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MATHEMATISCH-NATURWISSENSCHAFTLICHE FAKULTÄT
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Basic Physics Course with MATLAB's Symbolic Toolbox and Live Editor

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5.2 Quantization and Schrödinger equation (Computational example)

```
clear all
syms hbar m b V_HJG V_WG x t positive
syms psi(x,t) S(x,t) R(x,t) rho(x,t)
Par=[m==1 hbar==1 b==1]
```

Par = $(m = 1 \quad \text{hbar} = 1 \quad b = 1)$

1 Hamilton-Jacobi Equation (HJE)

The HJE expresses the energy by the concept of action S and thus has a clear physical meaning:

HJE: $\frac{\partial}{\partial t}S(x,t) + \frac{1}{2m}\left(\frac{\partial}{\partial x}S(x,t)\right)^2 + V_{HGJ}(x) = 0$

this results in the time evolution of the action: $\frac{\partial}{\partial t}S(x,t) = ...$

```
diff(S(x,t),t)+diff(S(x,t),x)^2/2/m+V_HJG==0
```

ans =

$$V_{\mathrm{HJG}} + \frac{\partial}{\partial t}\, S(x,t) + \frac{\left(\frac{\partial}{\partial x}\, S(x,t)\right)^2}{2\,m} = 0$$

```
e1=isolate(ans,diff(S(x,t),t))
```

e1 =

$$\frac{\partial}{\partial t}\; S(x,t) = -V_{\mathrm{HJG}} - \frac{\left(\frac{\partial}{\partial x}\; S(x,t)\right)^2}{2\,m}$$

2 Continuity equation (CE)

The CE describes the conservation of density ρ. As the density in a region changes $(\dot{\rho} \neq 0)$, a corresponding current $\vec{j} = \rho\vec{v} = \rho\vec{\nabla}S/m$ flows through the surface of the region. Therefore, the CE also has a clear physical meaning.

CE: $\dot{\rho}(x,t) + \vec{\nabla}\cdot\left(\rho(x,t)\frac{\vec{\nabla}S(x,t)}{m}\right) = 0$

From this follows the time evolution of the density root $R = \sqrt{\rho}$: $\frac{\partial}{\partial t}R(x,t) = ...$

```
diff(R(x,t)^2,t)==-diff(R(x,t)^2*diff(S(x,t),x)/m,x);
e2=isolate(ans,diff(R(x,t),t))
```

e2 =

$$\frac{\partial}{\partial t}\; R(x,t) = -\frac{R(x,t)\,\frac{\partial^2}{\partial x^2}\; S(x,t) + \frac{\partial}{\partial x}\; S(x,t)\,\frac{\partial}{\partial x}\; R(x,t)\; 2}{2\,m}$$

3 Wave function (WF)

The density describes the physical content, the action describes the dynamics. Both can be combined in one WF:

WF: $\psi(x,t) = R(x,t)exp\left(\frac{iS(x,t)}{\hbar}\right)$.

```
e3=psi(x,t)==R(x,t)*exp(1i*S(x,t)/hbar)
```

e3 =

$$\psi(x,t) = \mathrm{e}^{\frac{S(x,t)\,\mathrm{i}}{\mathrm{hbar}}}\; R(x,t)$$

4 Wave equation (WE)

We consider the wave equation

$$WE:\; -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V_{WG}(x)\psi(x,t)$$

The WE can be expressed via the WF through $S(x,t)$ and $R(x,t)$:

```
e4=-hbar/1i*diff(psi(x,t),t)==-hbar^2*diff(psi(x,t),x,2)/2/m+V_WG*psi(x,t)
```

e4 =

$$\mathrm{hbar}\,\frac{\partial}{\partial t}\;\psi(x,t)\;\mathrm{i} = V_{\mathrm{WG}}\,\psi(x,t) - \frac{\mathrm{hbar}^2\,\frac{\partial^2}{\partial x^2}\;\psi(x,t)}{2\,m}$$

```
sube(e4,[e3,e2,e1]);
eq4=expand(isolate(ans,V_WG))
```

eq4 =

$$V_{\mathrm{WG}} = V_{\mathrm{HJG}} + \frac{\mathrm{hbar}^2\,\frac{\partial^2}{\partial x^2}\;R(x,t)}{2\,m\,R(x,t)}$$

5 Classical interpretation

Choosing V_{WG} according to 4, the *WE* is mathematically equivalent to the coupled system of *HJE* and *CE*.

$$WE5:\; -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \left(V_{HJG}(x) + \frac{\hbar^2}{2m}\frac{1}{R(x,t)}\frac{\partial^2}{\partial x^2}R(x,t)\right)\psi(x,t)$$

The density ρ describes the statistical distribution of particles. $WE5$ is an

equation of classical, statistical physics.

```
sube(e4,eq4)
```

ans =

$$\mathrm{hbar}\,\frac{\partial}{\partial t}\;\psi(x,t)\;\mathrm{i} = \psi(x,t)\left(V_{\mathrm{HJG}} + \frac{\mathrm{hbar}^2\,\frac{\partial^2}{\partial x^2}\;R(x,t)}{2\,m\,R(x,t)}\right) - \frac{\mathrm{hbar}^2\,\frac{\partial^2}{\partial x^2}\;\psi(x,t)}{2\,m}$$

6 Quantization

In addition to the $WF\;\psi(x,t)$, $WE5$ also contains the density root $R(x,t)$. The unification of action and density (or dynamics and content) is incomplete.

The Schrödinger equation or the quantum mechanics are obtained by eliminating (omitting) the R-term in $WE5$:

Schrödinger equation $SG \sim WE6$:

$$WE6:\; -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V_{HJG}(x)\psi(x,t)$$

This elimination of the R term is called quantization.

Usually, the quantization is conceived a little differently: namely, by replacing certain terms in the energy function by operators. This also eliminates the R term.

The quantization changes the *HJG*. There V_{HJG} becomes

```
sube(V_WG,eq4)
```

```
ans =
```

$$V_{\mathrm{HJG}} + \frac{\mathrm{hbar}^2 \frac{\partial^2}{\partial x^2} R(x,t)}{2\, m\, R(x,t)}$$

The energy $E = -\frac{\partial}{\partial x} S(x,t)$ therefore depends on the root density $R(x,t) = \sqrt{\rho(x,t)}$.

```
sube(e1,V_HJG==ans)
```

```
ans =
```

$$\frac{\partial}{\partial t} S(x,t) = -V_{\mathrm{HJG}} - \frac{\left(\frac{\partial}{\partial x} S(x,t)\right)^2}{2\, m} - \frac{\mathrm{hbar}^2 \frac{\partial^2}{\partial x^2} R(x,t)}{2\, m\, R(x,t)}$$

The Newtonian separation of content and dynamics is thus cancelled out. The density ρ can no longer be interpreted as particle density. It becomes the probability for the response of a detector.

Starting from the classical description of absolute and objective world contents, quantization is a transition to the description of contents that appear exclusively in the observation and in relation to it.

Quantization is the basis of our modern technologies such as information processing or telecommunications.