

2.3 Feldoperatoren

$\psi_\nu(\underline{x})$ Basis in $\mathcal{H}^{(1)}$

$$\hat{\psi}(\underline{x}) = \sum_{\nu} \psi_{\nu}(\underline{x}) a_{\nu} \quad ; \quad a_{\nu} = \int \psi_{\nu}^*(\underline{x}) \hat{\psi}(\underline{x}) d\tau$$

$$\hat{\psi}^{\dagger}(\underline{x}) = \sum_{\nu} \psi_{\nu}^*(\underline{x}) a_{\nu}^{\dagger} \quad ; \quad a_{\nu}^{\dagger} = \int \psi_{\nu}(\underline{x}) \hat{\psi}^{\dagger}(\underline{x}) d\tau$$

Antikommutatorrelationen für Fermionen $\{A, B\} = AB + BA$

$$\{\hat{\psi}(\underline{x}), \hat{\psi}^{\dagger}(\underline{x}')\} = \delta(\underline{x} - \underline{x}') \cdot 1$$

Teilchenzahloperator $\hat{N} = \sum_{\nu=1}^{\infty} a_{\nu}^{\dagger} a_{\nu} = \int \hat{\psi}^{\dagger}(\underline{x}) \hat{\psi}(\underline{x}) d\tau$

Einteilchenenergieoperator

$$\hat{H} = \sum_{\lambda, \mu} A_{\lambda\mu} a_{\lambda}^{\dagger} a_{\mu} = \int \hat{\psi}^{\dagger}(\underline{x}) A(\underline{x}) \hat{\psi}(\underline{x}) d\tau$$

2.4 Elektronengas

A Spinoren in Schrödinger-Darstellung

$$\mathcal{H}^{(1)} = \mathcal{H}_0 \otimes \mathcal{H}_s$$

Einteilchenenergieoperator $h(\vec{r}, \vec{s}) = -\frac{\hbar^2}{2m} \Delta + v(\vec{r}, \vec{s})$

Spinor
$$\begin{pmatrix} \phi_{\frac{1}{2}}(\vec{r}) \\ \phi_{-\frac{1}{2}}(\vec{r}) \end{pmatrix} = \underbrace{\begin{pmatrix} h_{\frac{1}{2}\frac{1}{2}} & h_{\frac{1}{2}-\frac{1}{2}} \\ h_{-\frac{1}{2}\frac{1}{2}} & h_{-\frac{1}{2}-\frac{1}{2}} \end{pmatrix}}_{\text{Schrödinger-Gleichung}} \begin{pmatrix} \psi_{\frac{1}{2}}(\vec{r}) \\ \psi_{-\frac{1}{2}}(\vec{r}) \end{pmatrix} = E \begin{pmatrix} \psi_{\frac{1}{2}}(\vec{r}) \\ \psi_{-\frac{1}{2}}(\vec{r}) \end{pmatrix}$$

Schrödinger-Gleichung

B Feldoperatoren als Spinoren

$\psi_{\nu}(\vec{r})$ sei eine Basis in \mathcal{H}_0

$$\hat{\psi}_{\sigma}(\vec{r}) = \sum_{\nu=1}^{\infty} \psi_{\nu}(\vec{r}) a_{\nu\sigma} \quad ; \quad a_{\nu\sigma} = \int \psi_{\nu}^*(\vec{r}) \hat{\psi}_{\sigma}(\vec{r}) d^3r \quad \left| \sigma = \pm \frac{1}{2} \right.$$

$$\hat{\psi}_{\sigma}^{\dagger}(\vec{r}) = \sum_{\nu=1}^{\infty} \psi_{\nu}^*(\vec{r}) a_{\nu\sigma}^{\dagger} \quad ; \quad a_{\nu\sigma}^{\dagger} = \int \psi_{\nu}(\vec{r}) \hat{\psi}_{\sigma}^{\dagger}(\vec{r}) d^3r$$

Antikommutatorrelationen

$$\{a_{\nu\sigma}, a_{\mu\tau}^{\dagger}\} = \delta_{\nu\mu} \delta_{\sigma\tau} \cdot 1 \quad ; \quad \{\hat{\psi}_{\sigma}(\vec{r}), \hat{\psi}_{\tau}^{\dagger}(\vec{r}')\} = \delta_{\sigma\tau} \delta(\vec{r} - \vec{r}') \cdot 1$$

Teilchenzahloperator

$$\hat{N} = \sum_{\nu=1}^{\infty} \sum_{\sigma}^{\pm 1/2} a_{\nu\sigma}^{\dagger} a_{\nu\sigma} = \sum_{\sigma}^{\pm 1/2} \int \hat{\psi}_{\sigma}^{\dagger}(\vec{r}) \hat{\psi}_{\sigma}(\vec{r}) d^3r$$

$$\hat{N} = \sum_{\sigma}^{\pm 1/2} \int \hat{m}_{\sigma}(\vec{r}) d^3r \quad \text{mit} \quad \hat{m}_{\sigma}(\vec{r}) = \hat{\psi}_{\sigma}^{\dagger}(\vec{r}) \hat{\psi}_{\sigma}(\vec{r})$$

Teilchendichteoperator

C Energieoperator

Potenzialoperator

$$H \Psi_g(\vec{r}_1, \dots, \vec{r}_N) = E_g \Psi_g(\vec{r}_1, \dots, \vec{r}_N)$$

N-Elektronen-Schrödinger-Gl.

$$\langle \Psi_g | \Psi_g \rangle = 1$$

$$E_g = \langle \Psi_g | H | \Psi_g \rangle = \langle \Psi_g | T + V + V_{ee} | \Psi_g \rangle$$

Hartree-Fock-Näherung $\Psi_g \rightarrow \Psi_g^{SD}$

$$V \approx \langle \Psi_g^{SD} | \sum_{i=1}^N v(\vec{r}_i) | \Psi_g^{SD} \rangle$$

Thomas,
Fermi

$$= \sum_{k \in \text{besetzt}} \int |\varphi_{k_i}^*(\vec{r}_i) v(\vec{r}_i) \varphi_{k_i}(\vec{r}_i) d^3r_i$$

$$= \sum_{k \in \text{besetzt}} \int |\varphi_k(\vec{r})|^2 v(\vec{r}) d^3r = \int n(\vec{r}) v(\vec{r}) d^3r$$

$$\text{mit } n(\vec{r}) = \sum_{k \in \text{besetzt}} |\varphi_k(\vec{r})|^2$$

$$\hat{V} = \int \hat{m}(\vec{r}) v(\vec{r}) d^3r$$

$$V = \langle \Psi_g | \hat{V} | \Psi_g \rangle$$

$$= \int \langle \Psi_g | \hat{m}(\vec{r}) v(\vec{r}) | \Psi_g \rangle d^3r$$

$$= \int \langle \Psi_g | \hat{m}(\vec{r}) | \Psi_g \rangle v(\vec{r}) d^3r$$

$$= \int n_g(\vec{r}) v(\vec{r}) d^3r$$

⋮