Energy densities in quantum mechanics

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-- Introduction: why is there the problem?

-- Our approach

-- Applications to wave-packet and energy transfer

-- Joint work with Varazdat Stepanyan

Non-stationary quantum mechanics

$$i\hbar\dot{\phi} = H\phi, \qquad H \equiv -\frac{\hbar^2}{2m}\Delta + U.$$

Wave equaiton

$$\partial_t(\phi\phi^\dagger) + \boldsymbol{\nabla}\,\boldsymbol{I} = 0,$$

Coordinate-density conservation

What about energy density and its local conservation?

$$\dot{\rho} + \boldsymbol{\nabla}\boldsymbol{J} = 0,$$

$$\int \mathrm{d}^3 r\,\rho(\boldsymbol{r},t) = \int \mathrm{d}^3 r\,\phi^\dagger(\boldsymbol{r},t) H \phi(\boldsymbol{r},t),$$

Useful in all processes of energy transfer, e.g. group velocity of energy transfer

No obvious solution: *H and x* do not commute

$$\rho \stackrel{?}{=} \int \mathrm{d}^3 p \left(\frac{p^2}{2m} + U(\boldsymbol{r}) \right) W(\boldsymbol{p}, \boldsymbol{r})$$

Quasi-probabilities are not unique

Lagrangians for the Schroedinger equation are also not unique

What to expect in addition to local conservation?

ρ is quadratic over ϕ,

is a must

$$H\phi = E\phi \mapsto \rho \stackrel{?}{=} E\phi^*\phi,$$

Trivial in stationary?

$$\rho(\boldsymbol{r}, t) - U\phi^*(\boldsymbol{r}, t)\phi(\boldsymbol{r}, t) \stackrel{?}{\geq} 0$$

Positive kinetic energy density?

Program: start with Dirac's equation =>

Lagrangian and energy density are fixed by relativism

But do take the non-relativistic limit

$$i\hbar\dot{\psi} = \mathcal{H}\psi \equiv mc^2\beta\psi + U(\boldsymbol{r},t)\psi - i\hbar c(\boldsymbol{\nabla}\boldsymbol{\alpha}\psi),$$

Dirac's equation in the standard representation

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\dot{\varrho}(\boldsymbol{r},t) + \boldsymbol{\nabla}\boldsymbol{\mathcal{J}}(\boldsymbol{r},t) - \dot{U}(\boldsymbol{r},t)\psi^\dagger\psi = 0,$$

Local energy conservation

$$\varrho = \frac{i\hbar}{2}\left(\psi^\dagger\dot{\psi} - \dot{\psi}^\dagger\psi\right)$$

Energy density

Non-relativistic energy density

$$\psi = \begin{bmatrix} \varphi \\ \chi \end{bmatrix} e^{-\frac{i}{\hbar} mc^2 t},$$

$$\phi = \varphi + O(c^{-2})$$

Schroedinger equation holds for ϕ

$$\chi = -\frac{i\hbar}{2mc} \boldsymbol{\nabla\sigma}\phi + \mathcal{O}(c^{-3}).$$

$mc^2\chi^\dagger\chi$ is non-relativistic

$$\varrho = \rho + mc^2(\varphi^\dagger\varphi + \chi^\dagger\chi) + \mathcal{O}(c^{-2}),$$

Energy separation

$$\rho = -\frac{\hbar^2}{4m}\left([\Delta\phi^\dagger]\phi + \phi^\dagger\Delta\phi\right) + U\phi^\dagger\phi.$$

non-relativistic energy density

$$H\phi = E\phi \mapsto \rho = E\phi^*\phi,$$

Second form of non-relativistic energy

Locally conserved spin-dependent, non-relativistic energy

$$mc^2(\varphi^\dagger\varphi + \chi^\dagger\chi) = mc^2 n_0 + \rho_s,$$

$$n_0 \geq 0.$$

$$\rho_s = \nabla\boldsymbol{\Upsilon},$$

$$\boldsymbol{\Upsilon} = \frac{\hbar}{4m}\Re[\phi^\dagger\boldsymbol{\sigma} \times \boldsymbol{P}\phi]$$

$$\int \mathrm{d}r^3 \rho_s(\boldsymbol{r}, t) = 0 \quad \text{for} \quad \int \mathrm{d}r^3 \phi^\dagger(\boldsymbol{r}, t)\phi(\boldsymbol{r}, t) = 1.$$

$$\rho_s = 0$$

For finite stationary states without magnetic field

Wave-packet motion: energy is transferred faster than the coordinate

Holds for Gaussian and also Airy (moving without dispersion) wave packets

$$v_{\rm en}(t) = \frac{\int {\rm d}x\, J(x,t)}{\int {\rm d}x\, \rho(x,t)} = \frac{\langle P^3 \rangle}{m\langle P^2 \rangle},$$

Energy group velocity
for 1d finite
Wave packet

$$v_{\rm cor}(t) = (1/m)\langle P \rangle(t), \quad P = (i/\hbar)\partial_x.$$

coordinate
group velocity

$$v_{\rm en} - v_{\rm cor} \geq 0,$$

Summary

Dirac's equation => non-relativistic energy density

Spin-dependent non-relativistic energy

Non-relativistic energy densities can be negative

Energy moves faster than the coordinate

Lagrangians for the Schroedinger equation

$$\mathcal{L} = \frac{\hbar^2}{4m}\left(\phi^\dagger \Delta\phi + \Delta\phi^\dagger \phi\right) - U\phi^\dagger\phi + \frac{i\hbar}{2}(\phi^\dagger\dot{\phi} - \dot{\phi}^\dagger\phi).$$

$$\Lambda = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}\phi^\dagger\boldsymbol{\nabla}\phi - U\phi^\dagger\phi + \frac{i\hbar}{2}(\phi^\dagger\dot{\phi} - \dot{\phi}^\dagger\phi).$$