Kvantmekanik

Schrödinger ekvationen

$$H\boldsymbol{\psi}(\boldsymbol{r},t) = \left[-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\boldsymbol{r})\right]\boldsymbol{\psi}(\boldsymbol{r},t) = i\hbar\frac{\partial}{\partial t}\boldsymbol{\psi}(\boldsymbol{r},t)$$

Där H är en hamiltonoperator. Om H är tidsoberoende ger separation av variabler:

$$\boldsymbol{\psi}(\boldsymbol{r},t) = \boldsymbol{\Phi}(\boldsymbol{r}) \cdot e^{-\frac{i}{\hbar}Et}$$

$$\left[-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\boldsymbol{r})\right]\boldsymbol{\Phi}(\boldsymbol{r}) = E\boldsymbol{\Phi}(\boldsymbol{r})$$

Den generella tidsberoende lösningen är:

$$\boldsymbol{\psi}(\boldsymbol{r},t) = \sum_n a_n \cdot \boldsymbol{\Phi}(\boldsymbol{r})e^{-\frac{i}{\hbar}Et}$$

Där a_n bestäms ur randvillkoren ($t = 0$):

$$a_n = \int \boldsymbol{\Phi}_n * (\boldsymbol{r}) \cdot \boldsymbol{\psi}(\boldsymbol{r}, t = 0)\, d^3r$$