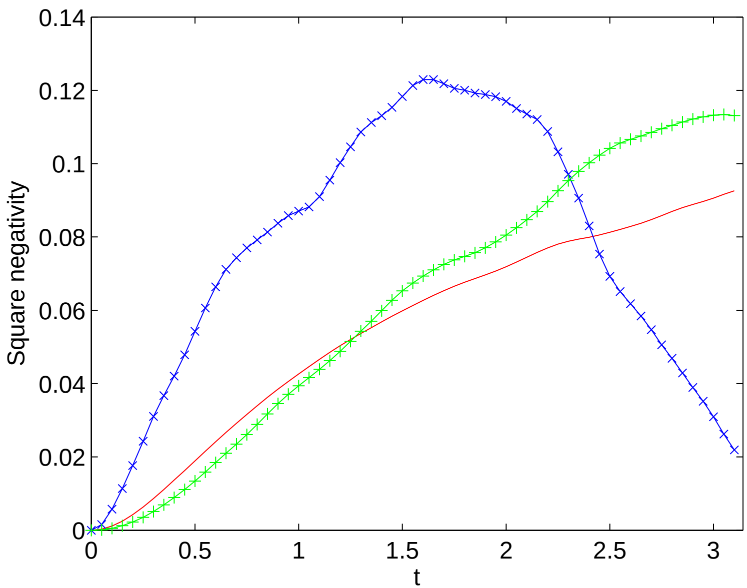
0.5
0.4
0.3
0.2
0.1
0
−0.1
−0.2
0
0.2
0.4
0.6
0.8
1
Im{⟨α⟩}
Re{⟨α⟩}

Identical to the preceding Figure except that $\hbar$ has been reduced by a factor of two, by setting $\kappa = 1, \mu = 1/4$.



Eigenvalue
t
Eigenvalue
t
t
Im{⟨α⟩}
Re{⟨α⟩}

Comparison of largest two and least two eigenvalues for classical (red), semiquantum (blue) and semiclassical (green) evolutions generated by $H_3 = H_1^3/E^2$, for the time interval $[0, \pi]$, with $\kappa = 2, \mu = 1/2, \alpha_0 = 1$. The quantum spectrum is $\{0, 1\}$. The evolution of the first moment is reproduced for comparison in the bottom RH corner. Values at the time-points $t = 1, 2, 3$ are marked.



0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
Square negativity
0
0.5
1
1.5
2
2.5
3
t

Comparison of “square-negativity” for classical (red), semiquantum (blue) and semiclassical (green) evolutions generated by $H_3 = H_1^3/E^2$ for the time-interval $[0, \pi]$, with $\kappa = 2, \mu = 1/2, \alpha_0 = 1.$

Conclusions

- SQ mechanics opens a new window on the quantum-classical interface.
- Need to look at more realistic Hamiltonians, for example

$$H = \frac{p^2}{2m} + V(q)$$

- Need to look at more degrees of freedom — what happens for classically chaotic systems, for example to the spectrum of the Groenewold operator?
- What is the relationship between SQ and SC approximations?
- What are the asymptotics of SQ approximations?

Further references:

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