

3.1 The correspondence principle

The Hamilton formalisms of classical mechanics defines the energy of a system by the Hamilton function

$$H(\vec{p}_i, \vec{r}_i) \quad (3.1)$$

In Quantum mechanics this function is replaced by an operator, the Hamilton operator

$$\mathbf{H}(\vec{\mathbf{p}}_i, \vec{\mathbf{r}}_i) \quad (3.2)$$

The correspondence principle allows to deduce the Hamilton operator from the Hamilton function just by replacing all momentum and space vectors by their corresponding operators.

- The resulting operator must be Hermitian which is not trivial.
- Often there exist several ways to get a symmetric operator (The Hamilton operator sometimes is not uniformly defined)
- For some systems the correct Hamiltonian is not known exactly.

The deduced operator is set equal to the time evolution operator in Eq. (2.7), leading to

The time dependent Schrödinger equation

$$\frac{\hbar}{i} \frac{\partial}{\partial t} \psi(t, \vec{r}_i) = \mathbf{H}(\vec{\mathbf{p}}_i, \vec{\mathbf{r}}_i) \psi(t, \vec{r}_i) \quad (3.3)$$

(This is often a representation in time and space since the Schrödinger equation is deduced from a classical point of view)

If the Hamilton operator is not explicitly time dependent, the Eigenvector system of Eq. (2.8) allows to calculate

The time independent Schrödinger equation

$$\hbar\omega\psi_0(\vec{r}_i) = E\psi_0(\vec{r}_i) = \mathbf{H}(\vec{\mathbf{p}}_i, \vec{\mathbf{r}}_i)\psi_0(\vec{r}_i) \quad (3.4)$$

(For solving the Schrödinger equation often an abstract representation is used)

The calculated energy Eigenvalues E_n and Eigenvectors f_n define how the quantum mechanical system evolves in time:

Let for $t = 0$ the system be in a state

$$\psi(0, \vec{r}_i) = \sum_n c_n f_n \quad . \quad (3.5)$$

We will find a time evolution of the state

$$\psi(t, \vec{r}_i) = \sum_n c_n f_n e^{\frac{iE_n t}{\hbar}} \quad . \quad (3.6)$$

The fraction of each Eigenvector to the sum of all states will change generally as a function of time.

⇒ The state of a system will normally change in time.

REMARKS:

- In physics the formalism of energy is much more fundamental than the formalism of using forces.
- All forces which apply to an electron may be included into the Hamiltonian by just adding the corresponding energy term. This allows to solve solid state physics by only one equation completely and correctly. But this equation is much too complex to use it as a starting point for any calculation. The "art" of solid state physics is to restrict the Hamiltonian to the necessary energy terms, in order to get computable equations ("Everything" means "Nothing").