# Energy flux balance in conservative mediums and fields

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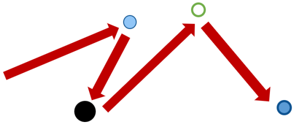
# Contents

# Introduction

# Diffusive and ballistic heat transfer

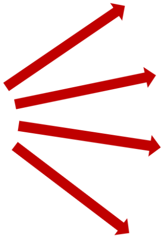
**Diffusive heat transfer:**

- Typical for macroscopic systems
- Result of reflection from defects and inhomogeneities
- Diffusion propagation of elastic waves

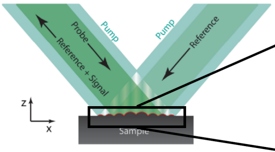


**Ballistic heat transfer:**

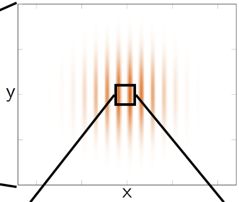
- Realized in microsystems
- Observed in ultrapure materials
- Ballistic propagation of elastic waves

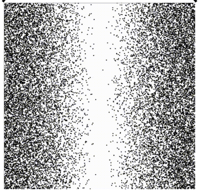


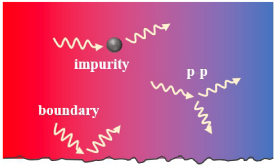
# Kinetic description of heat transfer in solids




Transient Thermal Grating (TTG) experiment, Huberman [1]






Phonon scattering mechanisms, Chen [2]

TTG simulation, Falco and Borisenkov

[1] S. Huberman et al. 2019. Science.
[2] H. Bao, J. Chen, X. Gu & B. Cao. 2018. ES Energy & Environment.

# Kinetic theory of heat transfer in solids

Waves are represented by quasiparticles (phonons). The quasiparticles motion is described by

$$\dot{f} + \nabla_{\mathbf{r}}(f\mathbf{v}) + \nabla_{\mathbf{v}}(f\mathbf{w}) = \mathrm{I}_{\mathrm{coll}}$$ — Boltzmann's kinetic equation[1]

**Results:**

- Description of heat transfer in crystalline dielectrics and other solids
- The second sound in a solid

**An open question:**

- Explicit connection to crystal lattice dynamics

[1] $f = f(t, \mathbf{r}, \mathbf{v})$ — particle density, $t$ — time, $\mathbf{r}$ — position vector, $\mathbf{v}$ — velocity, $\mathbf{w}$ — acceleration, $\nabla$ — gradient, $\mathrm{I}_{\mathrm{coll}}$ — collision integral

# Analogy in mass and energy transfer

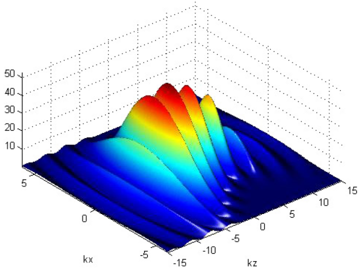
- Diffusive mass and energy transfer (classical diffusion and heat transfer)
- Ballistic mass transfer and wave energy transfer (matter dynamics and ballistic heat transfer)
- Corpuscular-wave dualism in solid state physics (phonons and other quasiparticles)
- Corpuscular-wave dualism in quantum mechanics (elementary particles and others)
- Kinetic description of wave processes: diffusion, anomalous and ballistic processes (energy and heat transfer)
- Energy transfer by electromagnetic field (the combined balance of the momentum of the field and matter)

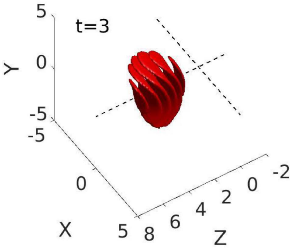
# Wave energy transfer

- propagation of mechanical waves in elastic media,
- heat transfer in crystalline solids,
- propagation of electromagnetic energy in a vacuum,
- probability transfer in quantum systems,
- gravitational waves on the surface of a liquid,
- mass transfer in general relativity,
- ...

**The question:** How can we uniformly describe these physically different processes?

# Localized disturbances

a) 


b) 


(a) The energy density of a localized acoustic pulse [1].
(b) The surface of the localized solution of the three-dimensional wave equation [2].

[1] J. Lekner. 2006. Localized oscillatory acoustic pulses. JPCM.
[2] A. B. Plachenov, P. Chamorro-Posada, A. P. Kiselev. 2023. Nonparaxial Tilted Waveobjects. JLT.

# Part I

# General theory

# Energy dynamics approach[1–3]

Carrier — substance (medium or field) in which wave energy transfer can be realized.

Phantom — *an effective* material body whose mass distribution is proportional to the energy distribution in the medium.

Energy dynamics — is a theory describing the wave transfer of energy based on an analogy with the classical dynamics of material bodies.

[1] A.M. Krivtsov. Dynamics of matter and energy. ZAMM. 2022.
[2] J.A. Baimova et al. Motion of localized disturbances in scalar harmonic lattices. PRE. 2023.
[3] V.A. Kuzkin. Acoustic transparency of the chain-chain interface. PRE. 2023.

# Energy dynamics in different branches of physics

| **Branches of physics** | **carrier** | **phantom** |
|---|---|---|
| Theory of elasticity | elastic medium | phantom |
| Solid state physics | crystal lattice | phonon |
| Electrodynamics | electromagnetic field | photon (group of photons) |
| Quantum mechanics | probability distribution | quantum particle |

# Local equations of balance

## Balance of energy

$$\dot{\epsilon} = -\nabla \cdot \mathbf{q},$$

$\epsilon$ — local energy (total specific energy of a small element of the medium),
$\mathbf{q}$ — local energy flux vector.

## Energy flux balance

$$\dot{\mathbf{q}} = -\nabla \cdot \mathbf{g} + \varphi,$$

$\mathbf{g}$ — superflux tensor (flux of the flux),
$\varphi$ — supply of energy flux.

The dot above the symbol — is a time derivative, $\nabla$ — nabla operator (vector operator of differentiation by spatial coordinates), point between symbols — scalar product of vector or tensor quantities.

# Global values

## Global balance equations

$$\dot{E} = 0, \qquad \dot{\mathbf{Q}} = \mathbf{\Phi},$$

where

$$E \stackrel{\text{def}}{=} \int \epsilon \, \mathrm{d}V, \qquad \mathbf{Q} \stackrel{\text{def}}{=} \int \mathbf{q} \, \mathrm{d}V, \qquad \mathbf{\Phi} \stackrel{\text{def}}{=} \int \boldsymbol{\varphi} \, \mathrm{d}V,$$

— global energy, flux and flux supply.

## Energy Center

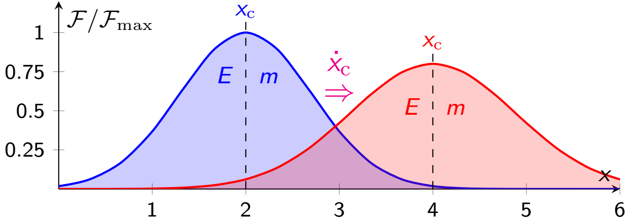
$$\mathbf{r}_{\mathrm{c}} \stackrel{\text{def}}{=} \frac{1}{E} \int \mathbf{r} \, \epsilon \, \mathrm{d}V \qquad \Rightarrow \qquad \mathbf{Q} = E \, \dot{\mathbf{r}}_{\mathrm{c}}.$$

Energy dynamics equation (analog of Newton's 2nd law):

$$E \, \ddot{\mathbf{r}}_{\mathrm{c}} = \mathbf{\Phi}.$$

# Analogy in energy and mass transfer

| | carrier | phantom | |
|---|---|---|---|
| energy | $E$ | $m$ | mass |
| energy flux | $\mathbf{Q}$ | $\mathbf{p}$ | impulse |
| energy flux supply | $\mathbf{\Phi}$ | $\mathbf{f}$ | external force |
| energy center | $\mathbf{r}_c$ | | center of mass |




Relationship between energy and mass quantities:

$$E = mc^2$$
$$\mathbf{Q} = \mathbf{p}c^2$$
$$\mathbf{\Phi} = \mathbf{f}c^2$$

# Part II

# Conservation of energy flux

# Scalar elastic medium

**The equation of motion** (the wave equation)

$$\rho \ddot{u} = C\nabla^2 u,$$

$u$ — displacement, $\rho$ и $C$ — density and stiffness of the medium.

**Local energy**

$$\epsilon = \frac{\rho}{2}\dot{u}^2 + \frac{C}{2}(\nabla u)^2.$$

**Local energy flux**

$$\mathbf{q} = -C\dot{u}\,\nabla u.$$

# Scalar crystal lattice

## Equation of motion

$$m\ddot{u} = \sum_\alpha C_\alpha (u_\alpha - u),$$

где $u$ — displacement the reference atom, $u_\alpha$ — displacement of the atom located by the vector $\mathbf{a}_\alpha$ (with respect to the reference atom), $\alpha$ — the number of the reference atom neighbour, $m$ — the atom mass, $C_\alpha$ — the stiffness of the interatomic bond.

## Local energy

$$\epsilon = \frac{m}{2}\dot{u}^2 + \sum_\alpha \frac{C_\alpha}{4}(u_\alpha - u)^2.$$

**Local energy flux** ($V_0$ — unit cell volume of the crystal lattice)

$$\mathbf{q} = -\frac{1}{2V_0}\sum_\alpha C_\alpha \mathbf{a}_\alpha \dot{u}\,(u_\alpha - u).$$

# Electromagnetic field in vacuum

**Equations of motion**

$$\dot{\mathbf{E}} = c^2 \nabla \times \mathbf{B}, \qquad \dot{\mathbf{B}} = -\nabla \times \mathbf{E},$$

$\mathbf{E}$ — electric field, $\mathbf{B}$ — magnetic field, $c$ — speed of light in vacuum, the cross is the vector product.

**Local energy**

$$\epsilon = \frac{1}{8\pi}\left(\mathbf{E}^2 + \mathbf{B}^2\right).$$

**Local energy flux** (Umov–Poynting vector)

$$\mathbf{q} = \frac{c}{4\pi}\mathbf{E} \times \mathbf{B}.$$

# Quantum particle in vacuum

**Schrodinger equation**

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\nabla^2\psi,$$

where $\psi$ — wave function, $i$ — complex unit, $\hbar$ — the reduced Planck constant, $m$ — particle mass, $U$ — the potential of the external field,
$\mathbf{r}$ — spatial coordinate.

**Local energy** ($E$ — the total energy of the disturbance)

$$\epsilon = E\,|\psi|^2.$$

**Local energy flux** ($\mathbf{j}$ — probability flux)

$$\mathbf{q} = E\,\mathbf{j}, \qquad \mathbf{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right).$$

# Energy flux in different branches of physics

| **Branches of physics** | **formula**[2] | **standard interpretation** |
|---|---|---|
| Theory of elasticity | $-C\dot{u}\,\nabla u$ | the flux of the mechanical energy |
| Solid State Physics | $\frac{1}{2V_0}\sum_\alpha C_\alpha \mathbf{a}_\alpha \dot{u}\,(u - u_\alpha)$ | photon impulse |
| Electrodynamics | $\frac{c}{4\pi}\mathbf{E}\times\mathbf{B}$ | Umov–Poynting vector |
| Quantum mechanics | $\frac{E\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$ | probability flux |

[2] The given formulas are for the local fluxes, the global fluxes are to be obtained by integration.

# Conservation of the energy flux

Balance equation, global energy flux and flux supply

$$\dot{\mathbf{Q}} = \boldsymbol{\Phi}, \qquad \mathbf{Q} \overset{\text{def}}{=} \int \mathbf{q}\, \mathrm{d}V, \qquad \boldsymbol{\Phi} \overset{\text{def}}{=} \int \varphi\, \mathrm{d}V.$$

For the considered cases $\varphi = 0$ and the flux is conserved:

$$\dot{\mathbf{Q}} = 0 \qquad \Longrightarrow \qquad \mathbf{Q} = \mathrm{const}$$

From the constancy of the flux it follows that the energy center velocity is constant:

$$\mathbf{Q} = E\,\dot{\mathbf{r}}_\mathrm{c} \qquad \Longrightarrow \qquad \dot{\mathbf{r}}_\mathrm{c} = \mathrm{const}.$$

The energy center velocity coincides with the average group velocity

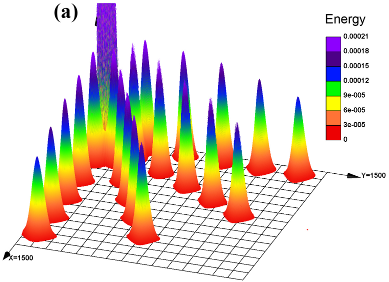
$$\dot{\mathbf{r}}_\mathrm{c} = \langle \mathbf{v}_\mathrm{g} \rangle, \qquad \mathbf{v}_\mathrm{g} \overset{\text{def}}{=} \frac{\mathrm{d}\omega}{\mathrm{d}\mathbf{k}},$$

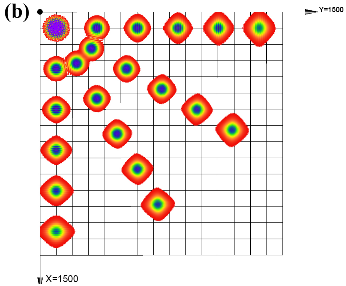
where $\omega$ — frequency, $\mathbf{k}$ — wave vector, $\langle \ldots \rangle$ — averaging over all harmonics.

# Example: phantoms in a two-dimensional lattice

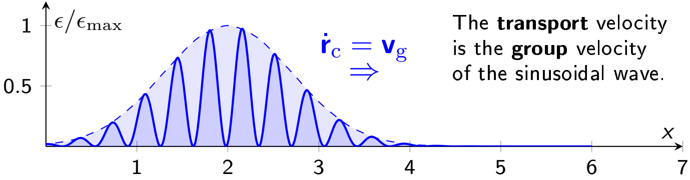
Transverse vibrations of a square homogeneous harmonic lattice.

The force is zero, the motion is uniform.




The structure of the phantom:




$\dot{\mathbf{r}}_c = \mathbf{v}_g$
$\Rightarrow$

The **transport** velocity is the **group** velocity of the sinusoidal wave.

J.A. Baimova, N.M. Bessonov, A.M. Krivtsov. PRE. 2023.

# Part III

# Change of the energy flux

# Change of the energy flux

The flux balance equation, the energy flux and the flux supply (the global ones)

$$\dot{\mathbf{Q}} = \mathbf{\Phi}, \qquad \mathbf{Q} \overset{\text{def}}{=} \int \mathbf{q}\,\mathrm{d}V, \qquad \mathbf{\Phi} \overset{\text{def}}{=} \int \varphi\,\mathrm{d}V.$$

For an inhomogeneous media $\varphi \neq 0$ and the flux is not conserved:

$$\dot{\mathbf{Q}} = \mathbf{\Phi} \qquad \Longrightarrow \qquad \mathbf{Q} \neq \mathrm{const}$$

Consequently, the energy center velocity is constant:

$$\mathbf{Q} = E\dot{\mathbf{r}}_\mathrm{c} \qquad \Longrightarrow \qquad \dot{\mathbf{r}}_\mathrm{c} \neq \mathrm{const}, \qquad E\ddot{\mathbf{r}}_\mathrm{c} = \mathbf{\Phi}.$$

The energy center velocity in an inhomogeneous medium can be considered as a generalization of the group velocity:

$$\mathbf{v}_\mathrm{g} \overset{\text{def}}{=} \frac{\mathbf{Q}}{E} \equiv \dot{\mathbf{r}}_\mathrm{c}.$$

# Scalar elastic medium

**Equation of motion** (inhomogeneous wave equation)

$$\rho\ddot{u} = \nabla\cdot(C\nabla u),$$

where $u$ — displacement, $\rho$ and $C$ — density and stiffness.

**Local energy**

$$\epsilon = \frac{\rho}{2}\dot{u}^2 + \frac{C}{2}(\nabla u)^2.$$

**Local energy flux**

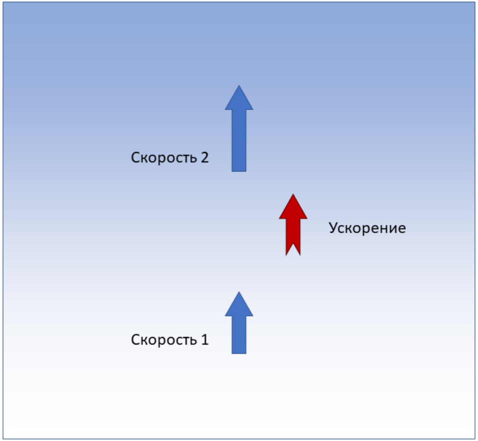
$$\mathbf{q} = -C\dot{u}\,\nabla u.$$

**Supply of the energy flux** ($\mathbf{I}$ — the unit tensor)

$$\varphi = C\left(\nabla u\nabla u - \frac{1}{2}(\nabla u)^2\,\mathbf{I}\right)\cdot\nabla\left(\frac{C}{\rho}\right).$$

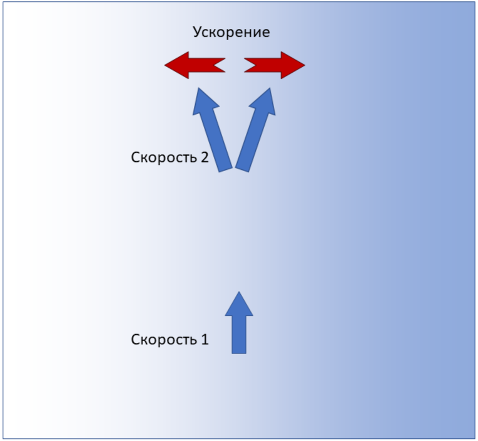
# Heterogeneous medium

## Motion along the gradient




The direction of acceleration is obvious

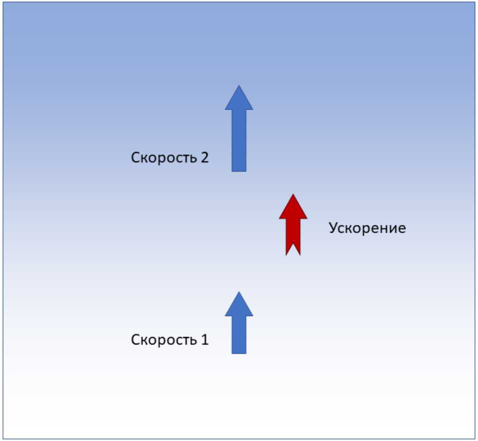
## Motion across the gradient




Which acceleration direction is correct?

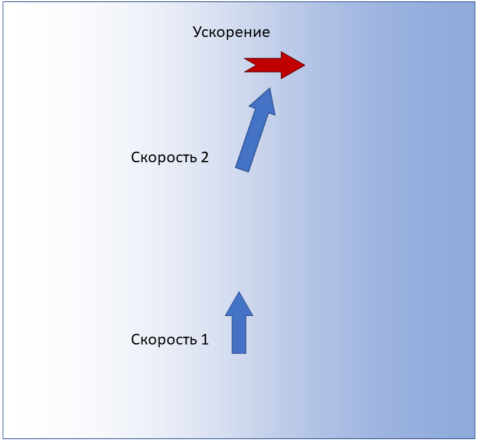
# Heterogeneous medium

Motion along the gradient




The direction of acceleration is obvious

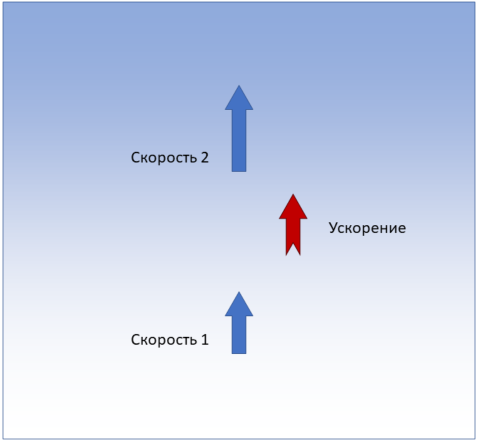
Motion across the gradient




Analogous direction

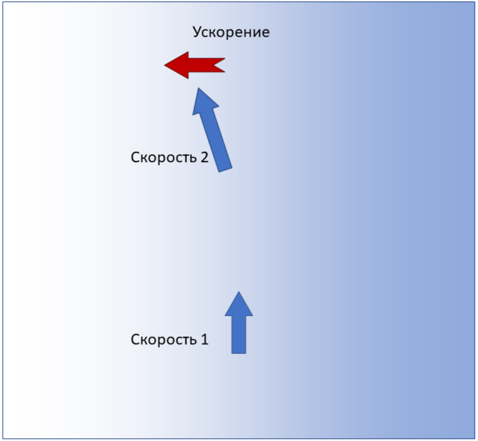
# Heterogeneous medium

## Motion along the gradient




The direction of acceleration is obvious

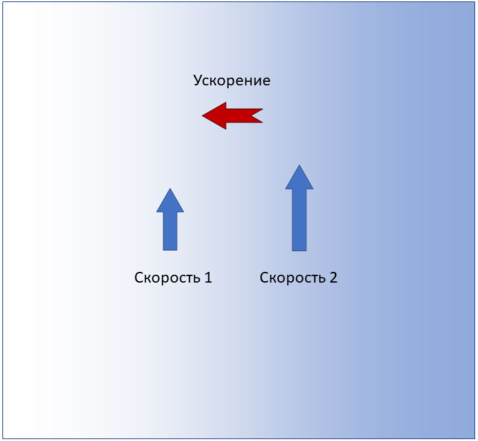
## Motion across the gradient




Correctly directed acceleration

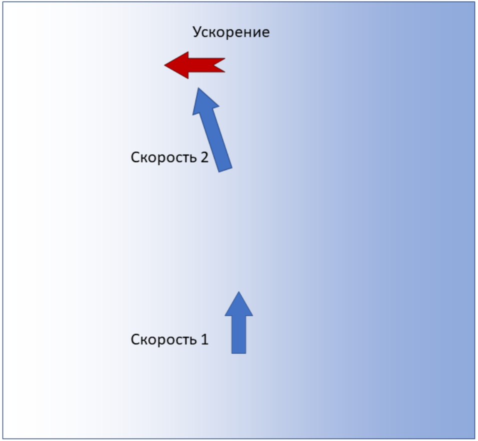
# Heterogeneous medium

Motion across the gradient




Explanation

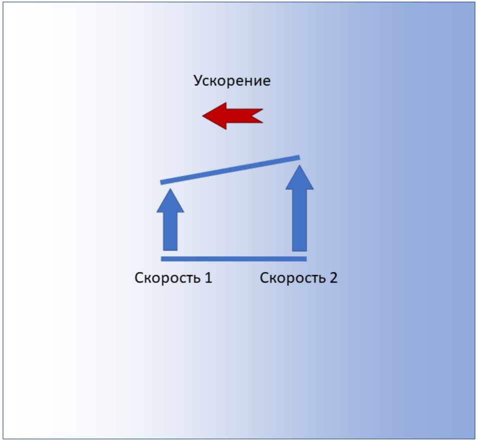
Motion across the gradient




Correctly directed acceleration

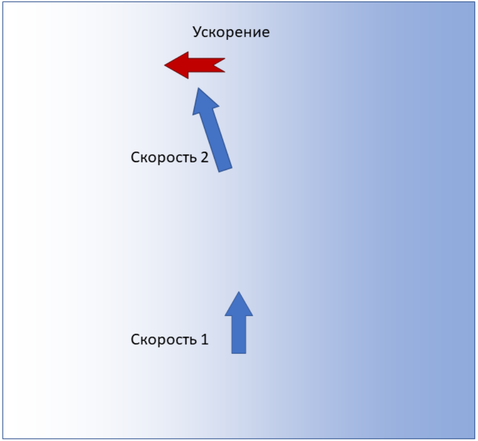
# Heterogeneous medium

Motion across the gradient




Explanation

Motion across the gradient




Correctly directed acceleration

# Scalar elastic medium: phantom motion

**Phantom dynamics equation** (further $\mathbf{r}_c = \mathbf{r}$ for brevity)

$$m\ddot{\mathbf{r}} = \mathbf{f}.$$

**An expression for the force acting on the phantom** (in a virial approximation)

$$\mathbf{f} = \frac{m}{2}(\nabla_{\|} - \nabla_{\perp})(c^2),$$

where

$$c = \sqrt{C/\rho}, \qquad \nabla_{\|} = \mathbf{e}\,\mathbf{e}\cdot\nabla, \qquad \nabla_{\perp} = \nabla - \nabla_{\|}, \qquad \mathbf{e} = \dot{\mathbf{r}}\,/\,|\dot{\mathbf{r}}|.$$

**The closed differential equation**

$$\ddot{\mathbf{r}} = \left(2\dot{\mathbf{r}}\dot{\mathbf{r}} - c^2\mathbf{I}\right)\cdot\nabla\ln c(\mathbf{r}).$$

# Ray description

Introduce the space coordinate $s$ along the trajectory:

$$\dot{\mathcal{F}} = \mathcal{F}'\,\dot{s} \qquad \Rightarrow \qquad \dot{\mathbf{r}} = \mathbf{r}'\,\dot{s},$$

dashed line denotes the derivative of $s$. Replacing $t$ by $s$ transforms the equation of motion of the energy point to the ray equation (used $|\dot{\mathbf{r}}| = c(\mathbf{r})$):

$$\ddot{\mathbf{r}} = \left(2\dot{\mathbf{r}}\dot{\mathbf{r}} - |\dot{\mathbf{r}}|^2\,\mathbf{I}\right)\cdot\nabla \ln c(\mathbf{r}) \qquad \Rightarrow \qquad \mathbf{r}'' = (\mathbf{r}'\mathbf{r}' - \mathbf{I})\cdot\nabla \ln c(\mathbf{r}),$$

which can be converted to the form ($\mathbf{e} = \mathbf{r}'$, $c = c(\mathbf{r})$)

$$(c^{-1}\,\mathbf{e})' = \nabla(c^{-1}).$$

This form of the ray equation is derived by other methods in the works Born and Wolf 1973 (p. 27). The ray equation describes the trajectory of the energy point, but does not provide information about its spatial position.

# A quantum particle in a potential field

**Schrodinger equation**

$$i\hbar\dot{\psi} = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\psi,$$

where $\psi$ — wave function, $i$ — complex unit, $\hbar$ — reduced Planck constant, $m$ — particle mass, $U$ — external potential, $\mathbf{r}$ — spatial coordinate.

**Local energy** ($E$ — total disturbance energy)

$$\epsilon = E|\psi|^2.$$

**Local energy flux** ($\mathbf{j}$ — probability flux)

$$\mathbf{q} = E\mathbf{j}, \qquad \mathbf{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right).$$

**Supply of energy flux**

$$\varphi = -E|\psi|^2\,\nabla U(\mathbf{r})/m.$$

# Mechanical interpretation of the quantum problem

**Model:** elastic medium with rotational degrees of freadom[3] in an elastic environment.

**Equation of dynamics of the medium** (is equivalent to the Schrodinger equation)

$$\rho \ddot{u} + C\Delta^2 u = 0, \qquad \Delta \overset{\text{def}}{=} \nabla^2 - \gamma(\mathbf{r}),$$

where $u$ — displacement, $\rho$ и $C$ — density and stiffness, $\gamma(\mathbf{r})$ — reduced stiffness of the elastic environment.

**Local energy and energy flux**

$$\epsilon = \frac{\rho}{2}\dot{u}^2 + \frac{C}{2}(\Delta u)^2, \qquad \mathbf{q} = C\left(\dot{u}\,\nabla\Delta u - \nabla\dot{u}\,\Delta u\right).$$

**Correlation with the characteristics of the quantum problem**

$$\psi = \frac{1}{\sqrt{2E}}\left(\sqrt{C}\Delta u - i\sqrt{\rho}\dot{u}\right), \qquad U(x) = \frac{\hbar^2}{2m}\gamma(x), \qquad \frac{\hbar}{m} = 2\sqrt{\frac{A}{\rho}}.$$

[3] In 1D — Euler–Bernoulli beam, in 2D — Kirchhoff–Love plate .

# Energy dynamics and Ehrenfest's theorem

**Dynamics equation** (for energy and mass, respectively; $E = mc^2$, $\boldsymbol{\Phi} = \mathbf{f}c^2$)

$$E\,\ddot{\mathbf{r}}_\mathrm{c} = \boldsymbol{\Phi} \qquad \Longleftrightarrow \qquad m\,\ddot{\mathbf{r}}_\mathrm{c} = \mathbf{f}.$$

**Ehrenfest's theorem** (the transition from quantum to classical mechanics; $\mathbf{F} = -\nabla U$):

$$m\langle\mathbf{r}\rangle^{\cdot\cdot} = \big\langle \mathbf{F}(\mathbf{r})\big\rangle \qquad \Longrightarrow \qquad m\langle\mathbf{r}\rangle^{\cdot\cdot} \approx \mathbf{F}(\langle\mathbf{r}\rangle),$$

where quantum, energy and mass interpretations of averaging:

$$\langle\mathcal{F}\rangle \stackrel{\mathrm{def}}{=} \int \mathcal{F}\,|\psi|^2\,\mathrm{d}V = \frac{1}{E}\int \mathcal{F}\,\epsilon\,\mathrm{d}V = \frac{1}{m}\int \mathcal{F}\rho\,\mathrm{d}V.$$

**Connection to energy dynamics**

$$\mathbf{r}_\mathrm{c} = \langle\mathbf{r}\rangle, \qquad \mathbf{f} = \langle\mathbf{F}\rangle.$$

# Conclusions

1. Along with the energy balance, the energy flux balance plays an important role in various brunches of physics.
2. The energy flux balance equation is an analogue to the momentum balance equation.
3. The mentioned analogy lays in the basis of the energy dynamics and it allows description of the wave energy transfer independently of the physical nature of the process.
4. In homogeneous medium the energy flux is being conserved[4], in non-homogeneous medium the change of the flux describes the dynamics of the energy transfer, and the flux can be used to generalize the notion of the group velocity.

[4] exactly for the scalar carrier and on average for the vector carrier

Thank you for your attention!

Additional information: tm.spbstu.ru/TC