I. Applications in quantum mechanics.
II. Singular points of the first order equations

O.M. Kiselev

Innopolis University

Schrödinger equation

Schrödinger equation in a simplest form can be written as

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi.$$

Here $\hbar$ is a Planck constant, m is a mass of a particle and $V(x)$ is a potential field which defines the behavior of the particle in a classical mechanics.

- Potential for a free particle is follows: $V(x) \equiv 0$.
- Potential for a linear oscillator is $V(x) = k\frac{x^2}{2}$.
- Potential for an electron of hydrogen atom: $V(\vec{x}) = -\frac{e^2}{\varepsilon_0 r}$.

Typical parameters of quantum systems

- $\hbar \sim 6.62607015 \times 10^{-34}$ J/Hz is the value of the Planck constant;
- $e \sim 1.602 \times 10^{-19}$ C is an electron charge;
- $m \sim 9.1 \times 10^{-31}$ kg is a mass of an electron;
- $r \sim 5.292 \times 10^{-11}$ m is a distance between the kernel and electron (Bohr radius);
- $\epsilon_0 \sim 8.8854 \times 10^{-12}$ F/m is a vacuum permittivity.

Wave motion

When we consider waves and its dependence on time we should understand a direction of wave motion.
let us consider two different solutions of a Schrödinger equation without external field:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2};$$

$$\tau = \frac{1}{h}t,\ \xi = \frac{\sqrt{2m}}{\hbar}x,$$

$$i\frac{\partial\Psi}{\partial \tau} = -\frac{\partial^2\Psi}{\partial \xi^2}.$$

Wave motion

In the simplest case two different solutions can be written:

$$\Psi_\pm = e^{-i\left(E\tau \pm \sqrt{E}\xi\right)}.$$

The wave phase with the sign $+$ is constant at line parallel by a straight-line $\xi = -\tau\sqrt{E}$. This means the wave moves in a negative direction with respect to ξ axis.
In contrast, the wave phase of the solution with $-$ is constant on all lines which are parallel by a straight-line $\xi = \tau\sqrt{E}$. This wave moves in a positive direction with respect to the axis ξ.

Oscillations in potential well

Let us consider oscillations in an infinite potential well $\xi \in (0, \lambda)$. The Schrödinger equation with additional boundary conditions is written as:

$$i\frac{\partial \Psi}{\partial \tau} = -\frac{\partial^2 \Psi}{\partial \xi^2}, \quad \Psi|_{\xi=0} = \Psi|_{\xi=\lambda} = 0.$$

A special solution which is periodic on time has a form:

$$\Psi(\xi, \tau) = e^{-iE\tau}\psi(\xi).$$

A substitution into the Schrödinger equation yields:

$$\psi'' + E\psi = 0, \quad \psi|_{\xi=0} = \psi|_{\xi=\lambda} = 0.$$

Solution can be written for discrete set of energy E_n:

$$\psi = \sin\left(\sqrt{E_n}\xi\right), \quad E_n = \frac{\pi^2}{\lambda^2}n^2, \quad n \in \mathbb{N}.$$

A barrier as a potential

Let us consider the potential with a threshold shape.

$$U(\xi) = \begin{cases} 0, & -\lambda < \xi; \\ u, & -\lambda \le \xi \le \lambda; \\ 0, & \lambda < \xi. \end{cases}$$

On left-hand side of the barrier a solution of the Schrödinger equation looks as

$$\Psi = e^{-i\left(E\tau - \sqrt{E}\xi\right)} + Re^{-i\left(E\tau + \sqrt{E}\xi\right)}.$$

Here first term is a falling wave. This waves move to the barrier. Second term is reflected wave, because this wave moves from the barrier.

On right-hand side of the barrier a solution contains a transmitted wave only:

$$\Psi = Te^{-i\left(E\tau - \sqrt{E}\xi\right)}.$$

Tunnel effect

The wave with the energy E for the Schrödinger equation looks like:

$$\Psi = e^{-i(E\tau)}\psi(\xi).$$

In this case the one-dimension Schrödinger equation looks like:

$$\psi'' + (E - U(\xi))\psi = 0.$$

If $u > E$ this means the energy to overcome this threshold is less that the threshold level. For the classical particle does not be passed through such threshold. Let us find a possibility to pass this threshold for quantum one.

Falling and reflected waves

General solution before the threshold:

$$\psi = e^{i\sqrt{E}\xi} + Re^{-i\sqrt{E}\xi}.$$

This formula contains the falling wave and reflected one.
At the threshold the solution has another form:

$$\psi = B_1 e^{\sqrt{u-E}\xi} + B_2 e^{-\sqrt{u-E}\xi}.$$

After the threshold the solution has transmitted wave only:

$$\psi = Te^{i\sqrt{E}\xi}.$$

Our problem is to find the transmitted and reflected waves.
Formally it means one should find the coefficients R and T.

A matching of the solutions

These solutions and their derivatives of first order should be matched at the point $\xi = -\lambda$:

$$
\begin{gathered}
e^{-i\omega\lambda} + Re^{i\omega\lambda} = B_1\, e^{-k\lambda} + B_2\, e^{k\lambda}, \\
i\omega\, e^{-i\omega\lambda} - i\omega\, R\, e^{i\omega\lambda} = k\, B_1\, e^{-k\lambda} - k\, B_2\, e^{k\lambda}.
\end{gathered}
$$

The same matching should be made at the point $\xi = \lambda$:

$$
\begin{gathered}
B_1\, e^{k\lambda} + B_2\, e^{-k\lambda} = Te^{i\omega\,\lambda}, \\
k\, B_1\, e^{k\lambda} - k\, B_2\, e^{-k\lambda} = i\omega\, T\, e^{i\omega\lambda}.
\end{gathered}
$$

Here $\omega = \sqrt{E}, \quad k = \sqrt{u - E}$.
So we have four equations with four unknown values R, T, B_1, B_2.
We are interested in R and T only.

The transmission coefficient

One can solve the system of four linear equations by hand or using some computer algebra system.
The transmission coefficient have the following form:

$$|T| = \frac{1}{\sqrt{\frac{u-E}{E}\sinh^2\left(\sqrt{u-E}\lambda\right) + \cosh^2\left(\sqrt{u-E}\lambda\right)}} \times \frac{1}{\sqrt{\frac{E}{u-E}\sinh^2\left(\sqrt{u-E}\lambda\right) + \cosh^2\left(\sqrt{u-E}\lambda\right)}}.$$

The transmission coefficient exponentially decreases with respect to width λ and height of the barrier $u - E$.

The reflection coefficient

$$|R| = \frac{2u\sinh(2\sqrt{u-E}\lambda)}{\sqrt{E\sinh^2(\sqrt{u-E}\lambda) + (u-E)\cosh^2(\sqrt{u-E}\lambda)}} \times \frac{1}{\sqrt{E\cosh^2(\sqrt{u-E}\lambda) + (u-E)\sinh^2(\sqrt{u-E}\lambda)}}.$$

Singular points of the first-order equations

Let's consider the first-order equations in the form:

$$\frac{dy}{dx} = \frac{a_1 y + b_1 x}{a_2 y + b_2 x}.$$

We will focus on neighborhood of the irregular point $(0, 0)$.
The first order equation connects to the two first-order equations for $x(t)$ and $y(t)$ as a parametric given function $y(x)$:

$$\frac{dy}{dt} = a_1 y + b_1 x,$$
$$\frac{dx}{dt} = a_2 y + b_2 x.$$

Exponents and eigenvalues

The solution of the linear system will be constructed as a vector:

$$\begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} e^{\lambda t}.$$

Substituting the formula into the system one obtains:

$$\lambda e^{\lambda t}\alpha_1 = a_1\alpha_1 e^{\lambda t} + b_1\alpha_2 e^{\lambda t},$$
$$\lambda e^{\lambda t}\alpha_2 = a_2\alpha_1 e^{\lambda t} + b_2\alpha_2 e^{\lambda t}.$$

It yields:

$$(a_1 - \lambda)\alpha_1 + b_1\alpha_2 = 0,$$
$$a_2\alpha_1 + (b_2 - \lambda)\alpha_2 = 0.$$

Eigenvalues

The system can be represented as

$$\begin{pmatrix} (a_1-\lambda) & b_1 \\ a_2 & (b_2-\lambda) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = 0$$

Non-trivial solutions exist if

$$\begin{vmatrix} (a_1-\lambda) & b_1 \\ a_2 & (b_2-\lambda) \end{vmatrix} = 0,$$

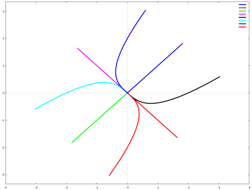
or

$$\begin{aligned} (a_1-\lambda)(b_2-\lambda) - a_2 b_1 = 0, \\ \lambda^2 - (a_1+b_2)\lambda + (a_1 b_2 - a_2 b_1) = 0, \\ \lambda_{1,2} = \frac{(a_1+b_2) \pm \sqrt{(a_1-b_2)^2 - 4a_2 b_1}}{2} \end{aligned}$$

The eigenvalues

- $(a_1 - b_2)^2 - 4a_2 b_1 > 0$, then $\lambda_{1,2} \in \mathbb{R}$;
- $(a_1 - b_2)^2 - 4a_2 b_1 = 0$, then $\lambda = (a_1 + b_2)/2$;
- $(a_1 - b_2)^2 - 4a_2 b_1 < 0$, then $\lambda_{1,2} \in \mathbb{C}$.

An unstable knot. $\lambda_1 > \lambda 2 > 0$.



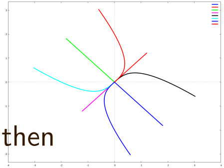
$$\frac{dy}{dt} = 2y + x, \quad \frac{dx}{dt} = y + 2x. \quad \left| \begin{array}{cc} (2-\lambda) & 1 \\ 1 & (2-\lambda) \end{array} \right| = 0,$$

$$\lambda_1 = 3,\ \alpha_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix},\ \lambda_2 = 1,\ \alpha_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^{3t} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + C_2 e^{t} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

A stable knot. $\lambda_1 < \lambda_2 < 0$



$$\frac{dy}{dt} = -2y + x, \quad \frac{dx}{dt} = y - 2x. \qquad \begin{vmatrix} (-2-\lambda) & 1 \\ 1 & (-2-\lambda) \end{vmatrix} = 0,$$

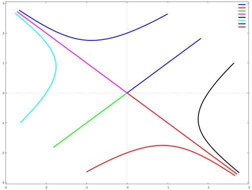
then

$$\lambda_1 = -3,\ \alpha_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix},\ \lambda_2 = -1\,\alpha_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^{-3t} \begin{pmatrix} 1 \\ -1 \end{pmatrix} + C_2 e^{-t} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

A saddle point. $\lambda_2 < 0 < \lambda_1$



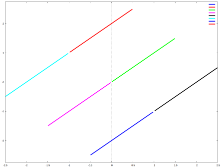
$$\frac{dy}{dt} = y + 2x, \quad \frac{dx}{dt} = 2y + x. \quad \begin{vmatrix} (1-\lambda) & 2 \\ 2 & (1-\lambda) \end{vmatrix} = 0.$$

$$\lambda_1 = 3,\ \alpha_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix},\ \lambda_2 = -1,\ \alpha_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^{3t} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + C_2 e^{-t} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

An unstable line. $\lambda_1 = 0,\ \lambda_2 > 0$



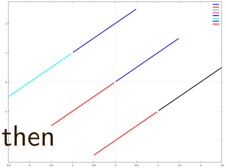
$$\frac{dy}{dt} = y + x, \quad \frac{dx}{dt} = y + x. \qquad \begin{vmatrix} (1-\lambda) & 1 \\ 1 & (1-\lambda) \end{vmatrix} = 0.$$

$$\lambda_1 = 0,\ \alpha_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix},\ \lambda_2 = 2,\ \alpha_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 \begin{pmatrix} 1 \\ -1 \end{pmatrix} + C_2 e^{2t} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

A stable line. $\lambda_1 < 0, \ \lambda_2 = 0$



$$\frac{dy}{dt} = -y - x, \qquad \frac{dx}{dt} = -y - x. \qquad \begin{vmatrix} (-1-\lambda) & -1 \\ -1 & (-1-\lambda) \end{vmatrix} = 0,$$

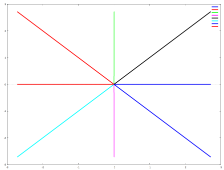
then

$$\lambda_1 = -2,\ \alpha_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix},\ \lambda_2 = 0,\ \alpha_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^{-2t} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + C_2 \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

A degenerated stable knot. One eigenvalue and two eigenvectors



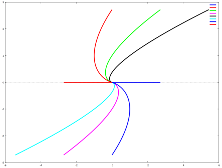
$$\frac{dy}{dt} = y, \quad \frac{dx}{dt} = x. \quad \begin{vmatrix} (1-\lambda) & 0 \\ 0 & (1-\lambda) \end{vmatrix} = 0,$$

$$\lambda_1 = 1,\ \alpha_1 = e^t \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ \lambda_2 = 1,\ \alpha_2 = e^t \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^t \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_2 e^t \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A degenerated unstable knot. Joint vector



$$\frac{dy}{dt} = y + x, \quad \frac{dx}{dt} = x. \qquad \begin{vmatrix} (1-\lambda) & 1 \\ 0 & (1-\lambda) \end{vmatrix} = 0,$$

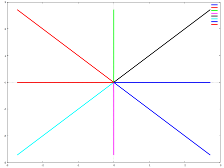
$$\lambda_1 = 1,\ \alpha_1 = e^t \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$\text{joint vector: } \alpha_2 = e^t \begin{pmatrix} t \\ 1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^t \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_2 e^t \begin{pmatrix} t \\ 1 \end{pmatrix}.$$

A degenerated stable knot. Two eigenvectors



$$\frac{dy}{dt} = -y, \quad \frac{dx}{dt} = -x. \qquad \begin{vmatrix} (-1-\lambda) & 0 \\ 0 & (-1-\lambda) \end{vmatrix} = 0,$$

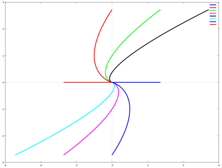
$$\lambda_1 = -1,\ \alpha_1 = e^{-t}\begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$\lambda_2 = -1,\ \alpha_2 = e^{-t}\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^{-t}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_2 e^{-t}\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A degenerated stable knot. Joint vector



$$\frac{dy}{dt} = -y - 5x, \quad \frac{dx}{dt} = -x. \qquad \begin{vmatrix} (-1-\lambda) & -5 \\ 0 & (-1-\lambda) \end{vmatrix} = 0,$$

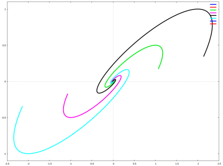
$$\lambda_1 = -1,\ \alpha_1 = e^t \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$\text{joint vector: } \alpha_2 = e^t \begin{pmatrix} t \\ -1/5 \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = C_1 e^{-t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_2 e^{-t} \begin{pmatrix} t \\ -1/5 \end{pmatrix}.$$

A stable focus. $\Re(\lambda_{1,2}) < 0$



$$\frac{dy}{dt} = y - 3x, \quad \frac{dx}{dt} = y - 2x. \qquad \begin{vmatrix} (1-\lambda) & -3 \\ 1 & (-2-\lambda) \end{vmatrix} = 0,$$

$$\lambda_1 = -\frac{1+i\sqrt{3}}{2}, \ \ \alpha_1 = e^{\lambda_1 t}\left(\begin{array}{c} 1 \\ \frac{3+i\sqrt{3}}{6} \end{array}\right),$$

$$\lambda_2 = \frac{-1+i\sqrt{3}}{2}, \ \ \alpha_2 = e^{\lambda_2 t}\left(\begin{array}{c} 1 \\ \frac{3-i\sqrt{3}}{6} \end{array}\right).$$

A general solution:

$$\left(\begin{array}{c} y \\ x \end{array}\right) = C_1 e^{\lambda_1 t}\left(\begin{array}{c} 1 \\ \frac{3+i\sqrt{3}}{6} \end{array}\right) + C_2 e^{\lambda_2 t}\left(\begin{array}{c} 1 \\ \frac{3-i\sqrt{3}}{6} \end{array}\right).$$

A real-valued solutions

Lemma

Suppose one get complex valued solution of a system with real coefficients. Then the real part of the solution and imaginary part of the solution are solutions of the system.

Proof.

Consider $y = u(t) + iv(t)$, $x(t) = p(t) + iq(t)$, where u, v, p, q are real-valued functions. Substitute the formulas into the system of equations and collect the real and imaginary parts.

Example of real solution

$$\begin{pmatrix} y_1 \\ x_1 \end{pmatrix} = e^{-t/2}\Re\left(\left(\cos\left(\frac{\sqrt{3}}{2}t\right) - i\sin\left(\frac{\sqrt{3}}{2}t\right)\right)\begin{pmatrix} 1 \\ \frac{3+i\sqrt{3}}{6} \end{pmatrix}\right) =$$

$$= e^{-t/2}\begin{pmatrix} \cos\left(\frac{\sqrt{3}}{2}t\right) \\ \frac{1}{2}\cos\left(\frac{\sqrt{3}}{2}t\right) + \frac{\sqrt{3}}{6}\sin\left(\frac{\sqrt{3}}{2}t\right) \end{pmatrix},$$

$$\begin{pmatrix} y_2 \\ x_2 \end{pmatrix} = e^{-t/2}\Im\left(\left(\cos\left(\frac{\sqrt{3}}{2}t\right) - i\sin\left(\frac{\sqrt{3}}{2}t\right)\right)\begin{pmatrix} 1 \\ \frac{3+i\sqrt{3}}{6} \end{pmatrix}\right) =$$

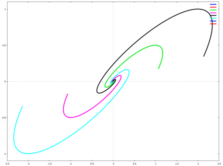
$$= e^{-t/2}\begin{pmatrix} -\sin\left(\frac{\sqrt{3}}{2}t\right) \\ \frac{1}{2}\sin\left(\frac{\sqrt{3}}{2}t\right) + \frac{\sqrt{3}}{6}\cos\left(\frac{\sqrt{3}}{2}t\right) \end{pmatrix}.$$

A general solution

$$\begin{pmatrix} y \\ x \end{pmatrix} = c_1 e^{-t/2} \begin{pmatrix} \cos\left(\frac{\sqrt{3}}{2}t\right) \\ \frac{1}{2}\cos\left(\frac{\sqrt{3}}{2}t\right) + \frac{\sqrt{3}}{6}\sin\left(\frac{\sqrt{3}}{2}t\right) \end{pmatrix} + c_2 e^{-t/2} \begin{pmatrix} -\sin\left(\frac{\sqrt{3}}{2}t\right) \\ \frac{1}{2}\sin\left(\frac{\sqrt{3}}{2}t\right) + \frac{\sqrt{3}}{6}\cos\left(\frac{\sqrt{3}}{2}t\right) \end{pmatrix}.$$

Here $c_{1,2} \in \mathbb{R}$.

An unstable focus. $\Re(\lambda_{1,2}) > 0$



$$\begin{array}{l} \frac{dy}{dt} = y - x, \\ \frac{dx}{dt} = y + \frac{1}{2}x. \end{array} \quad \begin{vmatrix} (1-\lambda) & -1 \\ 1 & (\frac{1}{2}-\lambda) \end{vmatrix} = 0,$$

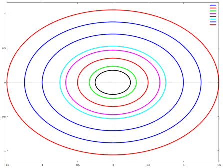
$$\lambda_1 = \frac{3 - i\sqrt{15}}{4}, \ \ \alpha_1 = e^{\lambda_1 t}\begin{pmatrix} 1 \\ \frac{1+i\sqrt{15}}{4} \end{pmatrix},$$

$$\lambda_2 = \frac{3 + i\sqrt{15}}{4}, \ \ \alpha_2 = e^{\lambda_2 t}\begin{pmatrix} 1 \\ \frac{1-i\sqrt{15}}{4} \end{pmatrix}.$$

A general solution:

$$\begin{pmatrix} y \\ x \end{pmatrix} = e^{3t/4}\left(C_1 e^{-i\frac{\sqrt{15}}{4}t}\begin{pmatrix} 1 \\ \frac{1+i\sqrt{15}}{4} \end{pmatrix} + C_2 e^{i\frac{\sqrt{15}}{4}t}\begin{pmatrix} 1 \\ \frac{1-i\sqrt{15}}{4} \end{pmatrix}\right).$$

Center. $\Re(\lambda_{1,2} = 0)$



$$\frac{dy}{dt} = 2x, \quad \frac{dx}{dt} = -y. \qquad \begin{vmatrix} (-\lambda) & 2 \\ -1 & (-\lambda) \end{vmatrix} = 0,$$

$$\lambda_1 = -i\sqrt{2}, \ \ \alpha_1 = e^{-i\sqrt{2}\,t} \left(\begin{array}{c} 1 \\ \frac{-i}{\sqrt{2}} \end{array} \right),$$

$$\lambda_2 = i\sqrt{2}, \ \ \alpha_2 = e^{i\sqrt{2}\,t} \left(\begin{array}{c} 1 \\ \frac{i}{\sqrt{2}} \end{array} \right).$$

A general solution:

$$\left(\begin{array}{c} y \\ x \end{array} \right) = a \left(\begin{array}{c} \cos(\sqrt{2}t) \\ -\frac{1}{\sqrt{2}}\sin(\sqrt{2}t) \end{array} \right) + b \left(\begin{array}{c} \sin(\sqrt{2}t)) \\ \frac{1}{\sqrt{2}}\cos(\sqrt{2}t) \end{array} \right).$$

Center. Real-valued solution

$$\begin{pmatrix} y \\ x \end{pmatrix} = r \begin{pmatrix} \cos(\sqrt{2}t + \phi) \\ -\frac{1}{\sqrt{2}} \sin(\sqrt{2}t + \phi) \end{pmatrix},$$

$$r = \sqrt{a^2 + b^2} > 0, \quad \phi = \arctan\left(\frac{b}{a}\right) \in [-\pi/2, \pi/2).$$

$$y^2 + 2x^2 = r^2.$$

Summary