General Complex Hamiltonian for Harmonic Oscillator

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Introduction

- Introduction of Quantum Hamilton Mechanics
- Intrinsic Hamiltonian
- Complex Trajectories of Harmonic Oscillator
- General Hamiltonian for Harmonic Oscillator
- Complex Energy
- Summary & Conclusions

Quantum Hamilton Mechanics

Schrödinger Eq.

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi$$

Transformation

$$\psi=e^{iS/\hbar},\ \text{or}\ S=-i\hbar\ln\psi$$

Quantum Hamilton -Jacobi Equation

$$\frac{\partial S}{\partial t}+\left[\frac{1}{2m}\mathbf{p}^2+V+\frac{i\hbar}{2m}\nabla\cdot\mathbf{p}\right]_{\mathbf{p}=\nabla S}=0$$

$$\frac{\partial S}{\partial t}+H(t,\mathbf{q},\mathbf{p})\Big|_{\mathbf{p}=\nabla S}=0$$

Quantum Hamiltonian

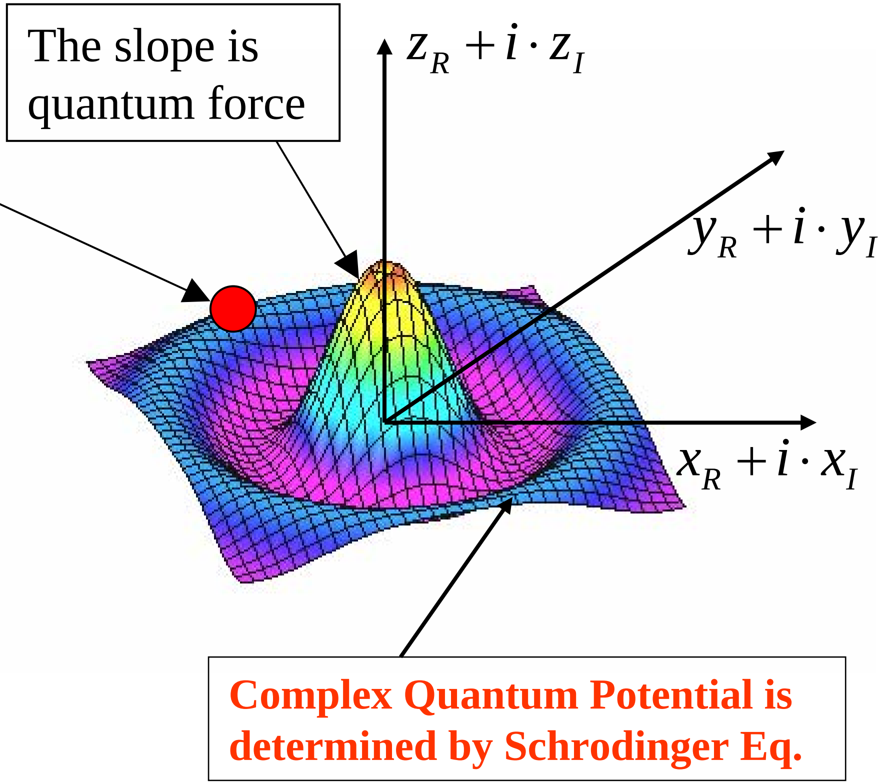
$$H=\frac{1}{2m}\mathbf{p}^2+V(\mathbf{q})+Q(\psi(\mathbf{q}))$$

Quantum Potential

Intrinsic Hamiltonian

Quantum Potential in Complex Space

- A quantum state ψ determines a quantum potential ***Q (ψ)*** which governs particle's quantum motion



quantum force = derivatives of *Q(Ψ)*

$$F_x = -\frac{\partial Q(\psi)}{\partial x}$$

$$F_y = -\frac{\partial Q(\psi)}{\partial y}$$

$$F_z = -\frac{\partial Q(\psi)}{\partial z}$$

Even for free particle (free from external force), the quantum force is not zero.

Quantum force is intrinsic and state-dependent.

Newton Law in Complex Space

Complex Position

$$x = x_R + i x_I$$

Complex Potential

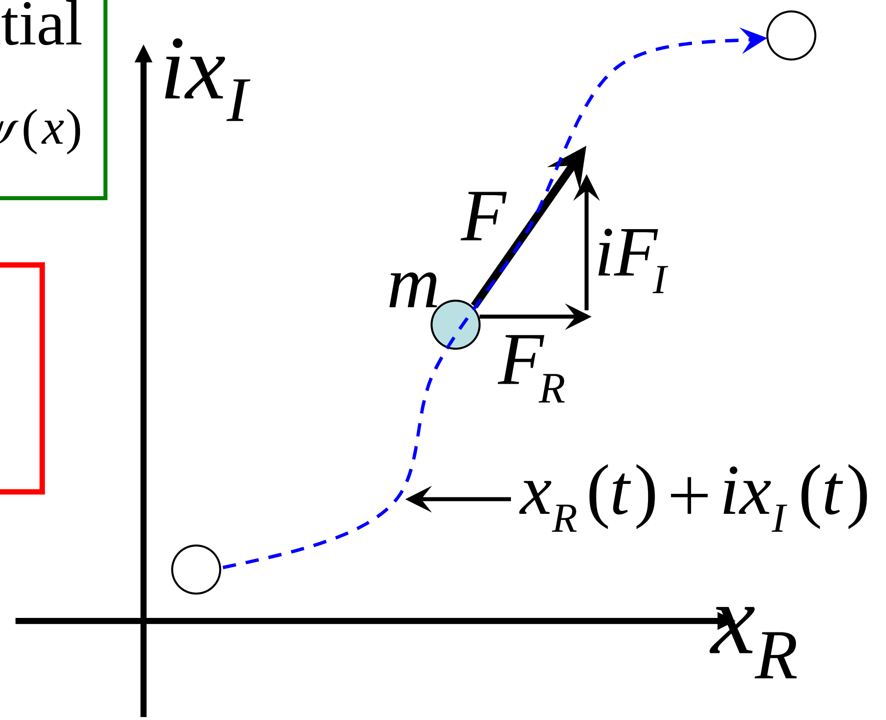
$$Q(\psi) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\ln\psi(x)$$

$$m\frac{d^2x}{dt^2} = F = -\frac{d}{dx}\left(Q(\psi) + V\right)$$

Complex Force

$$F = F_R + iF_I$$

Applied Potential



- Particle's trajectory $x_R(t) + ix_I(t)$ is on complex plane.
- Only the real part $x_R(t)$ can be measured.
- $x_R(t)$ is coupled to $x_I(t)$ in solving the complex ODE.
- $x_R(t)$ is measured under the influence of the unobservable $x_I(t)$

Dynamic Representation of Quantum State Ψ

A quantum state ψ has two physical meanings:

- Serve as probability density function
- Represent a dynamic system:
  - Determine Hamiltonian $H(\psi) = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{q}) + Q(\psi(\mathbf{q}))$
  - Determine Hamilton Equations of Motion

$$S_\psi \begin{cases} \frac{d\mathbf{q}}{dt} = \frac{\partial H(\psi)}{\partial \mathbf{p}} = \frac{1}{m}\mathbf{p} \\ \frac{d\mathbf{p}}{dt} = -\frac{\partial H(\psi)}{\partial \mathbf{q}} = -\frac{\partial}{\partial \mathbf{q}}\left[V(\mathbf{q}) - \frac{\hbar^2}{2m}\nabla^2 \ln \psi(\mathbf{q}) \right] \end{cases}$$

  - S_ψ is the dynamic representation of the abstract quantum state ψ

Quantum Mechanics

$$H_c = \frac{1}{2m} p^2 + V(x) \neq \text{constant}$$

$$p \to \hat{p} = -i\hbar(d/dx) \qquad x \to \hat{x} = x$$

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x}) = -\frac{1}{2m}\frac{d^2}{dx^2} + V(x)$$

$$\hat{H}\psi = E\psi \;\Rightarrow\; \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (E - V(x))\psi = 0$$

Eigenvalue E_n ⇒ Energy quantization

Eigenfunction ψ_n ⇒ Probability density

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{x} \psi \, dx$$

$$\langle Q \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{Q} \psi \, dx$$

Quantum Hamilton Mechanics

$$H = \frac{1}{2m} p^2 + V(x) - \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\ln\psi(x) = E = \text{constant}$$

$p = dS/dx$ ⇓ $\mathrm{p} = -i\hbar \, \mathrm{d} \ln \psi / \mathrm{dx}$

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (E - V(x))\psi = 0$$

Schrödinger Eq. is the energy conservation law in Complex space

Solve for ψ_n ⇓

Dynamic representation of ψ_n

$$\begin{cases} \dfrac{dx}{dt} = \dfrac{\partial H(\psi_n)}{\partial p} = \dfrac{1}{m} p, \\[2ex] \dfrac{dp}{dt} = -\dfrac{\partial H(\psi_n)}{\partial x} \end{cases}$$

Solve for $x(t),\ p(t)$ ⇓

Eigen-trajectory in ψ_n

The Origin of Quantum Operator

Till now, no formal proof is given to the quantization axiom $p \to \hat{p} = -i\hbar\nabla$
In complex mechanics, quantum operators arise naturally.

Complex Function Q ➡ $Q = \frac{1}{\psi}\hat{Q}\psi$ ➡ Quantum Operator $\hat{Q}$

1 $\mathbf{p} = \nabla S = -\mathrm{i}\hbar\nabla\ln\psi = \frac{1}{\psi}\left(-\mathrm{i}\hbar\nabla\right)\psi$ ➡ $p = \frac{1}{\psi}\hat{p}\psi$ ➡ $\hat{p} = -i\hbar\nabla$

2 $x = \frac{1}{\psi}x\psi$ ➡ $x = \frac{1}{\psi}\hat{x}\psi$ ➡ $\hat{x} = x$

3 $H = \frac{1}{2m}p^2 + V - \frac{\hbar^2}{2m}\nabla^2\ln\psi, \quad p = -i\hbar\nabla\psi$

$$= \frac{1}{2m}\left(-\mathrm{i}\hbar\nabla\ln\psi\right)^2 + V - \frac{\hbar^2}{2m}\nabla^2\ln\psi = \frac{1}{\psi}\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi = \frac{1}{\psi}\hat{H}\psi$$

➡ $\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V = \frac{1}{2m}\hat{p}^2 + V$

Notice: In quantum mechanics, we have $\hat{Q}$, but do not have Q . Without the connection to Q , the origin of $\hat{Q}$ is rather obscure.

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Intrinsic Complex Hamiltonian in Schrödinger Equation

Schrödinger Eq. ⇒

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Transformation ⇓

$$\Psi(t,\mathbf{q}) = e^{iS(t,\mathbf{q})/\hbar}$$

Quantum Hamilton -Jacobi Equation ⇒

$$\frac{\partial S}{\partial t} + \left[\frac{1}{2m}\mathbf{p}^2 + V + \frac{i\hbar}{2m}\nabla\cdot\mathbf{p}\right]_{\mathbf{p}=\nabla S} = 0$$

$$\Rightarrow \frac{\partial S}{\partial t} + H\,(t,\mathbf{q},\mathbf{p})\Big|_{\mathbf{p}=\nabla S} = 0$$

Intrinsic Hamiltonian ⇒

$$H = \frac{1}{2m}\mathbf{p}^2 + V(\mathrm{t},\mathbf{q}) + Q(\Psi(\mathrm{t},\mathbf{q}))$$

Quantum Potential ⇒

$$Q(\psi(\mathbf{q})) = \frac{\hbar}{2mi}\nabla\cdot\mathbf{p} = \frac{\hbar}{2mi}\nabla^2 S$$

$$= -\frac{\hbar^2}{2m}\nabla^2 \ln\Psi(\mathrm{t},\mathbf{q})$$

Quantum Harmonic Oscillator

$$H(\psi_n) = \frac{1}{2m}p^2 + \frac{1}{2}Kx^2 - \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\ln\psi_n(x) = E = \text{constant}$$

→ Intrinsic Hamiltonian for Harmonic Oscillator

Solve for ψ_n

$$\psi_n(x) = C_n H_n(\alpha x)e^{-\alpha x^2/2}, \quad n = 0,\ 1,\ 2, \cdots$$

H_n is the th-order Hermite polynomial

Dynamic motion

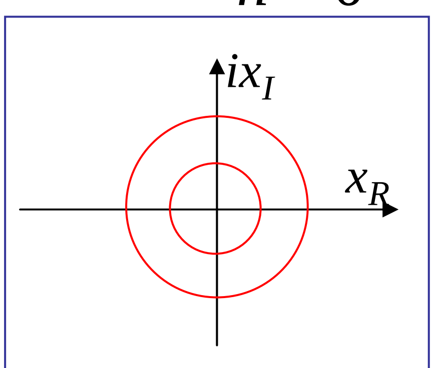
$$p = \frac{dx}{dt} = -i\hbar\frac{d}{dx}\ln\psi_n(x) = -\frac{i\hbar}{\psi_n}\frac{d\psi_n(x)}{dx}$$

→ Motion in complex plane

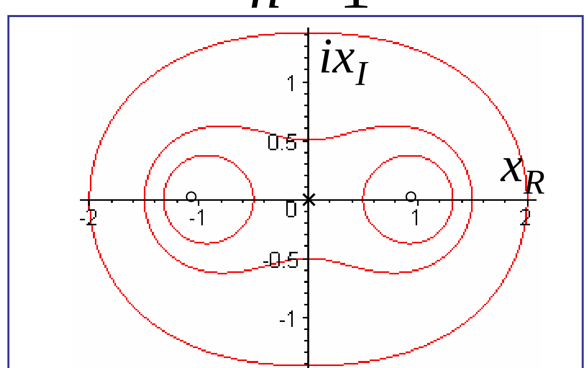
$$x(t) = x_R(t) + ix_I(t)$$

Eigen-trajectories

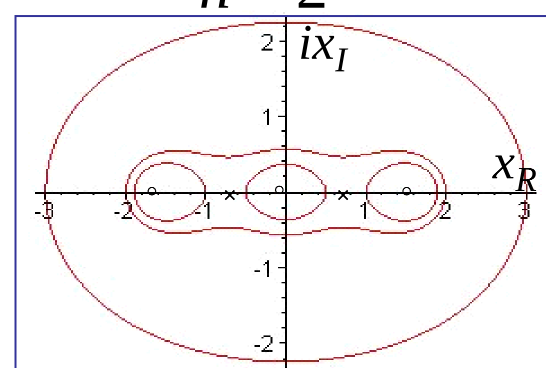
$n = 0$



$n = 1$



$n = 2$



Quantum Potential Disappears Beyond Nanoscale

Quantum Newton Law

$$m\frac{dx^2}{dt^2} = -\frac{dV}{dx} - \frac{dQ}{dx}, \quad x \in \Box$$

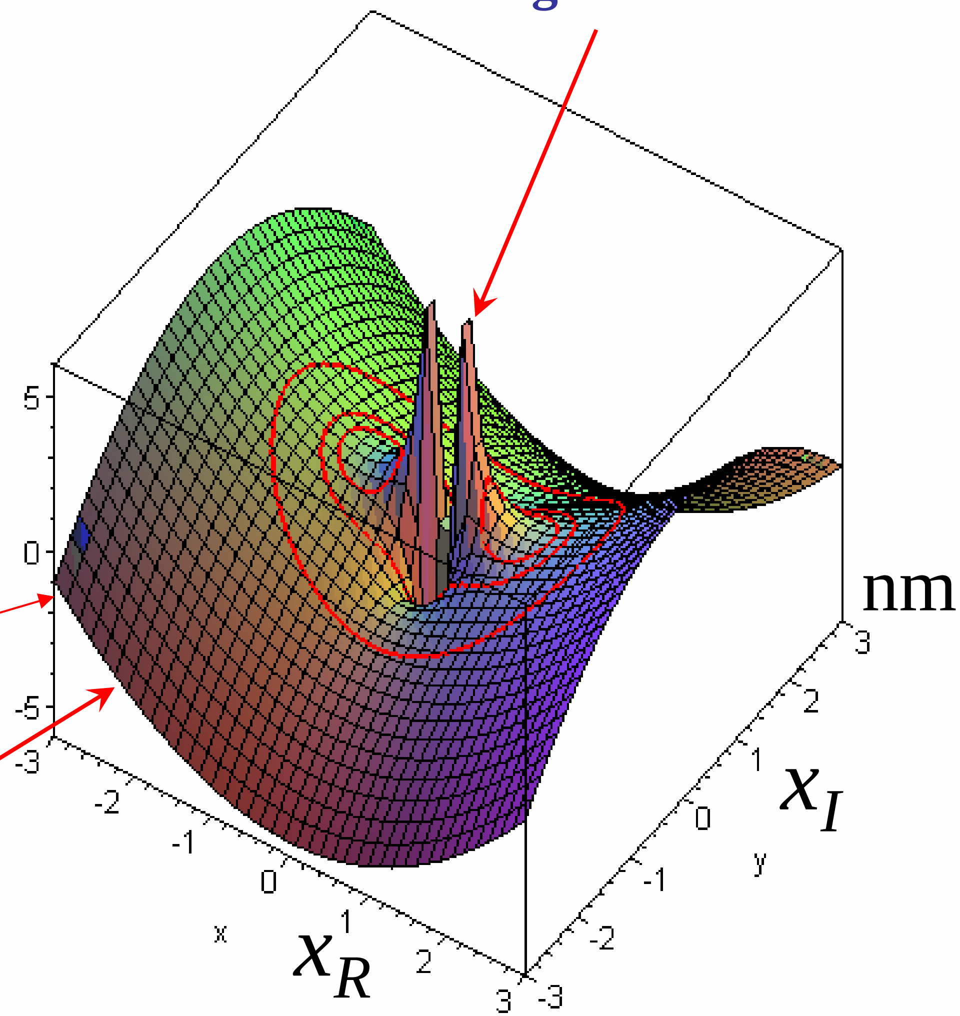
Large x $Q \rightarrow 0$

Classical Newton Law

$$m\frac{dx^2}{dt^2} = -\frac{dV}{dx}$$

Total potential

Quantum potential Q is significant only in a nano-scale region



$$V = \frac{1}{2}kx^2$$

$$Q \rightarrow 0$$

Quantization of Action Variable

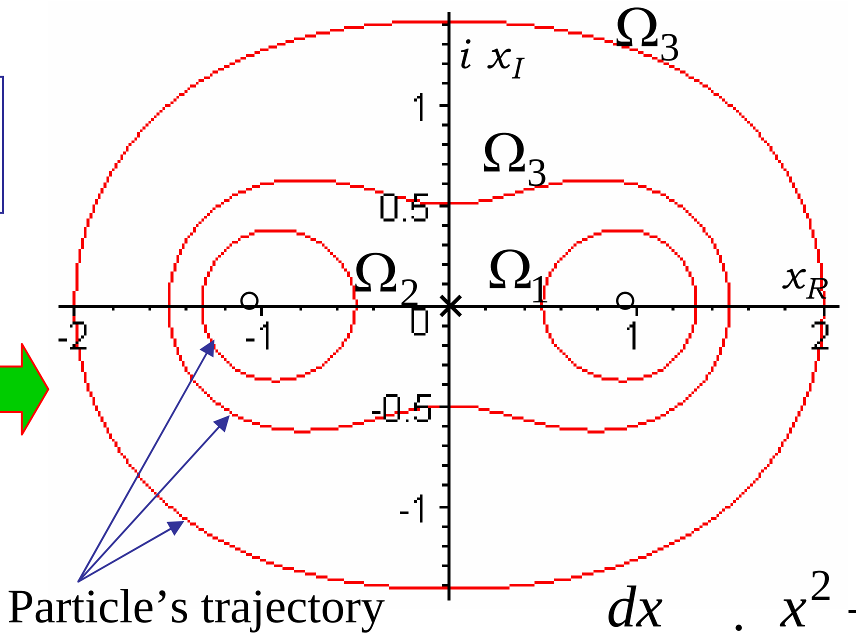
The action variable evaluated along any closed eigen-trajectory of harmonic oscillator satisfies the Sommerfeld-Wilson quantization rule

$$\int_c p\ dx = n_c h, \quad n_c = 0,\ 1,\ 2, \cdots$$

$$n = 1 \Rightarrow \int_c p\ dx = i\hbar \int_c \frac{x^2 - 1}{x}\, dx = \begin{cases} 0, & \forall c \in \Omega_1 \text{ or } \Omega_2 \\ h, & \forall c \in \Omega_3 \end{cases}$$

c is a Contour traced by a particle moving in complex plane

There are infinitely many contours, but the contour integration of pdx has only two discrete values, depending whether the pole is enclosed or not.



$$\frac{dx}{dt} = i\ \frac{x^2 - 1}{x}$$

The Origin of Quantization

Contour integration depends on the number of poles enclosed by the contour, but not on the shape of the contour.

General Hamiltonian for Harmonic Oscillator

$$H_G = \frac{1}{a}p'^2 + ax'^2 + bx' + c = \frac{1}{a}p'^2 + a\left(x' + \frac{b}{2a}\right)^2 - \frac{b^2}{4a} + c, \quad a,b,c \in \square$$

Schrödinger equation:

$$-\frac{1}{a}\frac{d^2}{dx'^2}\psi'(x') + \left[a\left(x' + \frac{b}{2a}\right)^2 - \frac{b^2}{4a} + c\right]\psi'(x') = E'\psi'(x')$$

Coordinate Transformation

Let $x = \sqrt{a}x' + b/2\sqrt{a}$

Schrödinger equation:

$$\frac{d^2}{dx^2}\psi(x) + \left(E - x^2\right)\psi(x) = 0$$

$$E = E' + b^2/4a - c$$

Ordinary wave function:

$$\psi_n(x) = C_n H_n(x) e^{-x^2/2}$$

Coordinate transformation: $x \to x'$

$$x' = 1/\sqrt{a}\, x - b/2\sqrt{a}$$

New Eigen Function:

$$\psi'_n(x') = C'_n H'_n(x') e^{-x'^2/2}$$
$$= C'_n H'_n\left(1/\sqrt{a}\, x - b/2a\right) e^{-\left(1/\sqrt{a}\, x - b/2a\right)^2/2}$$

New Eigenvalue: $E' = E - b^2/4a + c$

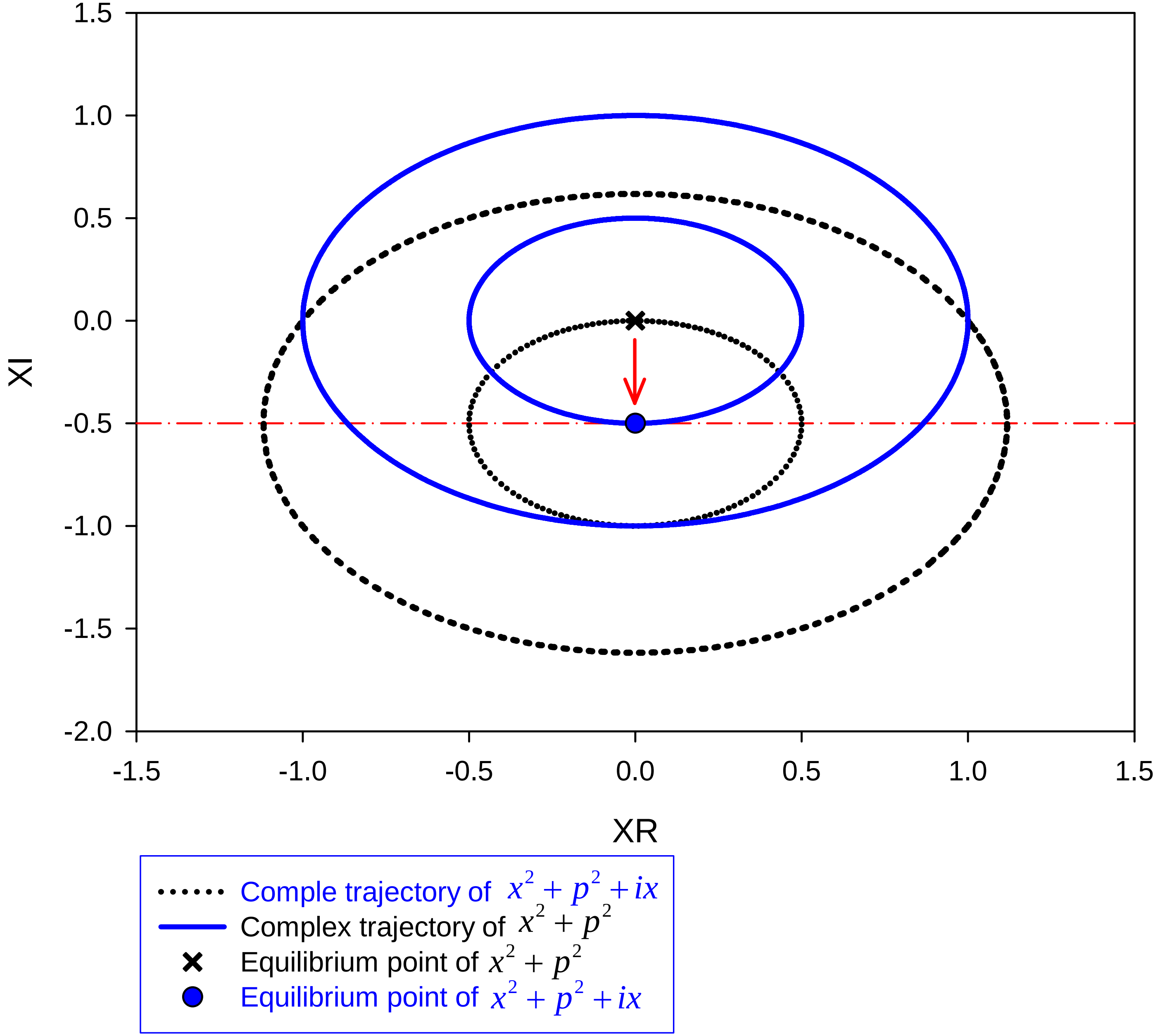
Trajectory movement:

Let $1/\sqrt{a} = re^{i\theta}$

r Multiple

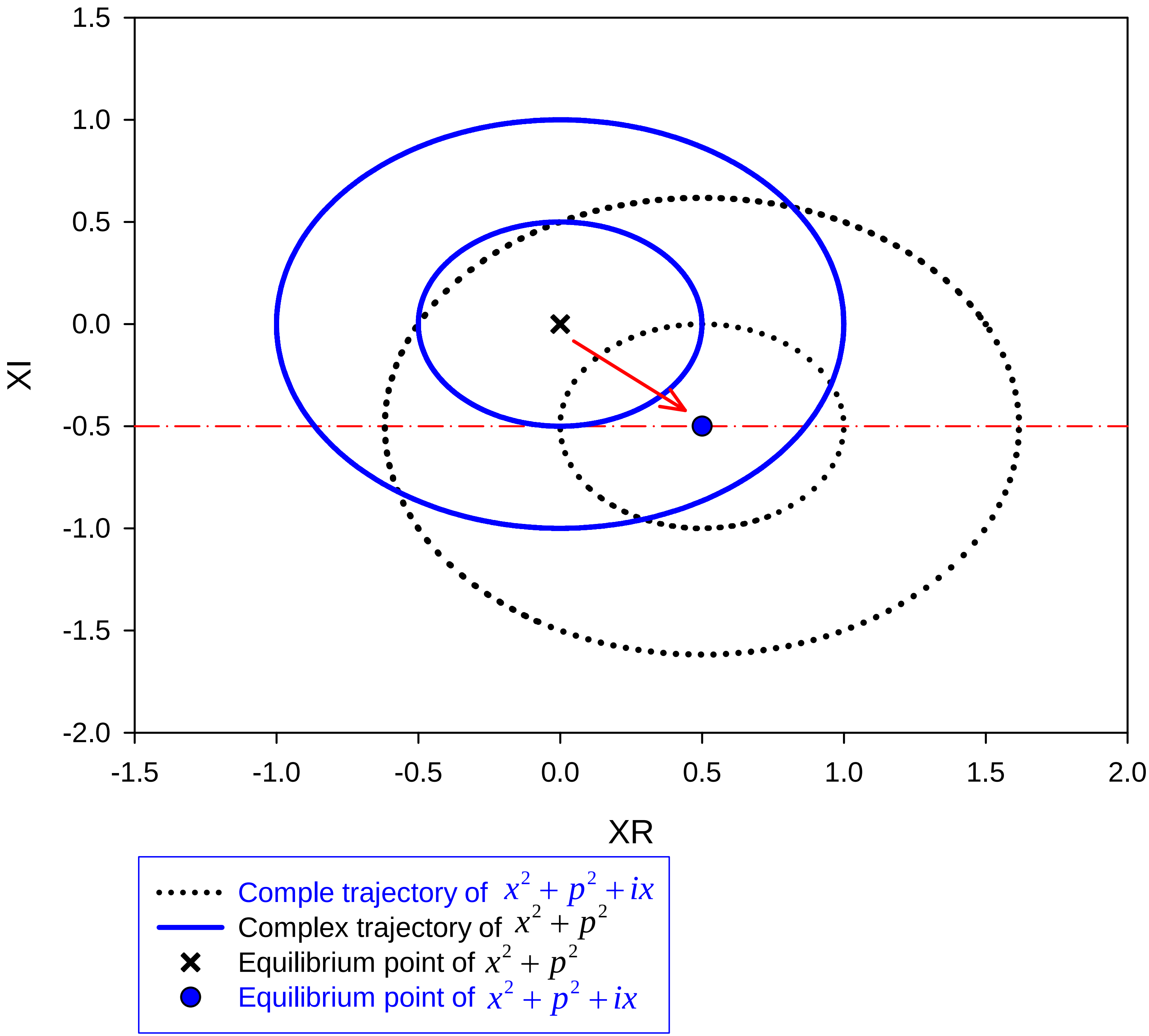
θ rotation

$-b/2a$ shift



$b = i,\ a = 1$

$i/2$ shift



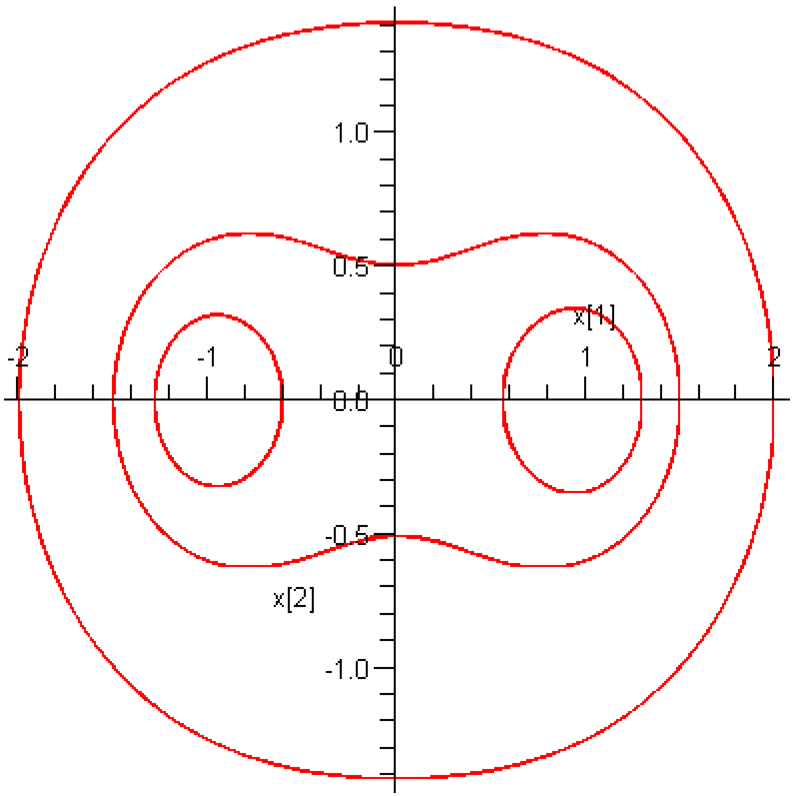
$ix - x$

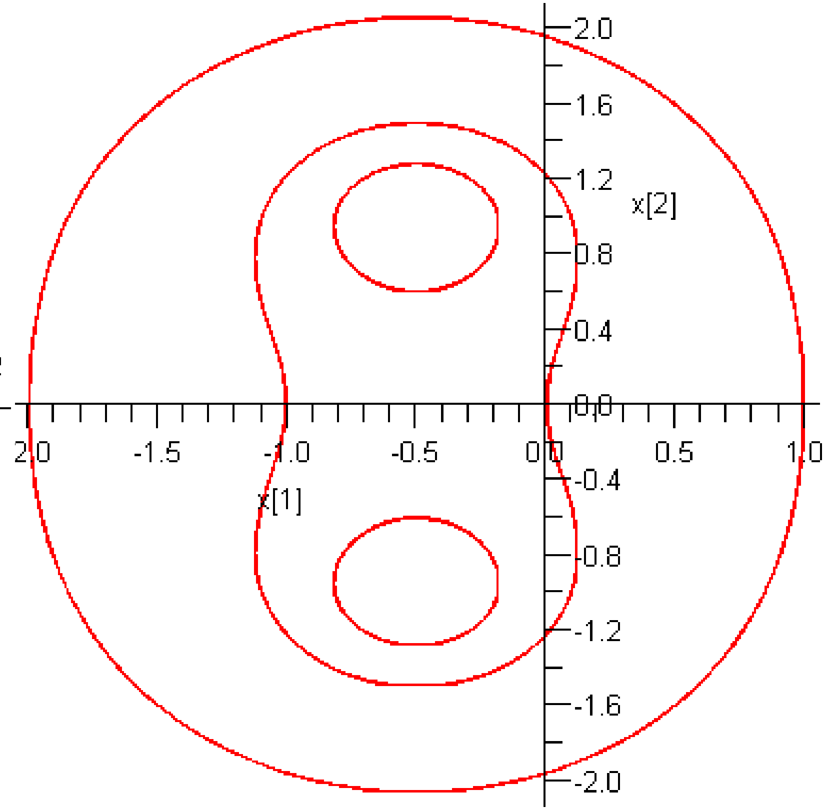
$+ i/2$

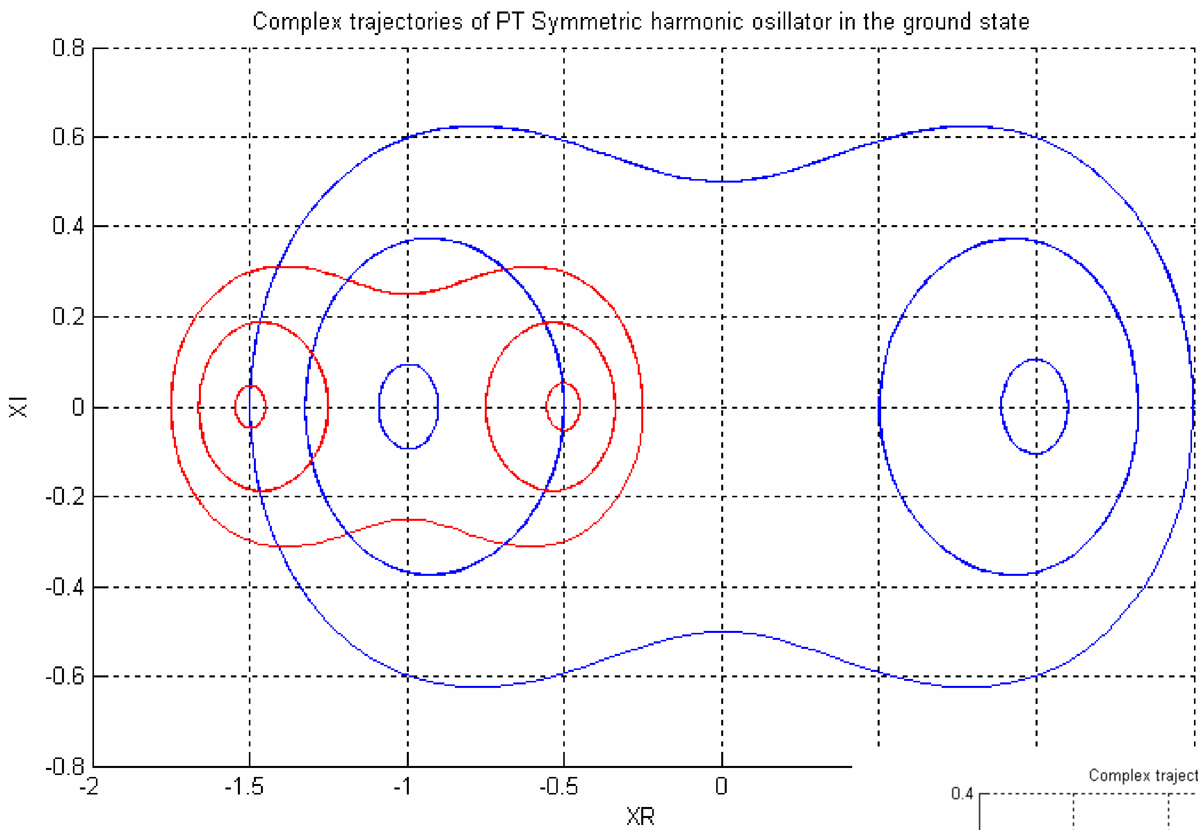
$1, \ a = 1$

shift

Rotate-Invariant Trajectory







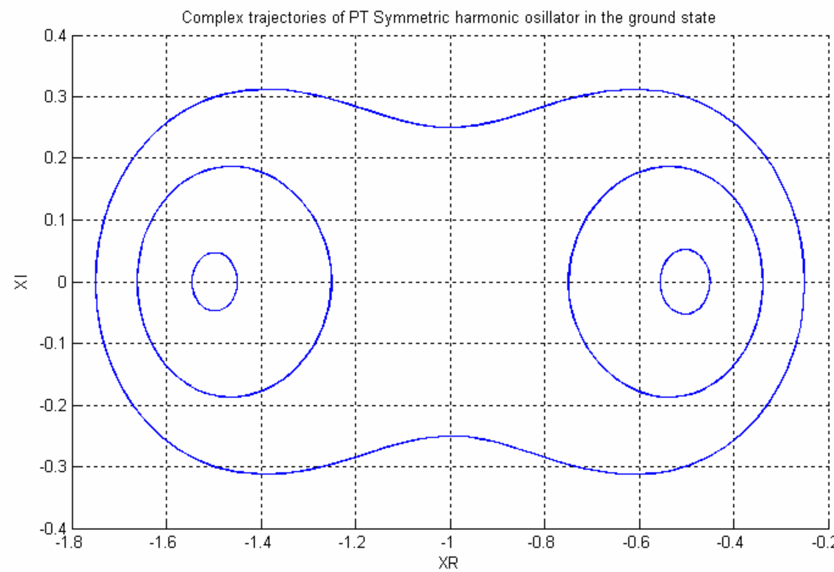
$$\psi_1(x) = 2xe^{-x^2/2}$$

$$\frac{dx}{dt} = i\,\frac{x^2 - 1}{x}$$

$$x' = x/2 - 1$$

$$\psi_1(x') = 2(2x'+2)e^{-(2x'+2)^2/2}$$

$$\frac{dx'}{dt} = i\,\frac{4x'^2 + 8x' + 3}{x'+1}$$

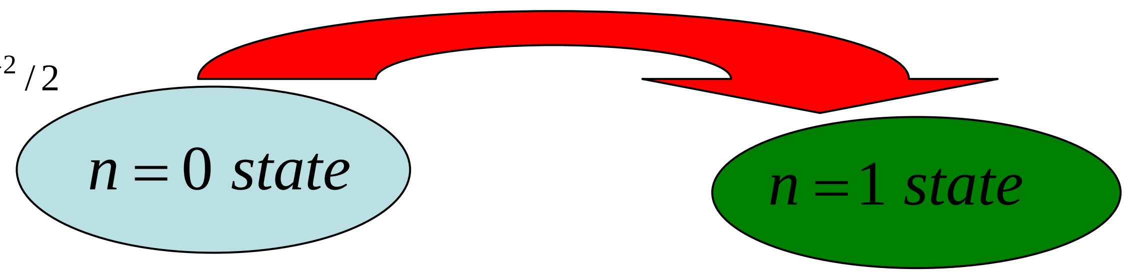


Complex Energy

- A system's total energy becomes complex when it has complex eigenvalue $H\left(\mathbf{q},\mathbf{p},t\right)=\frac{1}{2m}\mathbf{p}\cdot\mathbf{p}+V(\mathbf{q})+Q(\psi(\mathbf{q}))=-\frac{\partial S}{\partial t}=E=\text{constant}$
- Consider the state transition of harmonic oscillator

$\psi_0\left(\bar{x}\right)=e^{-\bar{x}^2/2}$

$\bar{E}_0=1/2$



$\psi_1\left(\bar{x}\right)=2\bar{x}e^{-\bar{x}^2/2}$

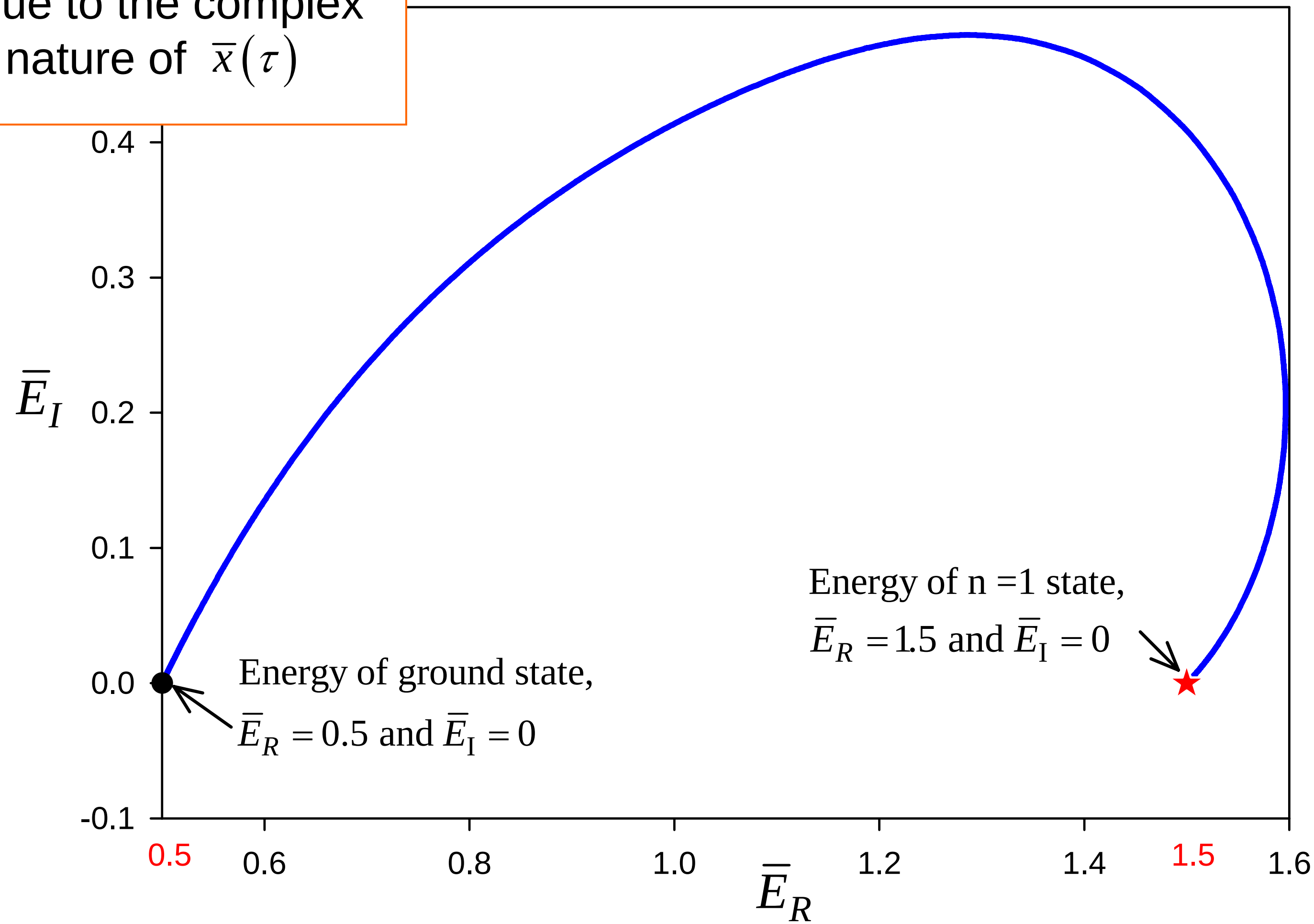
$\bar{E}_1=3/2$

Wave function of the whole transition process

$$\Psi_H(\bar{x},\tau)=\begin{cases} e^{-\bar{x}^2/2}e^{-i\bar{E}_0\tau} & \tau\le 0 \\ (1-\tau)e^{-\bar{x}^2/2}+2\tau\bar{x}e^{-\bar{x}^2/2}, & 0<\tau<1 \\ 2\bar{x}e^{-\bar{x}^2/2}e^{-i\bar{E}_1\tau} & \tau\ge 1 \end{cases}$$

Energy transfer from ground state to n=1 state on the complex plane

The total energy is complex valued due to the complex nature of $\bar{x}(\tau)$



Summary & Conclusions

- An intrinsic complex Hamiltonian and its related complex Hamiltonian equations of motion arise naturally within every quantum system.
- Schrödinger equation is just an expression for the total energy conservation of the accompanying intrinsic complex Hamiltonian.

$$H\left(\mathbf{q},\mathbf{p},t\right)=\frac{1}{2m}\mathbf{p}\cdot\mathbf{p}+V(\mathbf{q})+Q(\psi(\mathbf{q}))=-\frac{\partial S}{\partial t}=E=\text{constant}$$

- The PT-symmetric and the non-PT-symmetric complex Hamiltonian can be unified into a general class of complex Hamiltonian.

Summary & Conclusions

There is a general complex Hamiltonian for harmonic oscillator:

$$H_G = \frac{1}{a} p'^2 + a x'^2 + b x' + c, \quad a, b, c \in \square$$

Coordinate transformation/Eigenvalues:

$$x' = \frac{1}{\sqrt{a}} x - \frac{b}{2a} = r e^{i\theta} - \frac{b}{2a} \qquad E' = E - \frac{b^2}{4a} + c$$

$\Rightarrow$ r Multiple, θ rotation and $-b/2a$ shift

ex: $H = \frac{1}{i^2} p'^2 + i^2 x'^2 + i^2 x' + \frac{3}{4} \Rightarrow a = b = i^2, \; c = \frac{3}{4}$

$$x' = \frac{1}{\sqrt{a}} x - \frac{b}{2a} = \frac{x}{i} - \frac{1}{2} \qquad E' = 2n + 1 + \frac{1}{4} + \frac{3}{4} = 2n + 2$$

Summary & Conclusions

- When viewed from the complex domain, the boundary between Hermitian system, PT-symmetric system, and non-PT-symmetric system disappears.

Hermitian System → Real ψ and real E

PT-symmetric System → Imaginary ψ and real E

Non-PT-symmetric System → Imaginary ψ and imaginary E

Summary & Conclusions

- Their quantum trajectories and eigenfunctions can be made coincident by linear coordinate translation.

- One can obtain the eigenfunction and eigenvalue for a quantum system without solving the Schrödinger equation.

- The identical quantum trajectory can be obtain under linear coordinate transformation in complex plane.

- Complex energy has real physical meaning, however, the real energy reflects the eigenvalue of the system, only a small part in it.